Deterministic and stochastic partial differential equations arising in semiconductor theory and stellar dynamics

Óscar Sánchez Romero

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V.B. Director | El Doctorando

Fdo: Juan S. Soler Vizcaíno | Fdo: Óscar Sánchez Romero

A mi abuelo Pepe

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Introducción

El contenido de la memoria está orientado al estudio cualitativo de algunas soluciones de Ecuaciones en Derivadas Parciales (EDP). Más concretamente, se han tratado aspectos relacionados con la existencia y la estabilidad de soluciones estacionarias y comportamiento de las soluciones dependientes del tiempo de EDP originadas en teoría de transporte de carga en semiconductores y dinámica estelar. Evidentemente, dichos aspectos tienen interés *per se*, aunque el propio estudio proporciona las directrices para una posterior mejora en el modelado de los sistemas originales. Los trabajos que aquí se presentan buscan esta relación de retroalimentación entre el análisis y el modelado. En este sentido dos de los sistemas que se han planteado en la memoria son precisamente versiones modificadas de otros modelos que pretenden explicar la fenomenología observada que los originales no reflejan.

Los sistemas que se estudian tienen en común que representan a un gran número de partículas que interactuan entre si al moverse (bien sean los electrones que constituyen la corriente eléctrica, o las estrellas de una galaxia). La descripción de este tipo de sistemas depende de las las leyes físicas que rigen el sistema y de la escala de observación que se emplee. Así, podemos considerar un marco cuántico para describir el movimiento de los electrones y la teoría clásica para describir la dinámica de estrellas. En lo referente a las escalas de observación los problemas que trataremos en esta memoria son descripciones tanto microscópicas, cinéticas como hidrodinámicas.

Este capítulo está dedicado a la presentación de los modelos estudiados y los problemas concretos que hemos tratado. Completamos esta introducción anunciando los principales resultados obtenidos en cada caso y que desarrollaremos a lo largo de la memoria.

Dinámica estelar: el sistema de Vlasov-Poisson

Un sistema estelar es un conjunto acotado de estrellas. El número de elementos que los constituyen es muy variable, desde un sistema binario de estrellas, cúmulos estelares (de 10^2 a 10^6 estrellas) hasta galaxias (de 10^{10} a 10^{12} estrellas) o inmensos cúmulos constituidos por miles de galaxias. La rama de la física teórica que estudia estos sistemas gravitacionales se denomina dinámica estelar.

En general, la dinámica de un conjunto de N partículas (masas puntuales con masa 1) se puede determinar a partir de las leyes de la física que la rige. En el caso de electrones o átomos su movimiento puede estar descrito por la electrodinámica clásica (si se consideran como partículas clásicas) mientras que en el caso de las estrellas que constituyen una galaxia son las leyes clásicas de la gravitación (leyes del movimiento y gravitacional de Newton). Si se considera el conjunto de ecuaciones que determinan estas leyes se tiene lo que llamaremos en esta memoria una descripción microscópica. En el caso de los planetas y estrellas es la mecánica celeste la encargada de estudiar estos sistemas cuando el número de elementos del conjunto dinámico considerado no es muy grande.

En el caso de que N sea suficientemente grande se puede adoptar una descripción estadística del sistema. Ésta considera que la distribución de las partículas viene dada por una función $f(t,x,v)$ de manera que el número de partículas que se encuentran en el recinto $\Omega_x \subset \mathbb{R}^3$ y cuya velocidad está contenida en $\Omega_v \subset \mathbb{R}^3$ en el instante de tiempo t viene dado por

$$\int_{\Omega_x \times \Omega_v} f(t,x,v)\, dxdv \,.$$

Evidentemente, esta función f toma valores no negativos y permite obtener la densidad de partículas del sistema como

$$\rho(x) = \int_{\mathbb{R}^3} f(t,x,v)\, dv \,.$$

En consecuencia el número total de partículas viene dado por

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} f(t,x,v)\, dxdv \, = N.$$

El objeto de la mecánica estadística es el estudio de estos sistemas mediante la deducción y análisis de las ecuaciones cinéticas que verifican las funciones de distribución.

Si consideramos la descripción cinética de un conjunto cualquiera de partículas clásicas que interactuan mediante una ley de tipo Coulombiano, $u(r) = \gamma / r^2$, esta viene dada por la ecuación de Boltzman-Poisson (véase [31])

$$\begin{cases} \partial_t f + v \cdot \nabla_x f - \nabla_x \phi \cdot \nabla_v f = Q(f,f) \,, \\ \\ \Delta_x \phi = 4\pi\gamma\rho \,, \quad \lim_{|x|\to\infty} \phi(t,x) = 0 \,. \end{cases}$$

El potencial ϕ así descrito es una aproximación de campo medio, es decir se considera generado por la densidad de partículas ρ como solución de la ecuación de Poisson. La constante γ toma los valores 1 o -1 dependiendo de que las fuerzas de interación consideradas sean de tipo atractivo o repulsivo, respectivamente. Ejemplos típicos de sistemas modelados por esta ecuación son los sistemas electrodinámicos o gravitacionales. Q es un núcleo binario que aporta a la dinámica de las partículas el efecto de las posibles colisiones entre ellas. Para obtener el problema de valores iniciales asociado a este sistema tenemos que complementar las ecuaciones anteriores con una condición inicial $f(t=0,x,v) = f_0(x,v)$.

Si nos ceñimos al caso particular de las galaxias y grandes cúmulos estelares, donde las fuerzas gravitacionales son fuerzas de tipo Coulombiano atractivas, este sistema se considera una buena aproximación y además se puede asumir que no hay término de colisiones. En primer lugar el número de estrellas es lo suficientemente grande para poder asegurar que los efectos de las interacciones a corta distancia son despreciables frente a la colectividad de las interacciones a distancia superior. El razonamiento se basa en que el tiempo que una partícula ha de permanecer atravesando galaxias para que los efectos de las interacciones de corta distancia sean apreciables es superior a la edad del universo. Por lo tanto, el movimiento de cada estrella se puede ver a través de un campo medio generado por todas las partículas del sistema. En este caso, la razón entre el tiempo que una estrella emplea en recorrer una galaxia y la propia edad de la galaxia hace pensar que las posibles colisiones entre estrellas sean tan pocas que se pueden despreciar ([18, 33]). En el caso de que se consideren sistemas con menor número de elementos, o de menor dimensión estas simplificaciones pueden no ser razonables.

Puesto que no consideramos colisiones el sistema de Boltzman-Poisson se simplifica obteniendo el sistema de Vlasov–Poisson (VP) en el caso gravitacional

$$\begin{cases} \partial_t f + v \cdot \nabla_x f - \nabla_x \phi \cdot \nabla_v f = 0 \ , \\ \\ f(t=0,x,v) = f_0(x,v) \ , \\ \\ \Delta_x \phi = 4\pi\rho \ , \quad \lim_{|x|\to\infty} \phi(t,x) = 0 \ . \end{cases}$$

En los trabajos que se presentan en esta memoria vamos a tratar dos problemas relacionados con este sistema. En el Capítulo 2 analizamos el comportamiento de las soluciones del sistema de VP para tiempos largos. Para ello vamos a emplear tanto argumentos variacionales como invariancias del sistema. El Capítulo 3 propone un nuevo criterio de estabilidad para soluciones estacionarias del sistema de VP.

A continuación se citan algunas de las cantidades conservadas por las soluciones del sistema de VP con el fin de presentar los resultados que se obtendrán. Sea $f(t,x,v)$ una solución del sistema de VP. Se define la energía asociada a f como

$$E(f) := E_{KIN}(f) - E_{POT}(f)$$

donde la energía cinética y potencial vienen descritas respectivamente por

$$E_{KIN}(f) = \frac{1}{2}\int_{\mathbb{R}^6} |v|^2 f(t,x,v)\, dx\, dv \quad \text{y} \quad E_{POT}(f) = \frac{1}{8\pi}\int_{\mathbb{R}^3} |\nabla\phi|^2\, dx\,.$$

Para soluciones de VP clásicas se mantiene constante el valor de este funcional a lo largo de la evolución temporal así como las normas

$$\|f(t,\cdot,\cdot)\|_{\mathrm{L}^p(\mathbb{R}^6)} = \left|\int_{\mathbb{R}^6} |f(t,x,v)|^p\, dx\, dv\right|^{\frac{1}{p}} \qquad p \in [1,\infty]$$

(ver [57, 85]). En el caso particular $p = 1$ esto nos indica que las soluciones preservan la masa total del sistema:

$$M = \int_{\mathbb{R}^6} f_0(x,v)\, dx\, dv = \int_{\mathbb{R}^6} f(t,x,v)\, dx\, dv\,.$$

Otra cantidad conservada para las soluciones es el momento total

$$\langle v\rangle(f) := \int_{\mathbb{R}^6} v f(t,x,v)\, dx\, dv\,.$$

Los resultados que presentamos en el Capítulo 2 están centrados en el comportamiento de las soluciones dependientes del tiempo. Usualmente para analizar propiedades cualitativas de dichas soluciones se obtienen estimaciones sobre cantidades asociadas a éstas como normas L^p de la función de densidad o bien las energías potencial y cinética.

El primero de los resultados que obtenemos muestra cotas óptimas para la energía cinética de una solución. Se puede asegurar que las energías potencial y cinética de una solución del sistema VP verifican

(i) $E_{KIN}(f) \in \Big[\, K_-(E,M),\ K_+(E,M)\, \Big]$,

(ii) $E_{POT}(f) \in \Big[\, \max\{0, P_-(E,M)\},\ P_+(E,M)\, \Big]$,

(iii) $E_{POT}(f) \in \Big[\, 0,\ \sqrt{-4E_M E_{KIN}(f)}\, \Big]$, para todo instante de tiempo. Estos intervalos están determinados por la condición inicial de la solución mediante

$$K_{\pm}(E,M) = -2E_M \left(1 - \frac{E}{2E_M} \pm \sqrt{1 - \frac{E}{E_M}}\right) ,$$

$$P_{\pm}(E,M) = -2E_M \left(1 \pm \sqrt{1 - \frac{E}{E_M}}\right) ,$$

donde $M = \|f_0\|_{\mathrm{L}^1(\mathbb{R}^6)}$, $E = E(f_0)$ y E_M es el mínimo valor del problema

$$E_M := \inf \{E(f) \; ; \; f \in \Gamma_M\} \ , \tag{1}$$

con $\Gamma_M = \{f \; ; \; f(x,v) \geq 0 \, , \; \|f\|_{\mathrm{L}^1(\mathbb{R}^6)} = M \, , \; \|f\|_{\mathrm{L}^\infty(\mathbb{R}^6)} \leq 1\}$. Las cotas así presentadas son óptimas ya que las funciones que minimizan (1) son soluciones estacionarias del sistema de VP y para estas se tiene que

$$K_{\pm}(E,M) = E_{KIN}(f) = \frac{1}{2} E_{POT}(f) = P_{\pm}(E,M) \, .$$

La existencia de soluciones estacionarias indica que no podemos esperar en general obtener propiedades dispersivas para las soluciones del sistema de VP en contraste con las soluciones del mismo sistema de VP pero con potencial repulsivo. En el caso del sistema de Vlasov–Poisson con potencial repulsivo es conocido que las soluciones verifican la siguiente cota [58, 85]

$$\|\rho(t)\|_{\mathrm{L}^{\frac{5}{3}}(\mathbb{R}^3)} \leq \frac{C}{t^{\frac{3}{5}}} \, , \quad \forall t > 0 \, .$$

Esta desigualdad trivialmente implica que la densidad de partículas en cada dominio Ω desciende a lo largo de la evolución temporal.

En nuestro siguiente resultado obtenemos una condición que nos permite distinguir aquellas soluciones del sistema de VP atractivo en las que es imposible deducir cotas del estilo anterior de otras soluciones que son dispersivas en un sentido estadístico. Para ello combinamos las traslaciones Galileanas y la ecuación de dispersión que verifican dichas las soluciones. Para una condición inicial f_0 con masa y energía finita demostramos que:

i) si f_0 es tal que

$$E(f_0) < \frac{\langle v \rangle^2(f_0)}{2M} \, , \tag{2}$$

entonces, existe una constante $C > 0$, tal que la solución del sistema de VP asociada a f_0 verifica

$$\|\rho_f(t,\cdot)\|_{\mathrm{L}^{\frac{5}{3}}(\mathbb{R}^3)} \geq C \, , \quad \forall t \geq 0 \, .$$

ii) Si por el contrario f_0 verifica la desigualdad opuesta a (2) se tiene que para un cierto $t_0 > 0$

$$C_1 t^2 \leq \int_{\mathbb{R}^6} |x - \langle x \rangle|^2 f(t,x,v)\, dx\, dv \leq C_2 t^2 \quad \forall\, t \geq t_0 > 0\,, \tag{3}$$

y para cada $p \in [1, \infty)$,

$$\|\rho(t,x)\|_{\mathrm{L}^p(\mathbb{R}^3)} \geq \frac{C}{t^{3(p-1)/p}}, \quad \forall\, t > t_0\,,$$

donde $\langle x \rangle = \int_{\mathbb{R}^6} x f(t,x,v)\, dxdv$, y C_i, C son constantes positivas.

Obsérvese que aunque la estimaciónes obtenidas en *ii)* no se corresponden con las deducidas para el caso de potencial repulsivo, si que implican dispersión ya que la varianza de la distribución de densidad crece con orden t^2. Diremos pues que hemos deducido dispersión en sentido estadístico. Estos resultados extienden a los obtenidos en [13] para soluciones esféricamente simétricas.

Finalmente, la obtención en el primer resultado de soluciones estacionarias de VP como funciones mínimizantes de (1) también permite probar un criterio de estabilidad no lineal para dicha solución. La única función esféricamente simétrica donde se alcanza el mínimo para (1) coincide con una solución politrópica correspondiente a $\mu = 0$. En general la familia de soluciones politrópicas esféricas viene dada por la expresión

$$\nu_\mu = \nu(x,v) = c\left(E_0 - |v|^2/2 - \phi(|x|)\right)_+^\mu\,, \tag{4}$$

donde $(\cdot)_+$ es la función parte positiva, $\alpha < E_0 < 0$, $-1 < \mu$ y $c > 0$. La propiedad de estabilidad no lineal para ν_0 (estabilidad dinámica) se expresa en términos del funcional distancia

$$d(g,h) = E(g) - E(h) + \frac{1}{4\pi}\, \|\nabla\phi_g - \nabla\phi_h\|^2_{\mathrm{L}^2(\mathbb{R}^3)}\,,$$

donde ϕ_g y ϕ_h son las soluciones de la ecuación de Poisson asociadas a las densidades de g y h, respectivamente. Este resultado es consecuencia directa de los argumentos de minimización desarrollados para resolver (1). Este problema variacional presenta varias dificultades técnicas. El funcional energía es no convexo e invariante por traslaciones en la variable espacial. Por otro lado, el espacio funcional donde se plantea (1) está doblemente resgringido. Esto nos ha hecho estudiar el problema mediante argumentos de tipo compacidad por concentración y reordenamientos simétricos. Más concretamente, adaptamos las las técnicas desarrolladas en [48, 50] para el problema de minimización del funcional de Casimir que proporciona un criterio de estabilidad dinámica para soluciones politrópicas con $\mu \in (0, 3/2)$. Por lo tanto nuestro estudio viene a cubrir el caso crítico $\mu = 0$ (ver Capítulo 2 para más detalles). A lo largo de esta memoria trataremos otros problemas de minimización que tienen en común con este que el funcional a minimizar es no convexo e invariante por un grupo no compacto de simetrías, lo cual conlleva cierta complejidad técnica en su tratamiento, que se ha solventado mediante diversos argumentos.

El Capítulo 3 extiende este concepto de estabilidad a un concepto más fuerte, el de estabilidad orbital, y se aplica a un conjunto más grande de soluciones, las soluciones politrópicas esféricas para $\mu \in [0, 7/2)$. Para ello se resuelven los problemas de optimización

$$I^{\mu}_{M,J} := \inf \left\{ E(f)\,;\ f \in \Gamma^{\mu}_{M,J} \right\} \tag{5}$$

donde $\Gamma^{\mu}_{M,J} = \mathrm{L}^1_+(\mathbb{R}^6, M) \cap \mathrm{L}^{1+1/\mu}_+(\mathbb{R}^6, J)$ y $\mathrm{L}^p_+(\mathbb{R}^6, K) = \{f \in \mathrm{L}^p(\mathbb{R}^6); f \geq 0\,,\ \|f\|_{\mathrm{L}^p(\mathbb{R}^6)} = K\}$. Los argumentos empleados en este problema variacional nos permiten concluir que las soluciones politrópicas para $\mu \in [0, 7/2)$ son orbitalmente estables. Esencialmente este criterio establece que si una condición inicial f_0, con masa y norma $\mathrm{L}^{1+1/\mu}$ apropiadas, está suficientemente cerca de ν_μ (sus energías no difieren mucho) entonces la solución correspondiente estará cerca (en norma L^1) de la órbita de ν_μ definida por $\{\nu_\mu(\cdot - k, \cdot)\,;\ k \in \mathbb{R}^3\}$. Esta noción de estabilidad orbital es óptima ya que las invariancias Galileanas del sistema nos indican que efectivamente hay soluciones que *viajan* cerca de la órbita de ν_μ. El resultado es consecuencia directa del argumento de minimización empleado para resolver (5). En este caso reducimos (5) a un problema equivalente para las funciones de densidad. Combinando resultados para este problema reducido con el propio argumento de minimización del problema original podemos concluir la compacidad relativa en L^1 de cualquier sucesión minimizante (salvo traslaciones). Este resultado extiende a otros obtenidos en [48, 50] **Faltan citas** basados en resultados de minimización para el funcional Casimir o el de energía en espacios con restricción de masa o restricción de tipo Casimir-masa respectivamente.

Transporte de carga en semiconductores

El interés del estudio del transporte de carga en materiales semiconductores radica en su utilización como materia prima para construir dispositivos electrónicos. Desde la invención de los primeros transistores basados en el Germanio, ha sido el Silicio el material semiconductor que ha predominado en el campo tecnológico. Sin embargo, en los últimos años se han descubierto nuevas aplicaciones de los semiconductores, sobre todo como emisores y detectores de luz (células solares, diodos emisores de luz, lasers,...), que han motivado el estudio de otros materiales como pueden ser el Arsenuro de Galio (GaAs) o el Arsenuro de Aluminio (AlAs).

Clásicamente los semiconductores se caracterizan por ser materiales peores conductores que los metales sin llegar a ser materiales aislantes (clasificación que cuantitativamente se refleja en los valores de las conductividades típicas). Esta sencilla caracterización se hace actualmente mas compleja. Se distinguen además entre materiales superconductores y semimetales, donde estos últimos se diferencian de los semiconductores en que tienen conductividad algo mayor y a bajas temperaturas siguen manteniendo su carácter de conductores, mientras que los semiconductores se convierten en aislantes. No obstante si se pretende hacer un estudio detallado de estos materiales hay que tener en cuenta factores como la energía de gap, estructura cristalina, constante de la estructura, existencia de impurezas, etc... [6, 45].

Uno de motivos del éxito de los dispositivos semiconductores es que su tamaño es muy reducido si lo comparamos con los dispositivos electrónicos anteriores. De hecho, a lo largo de su evolución su tamaño ha seguido disminuyendo. Por ejemplo, el primer transistor de Germanio tenía un tamaño característico de $20\mu m$, mientras que los transistores de un procesador actual Pentium IV tiene un tamaño característico de $0.18\mu m$ y la Asociación de Industrias en Semiconductores (SIA) proyecta que para el final de 2009 los dispositivos emplearán tamaños del orden de $0.05\mu m$. Este proceso de miniaturización ha dado lugar a que los efectos cuánticos puedan ser relevantes en el proceso de transporte, ya que con los tamaños anteriores la hipótesis de transporte clásico se adaptaba bien a la evolución en estos semiconductores primitivos.

El transporte de un flujo de electrones a lo largo de un semiconductor sometido a una diferencia de potencial depende por tanto de numerosos factores: la naturaleza del propio material, las condiciones del medio (temperatura, fuerzas externas), tamaño del dispositivo, ... Por lo tanto son numerosos los modelos que han aparecido en la literatura para describir este proceso de transporte y el empleo de un modelo u otro dependerá de nuestro dispositivo particular. No obstante hay que destacar que éste es un campo en el que se sigue trabajando muy activamente [62, 82, 86].

Los principales factores que se tienen que tener en cuenta cuando se modela el transporte de carga en un semiconductor son:

i) La descripción del movimiento de muchas partículas. Esta puede ser una descripción microscópica, cinética o bien hidrodinámica. Por otro lado, dependiendo de si los efectos cuánticos son o no relevantes se puede considerar a los electrones como partículas clásicas con carga o bien como partículas cuánticas.

ii) La influencia de la red cristalina. Por ejemplo la periodicidad de la propia red cristalina implica que el potencial creado por los iones sea periódico. En este caso, si se desprecian otras interacciones, se deduce que los electrones se encuentran esencialmente en ciertos estados que se denominan estados de Bloch.

iii) Las interacciones entre las partículas, bien sean interacciones de tipo electrostático (interacciones a largo alcance de tipo Coulombiano) o bien colisiones entre las partículas que se encuentran en el semiconductor (denominadas genéricamente procesos de scattering).

Evidentemente, los distintos modelos que hay en la literatura responden a distintas formas de abordar estas cuestiones. Por supuesto, pueden aparecer otros factores que también influyen en el modelado como puede ser la existencia de impurezas en el semiconductor (dopaje) o bien el efecto de otro tipo fuerzas externas (como por ejemplo las generadas por un campo magnético).

La consistencia de un modelo proviene de su derivación a partir de primeros principios. En el caso del movimiento de electrones los primeros principios los establece la teoría cuántica. Esta considera que un electrón de masa m y carga elemental q que se mueve en el vacío bajo la acción de un campo eléctrico $E = E(x,t)$ viene descrito por la función de onda $\psi : \mathbb{R}^3 \times [0,\infty] \to \mathbb{C}$ que verifica la ecuación de Schrödinger

$$i\hbar \frac{\partial \psi}{\partial_t} = -\frac{\hbar}{2m}\Delta\psi - qV(x,t)\,. \tag{6}$$

En esta expresión $\hbar = h/2\pi$ es la constante de Planck reducida y $V(x,t)$ el potencial generado por el campo $E = -\nabla V$, e $i^2 = -1$. La función de densidad $n(x,t) = |\psi(x,t)|^2$ se interpreta como la distribución de probabilidad de encontrar al electron, es decir,

$$\int_\Omega n(x,t)\,dx$$

es la probabilidad de encontrar al electrón en la región Ω en el instante de tiempo t. Empleando esta teoría se puede describir microscópicamente un gas de electrones en una red cristalina. Dependiendo de los efectos considerados en el estudio se obtendrán diversos modelos.

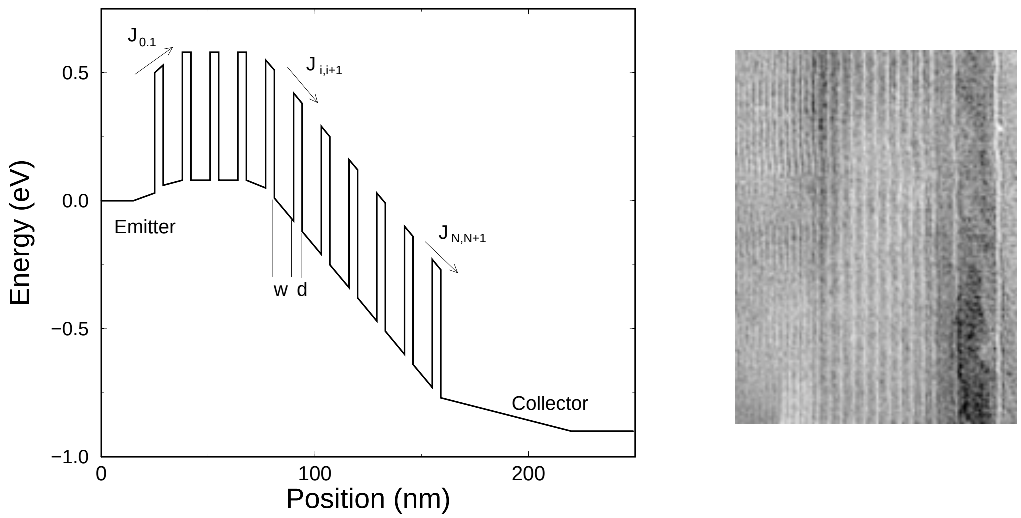

Figure 1: (*Izquierda*) Diagrama del perfil de potencial electrostático de una superred semiconductora SR. (*Derecha*) Sección transversal de una SR compuesta por capas de Si (bandas oscuras) y SiO2 (bandas claras) de distintas anchuras.

Este marco teórico se complica cuando los dispositivos semiconductores que se consideran son más complicados. En esta memoria vamos a presentar dos trabajos relacionados con unos dispositivos denominados superredes semiconductoras (SR). Éstas están compuestas por la superposición periódica de capas muy finas de dos semiconductores distintos cuyas dimensiones laterales son mucho mayores que la dimension l de un período. Puesto que los semiconductores que constituyen el dispositivo son distintos la banda de conducción de una superred puede verse como una consecución de pozos y barreras de tamaños d y w respectivamente donde $l = d + w$. La primera y última capas se ponen en conexión con los denominados contactos (ver Fig. 1).

Estos dispositivos propuestos por primera vez por L. Esaky en 1969 constituyen un claro ejemplo de lo que hoy día se conoce como sistemas cuánticos abiertos caracterizados por ser sistemas en los cuales hay un intercambio de partículas con el ambiente (en nuestro caso a través de los contactos). La modelización de estos dispositivos es bastante más complicada puesto que la corriente de electrones ha de pasar a través de un medio heterogéneo. Dependiendo pues de las características de la SR el desplazamiento de la carga se efectuará mediante unos mecanismos u otros.

El tuneleo resonante secuencial es uno de los tipos de transporte típico en estos dispositivos. Se denomina tuneleo al mecanismo por el cual los electrones pasan de unos pozos a otros atravesando la barrera que los separa. La teoría estblecida se basa en que los posibles estados de los electrones que se encuentran en cada pozo son estados estacionarios de la ecuación de Schrödinger, y por tanto la corriente se puede calcular empleando un coeficiente de transmisión del estado donde se encuentran los electrones antes de pasar la barrera a otro estado en el pozo siguiente. Según algunos autores esta descripción no es válida cuando se pretenden estudiar estados de no equilibrio [37]. Por lo tanto, se hacen necesarias descripciones dinámicas del comportamiento de los electrones en caso de no equilibrio.

En este ambiente se encuadran el resto de los trabajos que presentamos en esta memoria. Pasamos entonces a describir los problemas planteados y a mostrar los resultados obtenidos.

Evolución de partículas cuánticas

En este punto presentamos dos trabajos relacionados con el análisis de propiedades cualitativas de soluciones de dos sistemas de tipo Schr̆odinger-Poisson [60, 82]. Este modelo aparece en la literatura para modelizar un gas de electrones que se mueve en el vacío y se ven afectados por el campo eléctrico que ellos mismos producen. Pese a su generalidad, en los últimos años han aparecido diversos trabajos en los que se adapta este modelo a contextos particulares [91, 61, 81]. El estudio de estas propiedades es relevante para la fabricación de SR [2, 25, 109].

El primero de los modelos analizados es el propio sistema de Schrödinger-Poisson (SP) en el espacio tridimensional, que se define como

$$
\begin{aligned}
i\hbar\frac{\partial\psi}{\partial t} &= -\frac{\hbar^2}{2m}\Delta_x\psi + V\psi, & \lim_{|x|\to\infty}\psi(x,t) &= 0,\\
\psi(x,t=0) &= \phi(x), & &\\
\Delta_x V &= -\,n, & \lim_{|x|\to\infty} V(x,t) &= 0\,.
\end{aligned}
$$

El sistema de Schrödinger-Poisson se ha cerrado añadiendo condiciones de frontera en infinito y una condición inicial.

Aunque es bien conocido que las soluciones de estos sistemas tienen cantidades conservadas como la masa o la energía, otras cantidades como el momento de segundo orden o las normas L^p, donde $p > 2$, nos pueden indicar dispersión de la función de densidad. Analizaremos el comportamiento de tales cantidades en el contexto del estado individual (un único electrón) modelado por el sistema de SP aunque nuestro análisis puede ser sencillamente extendido al caso mixto (un número finito electrones). Hay que señalar que el estudio del comportamiento para tiempos grandes de las soluciones de este sistema ya ha sido tratado en trabajos anteriores [29, 59], siendo nuestro objetivo mejorar los resultados allí obtenidos. Obtenemos cotas inferiores y superiores de las normas $\mathrm{L}^p(\mathbb{R}^3)$ de las soluciones, con $2 < p < 6$, que nos delimitan fielmente el comportamiento que estas tienen. Es decir, para una condición inicial apropiada se puede demostrar que la solución asociada verifica

$$\frac{C_1}{|t|^{\frac{3p-6}{2p}}} \leq \|\psi(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq \frac{C_2}{|t|^{\alpha(p)}}, \quad \forall\, |t| \geq \xi,\ \forall\, p \in [2,6]\,,$$

donde C_i son constantes positivas, $\xi > 0$ y

$$\alpha(p) = \begin{cases} 1 - \frac{2}{p}, & \text{si } p \in [2,3], \\ \frac{2}{3} - \frac{1}{p} & \text{si } p \in [3,6]\,. \end{cases}$$

Las cotas superiores mejoran a las ya obtenidas en [29, 59] mientras que las cotas inferiores que se han obtenido son óptimas. Estas cotas son consecuencia de la ecuación de dispersión que verifican las soluciones de SP y de una desigualdad propuesta por P. Lions que relaciona las energías cinética y potencial con la norma L^3 de las funciones.

El segundo de los modelos cuánticos considerados es el de Scrödinger-Poisson-Slater (SPS) que responde a las ecuaciones

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta_x\psi + V\psi - C_S n^{\frac{1}{3}}\psi, \qquad \lim_{|x|\to\infty}\psi(x,t) = 0, \tag{7}$$

$$\psi(x,t=0) = \phi(x), \tag{8}$$

$$\Delta_x V = -\,n, \qquad \lim_{|x|\to\infty} V(x,t) = 0\,. \tag{9}$$

Este sistema se diferencia de SP en que aparece un nuevo término denominado corrección de Slater. La constante C_S se denomina por tanto constante de Slater. Los efectos de potencial Coulombiano parecen ser muy fuertes cuando se compara el comportamiento del sistema de SP con las simulaciones (ver [89, 111]). Hay distintas opciones para intentar corregir este efecto. El modelo de SPS aparece como una modificación del sistema de SP donde se corrige el potencial Coulombiano (ver [20] para un análisis detallado).

Al igual que en el caso del sistema SP este sistema presenta cantidades conservadas como la carga (norma $\mathrm{L}^2(\mathbb{R}^3)$) o la energía, que en este caso viene definida por

$$E[\psi]=\int_{\mathbb{R}^3}\left\{\frac{\hbar^2}{2m}|\nabla\psi(x,t)|^2 + \int_{\mathbb{R}^3}\frac{|\psi(x,t)|^2|\psi(x',t)|^2}{8\pi|x-x'|}dx' - \frac{3C_S}{4}|\psi(x,t)|^{\frac{8}{3}}\right\}dx\,.$$

La energía es la suma de la energía cinética, la energía potencial Coulombiana y la energía potencial proveniente de la corrección de Slater.

El análisis cualitativo de las soluciones del sistema SPS está cláramente marcado por el balance entre los dos términos de energía potencial. Un hecho relevante es que la energía potencial puede tomar valores negativos. Esto implica importantes diferencias entre el comportamiento de las soluciones del sistema de SP y el sistema SPS: 1) Existencia de soluciones estacionarias (es decir soluciones con densidad constante), 2) existen soluciones que no presentan carácter dispersivo (incluso con energía total positiva). Evidentemente, esto muestra importantes diferencias entre las soluciones de un modelo y otro. A continuación describimos los principales resultados obtenidos. En primer lugar planteamos el problema variacional

$$I_M = \inf\{E[\psi]\,;\ \psi \in \mathrm{H}^1(\mathbb{R}^3)\,,\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M\}. \tag{10}$$

Bajo ciertas hipótesis técnicas se puede asegurar que este problema alcanza un valor mínimo. El funcional energía en este problema de minimización es también no convexo y presenta invarianza por traslaciones espaciales. En este caso se proponen dos técnicas distintas para resolver el problema, compacidad por concentración y compacidad débil no nula. Resolver (10) nos permite obtener dos interesantes consecuencias.

En primer lugar podemos asegurar la existencia de soluciones estacionarias (con densidad invariante) del sistema de SPS de la forma $\psi(x,t) = e^{-i\beta t}\psi(x)$. Combinando este resultado con la invariancia Galileana se puede afirmar que también existen soluciones del sistema SPS (incluso con energía total positiva) que cuya norma $\mathrm{L}^p(\mathbb{R}^3)$ se mantiene constante en el tiempo. Estas soluciones por si solas nos indican claramente diferencias cualitativas con las soluciones del sistema SP.

Estas diferencias quedan reflejadas en el análisis cualitativo que se hace de soluciones dependientes del tiempo. En primer lugar se obtienen cotas óptimas para la energía cinética de las soluciones. Al igual que en el caso del sistema de VP, se demuestra que la energía de soluciones de SPS suficientemente regulares está limitada entre los valores

$$E^{\pm}_{KIN} = -2I_M\left(1 - \frac{E_0}{2I_M} \pm \sqrt{1 - \frac{E_0}{I_M}}\right), \tag{11}$$

donde M y E_0 son respectivamente la masa y la energía de la solución.

Al igual que en el caso del sistema de VP la invariancia Galileana de las soluciones del sistema permite deducir un criterio que distingue las funciones cuyas normas L^p no decaen de aquellas que presentan dispersión en sentido estadístico. Entonces dada ψ una solución del sistema de SPS con condición inicial ϕ tal que

$$E[\phi] < \frac{1}{2}\frac{|\langle x\rangle|^2}{\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}} \qquad \text{donde } \langle x\rangle := \int_{\mathbb{R}^3} x\phi\,dx$$

se sabe que existen constantes positivas C, C' y C'' tales que

$$\|\psi(t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \geq C, \quad E_{POT}[\psi] \leq -C', \quad \forall t \geq 0, \quad p \in [\frac{8}{3}, 6].$$

Si ϕ verifica la desigualdad opuesta

$$E[\phi] > \frac{1}{2}\frac{|\langle x\rangle|^2}{\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}},$$

se obtiene la siguiente cota inferior

$$\|\psi(\cdot,t)\|_{L^p(\mathbb{R}^3)} \geq \frac{C''}{t^{\frac{3p-6}{2p}}}, \quad \forall t > \xi > 0, \quad p \in [2,6],$$

y además hay dispersión de la solución en sentido estadístico

$$\int_{\mathbb{R}^3} |(x - \langle x\rangle)|^2 n(x)\,dx = O(t^2).$$

En conclusión, se ha demostrado que si se considera la corrección de Slater en el modelo de Schrödinger–Poisson hay un importante cambio cualitativo en las soluciones del sistema.

Modelo de Drift-Diffusion para superredes semiconductoras

En esta parte de la tesis se presentan dos trabajos realizados sobre un modelo de Drift-Diffusion para superredes semiconductoras débilmente acopladas. Estas superredes se caracterizan por tener el tamaño de las barreras mucho mayor que el inverso del número de onda típico de los electrones que están dentro de la barrera. En el caso opuesto la superred se denomina fuertemente acoplada. El principal motivo del comportamiento no lineal del desplazamiento de corriente en estos dispositivos es la formación de dominios de campo eléctrico (regiones en las que el campo toma valores homogéneos). Los electrones que constituyen la corriente pueden provenir de dopar el sistema o de excitarlos desde la banda de valencia. Dependiendo de la densidad de electrones que hay en la superred se observan distintas modalidades de soluciones típicas del sistema. Estas soluciones dan lugar a una relación entre el voltaje aplicado al dispositivo, V, y la corriente de la solución típica que se obtiene, I, cuya representación se conoce como diagrama $I-V$. Cuando la densidad de electrones es suficientemente pequeña el campo eléctrico es casi uniforme dentro de todo el dispositivo y el diagrama $I-V$ presenta un perfil regular. Este tipo de soluciones se hacen inestables cuando la densidad de carga aumenta. Entonces aparecen soluciones cuyo campo eléctrico esta constituido por dos dominios conectados por una delgada región frontera que generalmente esta situada en uno o dos períodos. El diagrama $I-V$ pasa a estar constituido por un conjunto de ramas entre las que hay una discontinuidad (ver Capítulo 6). Las discontinuidades en este diagrama corresponden a desplazamientos de la frontera entre los dominios de campo de manera que pasan de estar centrados en un período a otro adyacente. Por último para valores intermedios de carga en la superred pueden aparecer soluciones de tipo oscilatorio [22].

A continuación se presenta el modelo de Drift–Diffusion que hemos adoptado en nuestros trabajos para estudiar estos dispositivos. El mecanismo principal de transporte en superredes débilmente acopladas es el tuneleo resonante secuencial. El desplazamiento de un electrón de un pozo al siguiente se puede subdividir en tres etapas, scattering, relajación y tuneleo. En el scattering un electrón situado originalmente en una subbanda excitada de un pozo pierde energía y cae a la primera subbanda del mismo pozo. Tras esta pérdida el electrón pasa un tiempo en este nivel básico antes de saltar al siguiente pozo. El tiempo medio de espera se conoce como relajación. Y por último el electrón tunelea hacia una subbanda del pozo siguiente y comienza de nuevo el proceso. En superredes débilmente acopladas el tiempo de scattering es mucho menor que el tiempo de tuneleo (o tiempo de escape) y éste a su vez es mucho menor que el tiempo de relajación. Por lo tanto, el proceso dominante en el transporte es el tuneleo resonante donde únicamente la primera subbanda de cada pozo está ocupada y la corriente de tuneleo es cuasiestacionaria (la corriente de tuneleo se calcula asumiendo valores constantes del campo y de la densidad de electrones en los pozos adjuntos a la barrera). En la situación mas sencilla, el centro de cada pozo cuántico esta n-dopado y la energía térmica es grande en comparación con la minibanda menor. Entonces el transporte en estos dispositivos se puede describir mediante una ecuación de Drift-Difusión; ver [1, 23, 22, 107]. El modelo considera un conjunto de $N+1$ celdas consecutivas, que son pares pozo-barrera, etiquetadas por el índice $i \in \{0, \ldots, N\}$. La barrera que separa el contacto emisor del primer pozo de la SR se considera como la barrera número 0, mientras que la N-ésima barrera separa el N-ésimo pozo del colector. El modelo asume que los electrones están concentrados en una sección bidimensional de la SR situada en el centro de cada pozo. Las variables que describen el transporte son la densidad de electrones bidimensional n_i $i = 1, \ldots, N$, y el campo eléctrico medio F_i, $i = 0, \ldots, N$, en cada celda. Estas cantidades están relacionadas mediante la siguiente ecuación de Poisson discreta:

$$F_i - F_{i-1} = \frac{e}{\overline{\varepsilon}}(n_i - N_D^w), \quad i \in \{1, \ldots, N\}. \tag{12}$$

En (12), N_D^w representa el dopaje bidimensional en cada pozo, que se supone constante, mientras que $\overline{\varepsilon}$ es la permitividad media en la SR y $e = -q$ es menos la carga del electrón. Por otro lado, si denotamos por $eJ_{i\to i+1}$ la densidad de corriente de tunel en la barrera que separa los pozos i y $i+1$, la densidad de carga que pasa a traves de la i-ésima barrera verifica la siguiente ecuación de continuidad

$$\frac{dn_i}{dt} = J_{i-1\to i} - J_{i\to i+1}, \quad i \in \{1, \ldots, N\}. \tag{13}$$

A partir de estas expresiones si diferenciamos (12) y sustituimos en (13) observamos que la cantidad

$$\frac{\overline{\varepsilon}}{e}\frac{dF_i}{dt} + J_{i\to i+1} = J(t), \quad i \in \{0, \ldots, N\} \tag{14}$$

no depende de la celda que consideremos. Esta relación es conocida como Ley de Ampere, donde $eJ(t)$ es la densidad de corriente total a través de la SR (la cual no depende del índice i).

El modelo se completa con una ley constitutiva que define las densidades de corriente $eJ_{i\to i+1}$ como función de los pares (n_k, F_k). La densidad de corriente depende de los potenciales electroquímicos en las celdas i y $(i+1)$ y del campo eléctrico medio F_i [22, 107]. Los potenciales electroquímicos en las celdas a su vez son funciones de la densidad de electrones y por tanto podemos considerar que la corriente de tuneleo $eJ_{i\to i+1}$ depende de n_i, n_{i+1} y F_i [22, 107]. No se ha obtenido una deducción de $eJ_{i\to i+1}$ a partir de primeros principios de manera rigurosa. En la literatura han aparecido algunas aproximaciones, bien a partir de ecuaciones cinéticas cuánticas para las funciones de Green [107] o bien a partir una version del método WKB para sistemas de muchas partículas ("transfer Hamiltonian formalism") [1, 23, 22]. Todas estas fórmulas implican que la corriente de tuneleo está dada por la diferencial de un término de convección ("drift") y otro de difusión ("diffusion") dada por

$$J_{i\to i+1} = \frac{n_i v(F_i)}{\ell} - \frac{D(F_i)(n_{i+1} - n_i)}{\ell^2}, \quad i \in \{1, \ldots, N-1\}. \tag{15}$$

La velocidad *de arrastre* y la *difusividad* vienen definidas por v y D, funciones del campo eléctrico, que dependen de las propiedades físicas de los materiales que constituyen la SR, ver [22] para más detalles. La naturaleza especial de los contactos (emisor y colector) se considera en la deducción de las densidades de tuneleo en dichos contactos. Empleando el formalismo "tranfer Hamiltonian", se obtienen las siguientes aproximaciones [23]

$$J_{0\to 1} = j^{(e)}(F_0) - \tfrac{n_1 W^{(b)}(F_0)}{\ell}, \tag{16}$$

$$J_{N\to N+1} = \tfrac{n_N W^{(f)}(F_N)}{\ell}. \tag{17}$$

Estas ecuaciones involucran la densidad de corriente $ej^{(e)}$ y la velocidad *hacia atrás* $W^{(b)}$ en el emisor, y la velocidad *hacia adelante* $W^{(f)}$ en el colector, las cuales son funciones del campo eléctrico. Todos los coeficientes v, D, $W^{(b)}$, $W^{(f)}$ y $j^{(e)}$ toman valores no negativos y son funciones suficientemente regulares. Perfiles típicos de estas funciones se pueden encontrar en el Capítulo 6.

Este sistema de ecuaciones todavía no está cerrado, puesto que hay una incógnita más que ecuaciones. Generalmente, se emplea una condición sobre el voltaje al que se somete el dispositivo

$$\ell \sum_{i=-N}^{1} F_i = V, \tag{18}$$

donde V es el voltaje. Dependiendo de que consideremos el dispositivo sometido a corriente continua (DC) constante o bien alterna (AC) V será una constante o bien una función periódica.

Las expresiones (12), (13) y (18) constituyen un sistema cerrado de ecuaciones para las incógnitas n_i con $i \in \{1, \ldots, N\}$ y F_i con $i \in \{0, \ldots, N\}$ al que nos referiremos a lo largo de esta memoria como modelo discreto de Drift-Diffusion (DDD).

Algunas de las variables que se han descrito en el modelo son observables en el laboratorio. Tanto el voltaje V como la corriente total eJ son variables perfectamente medibles, lo cual nos permite comparar la evidencia experimental con la simulación numérica. Es por ésto que nos referiremos al diagrama $I - V$ frecuentemente en la memoria. Sin embargo, otro tipo de medidas más complejas (relacionadas con la fotoluminiscencia) han permitido por ejemplo confirmar la existencia de dominios de campo en las SR.

El trabajo que se presenta en el Capítulo 6 está motivado por los resultados obtenidos en experimentos de recolocación [92]. Como ya hemos comentado, cuando la densidad de carga dentro de la SR es suficientemente grande aparecen soluciones estacionarias con dos dominios de campo conectados por una barrera localizada en un período. Estas soluciones presentan un diagrama $I - V$ constituido por numerosas ramas que presentan discontinuidades entre ellas. El motivo de esta discontinuidad es que las soluciones que dan lugar a cada una de las ramas tienen la barrera que conecta los dominios en una celda distinta. De hecho, si a una solución estacionaria para un determinado valor de voltaje V_0 se le aplica un incremento repentino de voltaje a un valor V_f que está en la siguiente rama del diagrama $I - V$ la solución inicial evolucionará hasta alcanzar el nuevo estado (estacionario). Esta evolución implica que la barrera que une los dominios de campo se ha de desplazar de una celda a la contigua. El tiempo que el sistema emplea en adaptarse a las nuevas condiciones se denomina tiempo de recolocación. Los experimentos de recolocación consisten en medir estos tiempos de adaptación cuando se consideran soluciones que parten de un mismo voltaje inicial V_0 y a las que sin embargo se les aplica distintos incrementos de manera que tienen que alcanzar distintos voltajes finales V_f que están en la siguiente rama del diagrama. En las primeras observaciones realizadas al respecto se comprobó que los tiempos de recolocación eran mayores cuando el voltaje final V_f tomaba valores más cercanos a la discontinuidad entre las ramas que contienen a V_0 y V_f. Además, estos tiempos de recolocación presentaban un comportamiento estocástico. En este mismo trabajo se presentan las distribuciones de probabilidad de estos tiempos de recolocación para distintos valores finales de voltaje. Éstas presentan diferencias cualitativas dependiendo de que los valores finales del voltaje estén cerca o lejos de la discontinuidad. En el Capítulo 6 proponemos y contrastamos numéricamente un modelo estocástico discreto de Drift-Diffusion para explicar estos experimentos. El modelo estocástico se obtiene a partir del modelo de DDD donde se introducen efectos de ruido de tipo “shot”, originado en los dispositivos semiconductores por la cuantización de la carga [19]. Dicho modelo ha sido testado numéricame empleando métodos de simulación numérica para ecuaciones estocásticas, cuidando especialmente que el ruido numérico no perturbe las conclusiones.

Los resultados numéricos coinciden cualitativamente con los observados en el laboratorio lo cual nos permite asegurar que las fluctuaciones allí observadas son debidas a estos efectos aleatorios de tipo “shot”.

El trabajo presentado en el Capítulo 7 está motivado por superredes donde la densidad de carga presenta valores intermedios. En estos dispositivos se han observado tanto corrientes con oscilaciones autosostenidas como corrientes estacionarias dependiendo del voltaje aplicado. El modelo de DDD representa esta fenomenología, y de hecho el límite al continuo (hiperbólico) del modelo DDD se ha usado en la literatura para explicar el comportamiento de las soluciones oscilatorias. Dependiendo del voltaje que se considere el campo eléctrico dentro de la superred toma valores mayores o menores. En particular para valores bajos de voltaje se obtienen soluciones estacionarias con valores bajos de campo. En Capítulo 7 presentamos la deducción rigurosa de el límite al continuo (parabólico) del modelo de DDD en un régimen de campos bajos. Más concretamente hemos probado que las soluciones del sistema DDD se pueden aproximar por las soluciones de del sistema:

$$\begin{cases} \partial_t n + \partial_x J(F,n) = 0, \\ J(F,n) = v(F)n - D(F)\partial_x n \\ \partial_x F = n - N_D \\ \int_X F = V \\ J(F,n)(X) = W^{(f)}(F)n(X) \\ J(F,n)(-X) = (j^{(e)}(F) - W^{(b)}(F)n)(-X) \end{cases} \tag{19}$$

El tratamiento riguroso de este límite presenta varias dificultades. En primer lugar el caracter discontinuo de las soluciones del sistema discreto (se pueden ver como funciones escalonadas) obliga a considerar las soluciones en espacios de funciones integrables donde las derivadas son medidas. Por otro lado las densidades de corriente en los contactos hacen necesarias un tratamiento particular del límite en estas regiones. Finalmente hemos de señalar que para poder pasar al límite la condición de voltaje la hemos sustituido en una primera aproximación por una condición artificial sobre el campo en el emisor y en una etapa posterior hemos empleado este estudio para considerar el problema original.

Chapter 1

Introduction

The contents of this thesis are concerned with to the qualitative analysis of solutions to Partial Differential Equations (PDEs). We focus our attention on problems of existence and stability of steady states as well as asymptotic behaviour of time dependent solutions of some PDEs arising in semiconductor charge transport theory and in stellar dynamics. This analysis is interesting *per se*, although the knowledge of these properties also provides the guidelines for a further improvements of the models originally proposed. Our work follows this feedback relation between the analysis and the modeling. In this direction, two of the systems proposed here are modified versions motivated by observed phenomena which cannot be explained by using the original models.

The analyzed models describe the dynamics of an ensemble of interacting particles (e.g. electrons in a semiconductor device or stars in a galaxy). This description depends on the physics of the problem and on the observation scale employed. Thus, we can consider the electrons in a semiconductor device as quantum particles meanwhile the stars in a galaxy can be framed in the classical gravitational theory. The problems dealt with in this thesis stem from microscopic, kinetic and hydrodynamic descriptions.

In this chapter we introduce the models and the particular problems to be studied. We also announce our main results.

Stellar dynamics: the Vlasov-Poisson system

A stellar system is a bounded ensemble of stars. The size of the system can vary from a binary system, stellar clusters (10^2 to 10^6 stars) to galaxies (10^{10} to 10^{12} stars) or enormous clusters constituted by thousand of galaxies. The part of the theoretic physics studying the stellar systems is called Stellar Dynamics.

In a general case, the dynamics of a set of N particles (point masses with mass 1) can be determined by the physics of the system. If the particles are electrons or atoms we can assume a classical description by considering classical electrodynamics (if we see them as classical particles), meanwhile in the case of stars constituting a galaxy the classical gravitational laws yield this description. The set of equations provided by these theories constitutes which we shall refer as microscopic description. Celestial Mechanics addresses this sort of problems when the number of stars considered in the stellar system is small.

If N is high enough we can adopt a statistical description of the system. This considers the particle distribution given by a function $f(t,x,v)$, providing the number of particles in a domain $\Omega_x \in \mathbb{R}^3$ with velocity $\Omega_v \in \mathbb{R}^3$ at the time instant t

$$\int_{\Omega_x \times \Omega_v} f(t,x,v)\, dx dv \,.$$

Obviously, the function f only achieves nonnegative values and allows to write the particle density of the system as

$$\rho(x) = \int_{\mathbb{R}^3} f(t,x,v)\, dv \,.$$

As consequence, the total number of particles is

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} f(t,x,v)\, dx dv \, = N.$$

The subject of Statistical Mechanics is the study of this kind of systems by deriving and analyzing the kinetic equations verified by the particle distribution function.

The kinetic description of a set of classical particles interacting by a Coulombian interaction law, $u(r) = \gamma/r^2$, is given by the Boltzmann–Poisson equation (see [31])

$$\begin{cases} \partial_t f + v \cdot \nabla_x f - \nabla_x \phi \cdot \nabla_v f = Q(f,f) \,, \\ \\ \Delta_x \phi = 4\pi\gamma\rho \,, \quad \lim_{|x|\to\infty} \phi(t,x) = 0 \,, \end{cases}$$

where ϕ is a mean–field approximation potential generated by the particle density as solution to the Poisson equation. Also, the constant γ is 1 or -1 depending on the interactions considered, attractive or repulsive, respectively. Typical examples of physical systems governed by this equation are gravitational systems and electro–dynamical systems. Finally, Q is a binary kernel modeling the effect of the interactions between the particles. The initial value problem associated with this system is obtained by coupling these equations with an initial condition $f(t=0,x,v) = f_0(x,v)$.

In the particular case of galaxies and big stellar clusters, where the gravitational forces are attractive and Coulombian, the Boltzmann–Poisson system constitutes an admissible approach. Furthermore, we can assume that it is a collisionless system, i.e. $Q = 0$. The high amount of constituent particles allows us to consider that any particle moves under the influence of the mean potential generated by all the others. Forces due to nearby stars are inessential even though gravitational attraction decreases with the square of the distance. The reason of this is based on a comparison between the relaxation time and the age of the universe. The relaxation time is the smallest time needed to perturb the trajectory of a particle crossing a galaxy by short range interactions. When the number of particles is high enough the relaxation time is much bigger than the age of the universe, which assures that the mean–field approximation is admissible. On the other hand, the relation between the crossing time (time needed by a particle for crossing the galaxy) and the age of the galaxy allows us to consider that the number of possible collisions between particles is small enough to neglect their effect ([18, 33]). If we consider systems with a smaller number of constituent particles or smaller typical length, these assumptions may become nonadmissible.

Under this last assumption the Boltzmann–Poisson system reads in the following simpler form:

$$\begin{cases} \partial_t f + v \cdot \nabla_x f - \nabla_x \phi \cdot \nabla_v f = 0 \ , \\ \\ f(t=0, x, v) = f_0(x, v) \ , \\ \\ \Delta_x \phi = 4\pi\rho \ , \quad \lim_{|x| \to \infty} \phi(t, x) = 0 \ . \end{cases}$$

This is the gravitational Vlasov–Poisson (VP) system. Two of the chapters of this thesis are devoted to this system. In Chapter 2 we analyze the behaviour for large times of the solutions to the VP system. We employ variational arguments as well as invariances of the system. In Chapter 3 a new stability criterium for stationary solutions of the (VP) system is proposed.

Let us define some of the time preserved quantities associated with the VP solutions in order to present the results achieved in both chapters. Let $f(t, x, v)$ a solution to the VP system. The energy associated with f is given by

$$E(f) := E_{KIN}(f) - E_{POT}(f)$$

where the kinetic and potential energies are

$$E_{KIN}(f) = \frac{1}{2} \int_{\mathbb{R}^6} |v|^2 f(t, x, v) \, dx \, dv \quad \text{and} \quad E_{POT}(f) = \frac{1}{8\pi} \int_{\mathbb{R}^3} |\nabla \phi|^2 \, dx \ ,$$

respectively. This functional is time preserved for classical solutions to the VP system as well as the norms

$$\|f(t,\cdot,\cdot)\|_{L^p(\mathbb{R}^6)} = \left|\int_{\mathbb{R}^6} |f(t,x,v)|^p \, dx\, dv\right|^{\frac{1}{p}} \qquad p \in [1,\infty]$$

(see [57, 85]). In case of $p = 1$, we actually have mass conservation:

$$M = \int_{\mathbb{R}^6} f_0(x,v)\, dx\, dv = \int_{\mathbb{R}^6} f(t,x,v)\, dx\, dv\,.$$

Another conserved quantity is the velocity moment

$$\langle v\rangle(f) := \int_{\mathbb{R}^6} v f(t,x,v)\, dx\, dv\,.$$

The purpose of Chapter 2 is to study the asymptotic behaviour of the solutions to the VP system. Typically, qualitative properties of solutions to this system are derived from estimates of some L^p norm of the density function or of the potential or kinetic energy.

Our first result determines an optimal interval for the kinetic and potential energies in terms of the total energy, the total mass being fixed. Indeed, the potential and kinetic energies associated with a VP solution verify

(i) $E_{KIN}(f) \in \Big[\ K_-(E,M),\ K_+(E,M)\ \Big]$,

(ii) $E_{POT}(f) \in \Big[\ \max\{0, P_-(E,M)\},\ P_+(E,M)\ \Big]$,

(iii) $E_{POT}(f) \in \Big[\ 0,\ \sqrt{-4E_M E_{KIN}(f)}\ \Big]$,

for all times (see Theorem 2.1, pag. 22). These intervals depends on the initial condition, since

$$K_\pm(E,M) = -2E_M\left(1 - \frac{E}{2E_M} \pm \sqrt{1-\frac{E}{E_M}}\right)\,,$$

$$P_\pm(E,M) = -2E_M\left(1 \pm \sqrt{1-\frac{E}{E_M}}\right)\,,$$

where $M = \|f_0\|_{L^1(\mathbb{R}^6)}$, $E = E(f_0)$ and E_M is the minimum value of

$$E_M := \inf\left\{E(f)\,;\ f \in \Gamma_M\right\}\,, \tag{1.1}$$

with $\Gamma_M = \{f\,;\ f(x,v) \geq 0\,,\ \|f\|_{L^1(\mathbb{R}^6)} = M\,,\ \|f\|_{L^\infty(\mathbb{R}^6)} \leq 1\}$. These intervals are optimal in the sense that they reduce to a point when we consider a minimizer of (1.1), which is a stationary solution to the VP system. Indeed,

$$K_\pm(E,M) = E_{KIN}(f) = \frac{1}{2}\, E_{POT}(f) = P_\pm(E,M)\ .$$

The existence of stationary solutions shows that in general for the gravitational case a dispersive behaviour can not be expected contrary to that what happens in the plasma physical case (repulsive potential). It is well known that the solutions to the VP system in the repulsive case verify [58, 85]

$$\|\rho(t)\|_{L^{\frac{5}{3}}(\mathbb{R}^3)} \leq \frac{C}{t^{\frac{3}{5}}}\,, \quad \forall t > 0\,. \tag{1.2}$$

Obviously, this inequality says that the number of particles of the system in any arbitrary bounded domain Ω decreases with time.

Our next result shows a necesary condition for the initial data which allows to distinguish between those solutions to the attractive VP system which cannot satisfy a decay bound like (1.2) those which satisfy some dispersion properties (in a statistical sense). The result is based on the Galilean translations and the dispersion equation verified by those solutions. Let $f_0 : \mathbb{R}^6 \to \mathbb{R}$ be a nonnegative function with finite mass and energy. We have

i) If

$$E(f_0) < \frac{\langle v\rangle^2(f_0)}{2M} \tag{1.3}$$

holds, then, there exists a constant $C > 0$, such that the corresponding solution to the VP system with initial condition f_0 verifies

$$\|\rho_f(t,\cdot)\|_{L^{\frac{5}{3}}(\mathbb{R}^3)} \geq C\,, \quad \forall t \geq 0\,.$$

ii) Otherwise there exists $t_0 > 0$ such that statistical dispersion occurs:

$$C_1\, t^2 \leq \int_{\mathbb{R}^6} |x - \langle x\rangle|^2 f(t,x,v)\, dx\, dv \leq C_2 t^2 \quad \forall\, t \geq t_0 > 0\ . \tag{1.4}$$

We can then deduce

$$\|\rho(t,x)\|_{L^p(\mathbb{R}^3)} \geq \frac{C}{t^{3(p-1)/p}}, \quad \forall\, t > t_0\ ,$$

where $p \in [1,\infty)$, $\langle x\rangle = \int_{\mathbb{R}^6} x f(t,x,v)\, dxdv,$, and C_i, C are positive constants.

See Propositions 2.2 and 2.4 (pages 38 and 42) for more details. We remark that in *ii)* we get only lower time decreasing estimates for the density (which do not imply dispersion), although the increasing character of the variance leads to dispersion in a statistical sense. These results extend those obtained in [13] for spherically symmetric solutions.

Besides, the construction of stationary solutions to the VP system as minimizers of (1.1) allows to prove an stability criterium for that solutions. The unique spherically symmetric minimizer of (1.1) coincides with a polytropic solution. The family of spherical polytropic solutions is defined by

$$\nu_\mu = \nu(x,v) = c\left(E_0 - |v|^2/2 - \phi(|x|)\right)_+^\mu , \tag{1.5}$$

where $(\cdot)_+$ is the positive part function, $\alpha < E_0 < 0$, $-1 < \mu$ and $c > 0$. The minimum of (1.1) is achieved in ν_0 with $c = 1$. The nonlinear stability criterium (dynamical stability) for this solution is given in terms of the functional

$$d(g,h) = E(g) - E(h) + \frac{1}{4\pi}\left\|\nabla\phi_g - \nabla\phi_h\right\|^2_{\mathrm{L}^2(\mathbb{R}^3)} ,$$

where ϕ_g and ϕ_h are solutions to the Poisson equation with densities g and h, respectively (See Theorem 2.3 pag. 37). The criterium is directly derived from the minimization arguments developed to solve (1.1). This variational problem exhibits several technical difficulties. The energy is a nonconvex functional and is invariant by space translations. Furthermore, the functional space where the minimization problem is proposed has two constraints. We have studied this problem by concentration–compactness techniques and symmetric rearrangements. Actually, we adapt the arguments developed in [48, 50] for the Casimir minimization problem, which provides a similar dynamical stability criterium with $\mu \in (0, 3/2)$. Then, our work does include the critical exponent $\mu = 0$ (see Chapter 2 for more details). Along this thesis we deal with some other minimization problems related to (1.1). The functionals considered are nonconvex and invariant by a noncompact group of symmetries. This implies certain technical complexity.

Chapter 3 extends the dynamical stability criterium to a stronger one in terms of the orbital stability, which can be deduced for the wider range of polytropic solutions with $\mu \in [0, 7/2)$. In this case, we have to study the minimization problem

$$I^\mu_{M,J} := \inf\left\{E(f)\,;\ f \in \Gamma^\mu_{M,J}\right\} , \tag{1.6}$$

where $\Gamma^\mu_{M,J} = \mathrm{L}^1_+(\mathbb{R}^6, M) \cap \mathrm{L}^{1+1/\mu}_+(\mathbb{R}^6, J)$ and $\mathrm{L}^p_+(\mathbb{R}^6, K) = \{f \in \mathrm{L}^p(\mathbb{R}^6); f \geq 0\,,\ \|f\|_{\mathrm{L}^p(\mathbb{R}^6)} = K\}$. The minimization arguments used to solve these problems allow to conclude that polytropic solutions with $\mu \in [0, 7/2)$ are orbitally stable. This criterium basically claims that if the initial condition f_0, with appropriate mass and $L^{1+1/\mu}$ norm, is close enough to ν_μ (in terms of the energies), then the corresponding solution remains close (in L^1 norm) to the orbit of ν_μ defined by $\{\nu_\mu(\cdot - k, \cdot)\,;\ k \in \mathbb{R}^3\}$. This concept of stability is optimum thanks to the Galilean invariance of the system, as we shall see in Chapter 3. The stability criterium is a consequence of the variational argument employed to solve the minimization problem (1.6). Now, we reduce (1.6) to an equivalent problem for the density functions. Combining the minimization arguments for the reduced problem with the original one we can conclude the relative compactness in L^1 of any minimizing sequence (up to translations). This result extends the results obtained in other works [48, 50, 51] based on minimization problems for the Casimir or energy functionals in spaces with mass or Casimir–mass constraints, respectively.

Transport in semiconductor devices

The interest of the study of charge transport in semiconductor materials relies on their use to develop electronic devices. Since the first built transistors, based on germanium, has been the Silicon the semiconductor material dominating the technological applications. Nevertheless, a lot of different devices for special applications have been invented in last decades (solar cell, light–emitting diodes, lasers, ...). This has motivated the study of other semiconductor materials as the Gallium Arsenide (GaAs) or the Aluminium Arsenide (AlAs). Historically, the semiconductors are materials with a much higher conductivity than insulators, but much lower conductivity than metals. This simple classification is nowadays more complete. Actually, it distinguishes also between semimetals and superconductors. The difference between semiconductors and semimetals is that the latter retain their metallic conductivity at low temperatures while semiconductors are transformed into insulators at very low temperatures. A more detailed analysis of these materials requires to consider factors as the gap energy, the crystal structure, lattice constant, impurities, etc.... [6, 45].

A very important fact for the success of semiconductor devices is that the device length is very small compared to previous electronic devices. Indeed, the typical device length is continuously decreasing. The first Germanium transistor had a characteristic length of $20\mu m$ and the transistors in a modern Pentium IV have a characteristic length of $0.18\mu m$. In fact, the Semiconductor Industry Association (SIA) announced that the devices in 2009 will have lengths around $0.05\mu m$. This miniaturization process has motivated increasing interest in the study of quantum effects in transport processes. Thus, the hypothesis of classic transport valid for large enough devices becomes fruitless for these small devices.

The transport of electrons in a semiconductor generated by the applied bias depends on several factors: the semiconductor material employed, the external conditions (temperature, external forces), size of the device, ... As consequence, a considerable quantity of models has been proposed in the literature to describe the transport process, and the selection of an appropriate model depends on the specific properties of the device. We remark that there is a great interest in this field [62, 82, 86].

Determinant factors in the modeling of charge transport in a semiconductor device are

i) The description of the dynamics of the electrons. This can be a microscopic, kinetic of hydrodynamic description. On the other hand, electrons can be considered like classical or quantum particles depending on the relevance of the quantum effects in the transport mechanism.

ii) The influence of the semiconductor crystal lattice. The periodicity of the semiconductor crystal lattice implies that the potential created by the ions is also periodic. In this case, if we neglect other interactions, we can deduce the existence of certain electronic states called Bloch states.

iii) The interactions between particles. We can consider electrostatic interactions (long–range interactions of Coulombian type) or collisions between particles (also called scattering processes).

The different models studied in the literature correspond to different answers to these questions. Of course, other relevant factors may appears in the modeling such as the existence of impurities in the semiconductor (doping) or the effect of other external forces (for example, an external magnetic fields).

The consistency of a model comes from its derivation from first principles. In the case of the electron dynamics the first principles are dictated by Quantum Mechanics. A single electron of mass m and charge q moving in a vacuum under the action of an electric field $E = E(x,t)$ is described by the complex wave function $\psi : \mathbb{R}^3 \times [0,\infty] \to \mathbb{C}$, which is governed by the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial_t} = -\frac{\hbar}{2m}\Delta\psi - qV(x,t)\,. \tag{1.7}$$

Here, $\hbar$ is the reduced Plank constant and $V(x,t)$ is the potential related to the electric field $E = -\nabla V$. The density function $n(x,t) = |\psi(x,t)|^2$ is

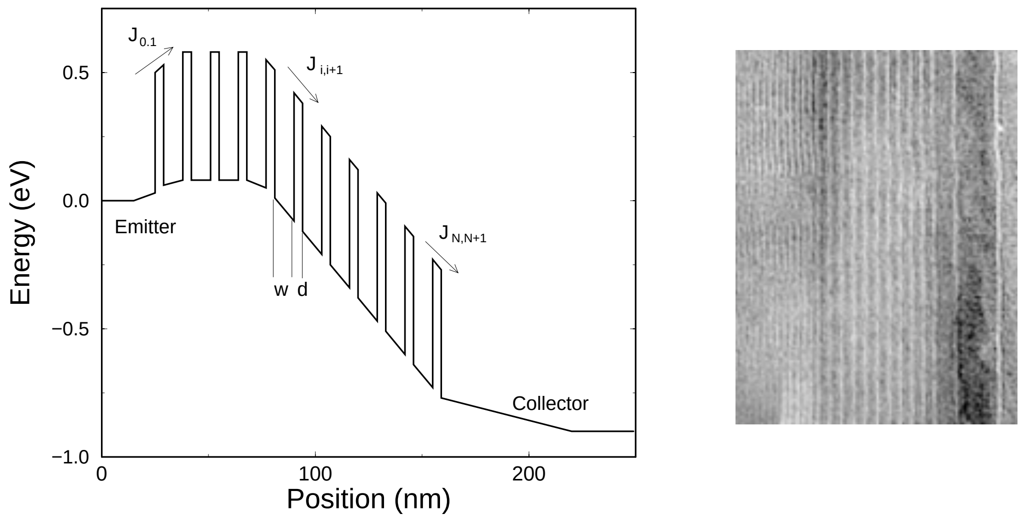

Figure 1.1: (*Left*) Conduction band diagrams of a semiconductor superlattice (*Right*) Transversal cross section of a SL constituted by layers of Si (dark bands) and SiO2 (light bands) of various thicknesses.

considered as the probability function of finding the electron, i.e.

$$\int_{\Omega} n(x,t)\,dx$$

is the probability of finding the electron in the domain Ω in the time instant t. Depending on the effects under consideration we will derive different models.

This theoretical framework is more complex when the devices considered are not simple semiconductor materials under applied bias. Along this thesis we shall present two works concerning a semiconductor devices, called semiconductor superlattices (SL). They are constituted by a periodic array of layers of two different semiconductors whose lateral dimension is much larger than the length l of one period. Since two semiconductors have different energy gaps, the conduction band of a superlattice can be viewed as a periodic array of potential wells and barriers, of widths d and w respectively, with $l = d + w$. The first and the last layers are connected to the emitter and the collector, which constitute the contacts (see Fig. 1.1).

These devices, proposed originally by L. Esaky in 1969, are a typical example of open quantum system, which are systems that can exchange locally conserved particles with its environment. The modeling of these devices is rather more complicated because the electron flux is crossing an heterogeneous medium. Depending on the characteristics of the SL, the displacement of charge can be due to several mechanisms.

Resonant tunneling is a typical mechanism of transport in these devices. Tunneling is the mechanism by which the electrons go from one well to the next on crossing the intermediate barrier. For the case of tunneling structures, the standard theory assumes that the electron states are stationary scattering–state solutions of Scrhödinger equations. Thus, the current can be calculated by using transmission coefficients between these elemental states. Some authors claim that this description is not adequate in general for nonequilibrium phenomena [37]. Thus, dynamical descriptions of the electrons in the nonequilibrium case are needed.

Quantum transport models

Here we present two works devoted to the analysis of the asymptotic dispersive character of the solutions to systems of Schr̈odinger–Poisson type [60, 82]. The Schr̈odinger–Poisson system models a gas of electrons in vacuum which are affected by the self–consistent electric field created by themselves. In last years, different adaptations of this general model have appeared in the literature for electron transport under particular contexts [91, 61, 81]. The study of dispersive properties is relevant for the fabrication of semiconductor superlattices [2, 25, 109].

The first model we have studied is the Schrödinger–Poisson (SP) system in the 3–dimensional space, defined by

$$
\begin{aligned}
i\hbar\frac{\partial\psi}{\partial t} &= -\frac{\hbar^2}{2m}\Delta_x\psi + V\psi, && \lim_{|x|\to\infty}\psi(x,t) = 0,\\
\psi(x,t=0) &= \phi(x),\\
\Delta_x V &= -\,n, && \lim_{|x|\to\infty} V(x,t) = 0\,.
\end{aligned}
$$

This system is closed with appropriate boundary and initial conditions. As it is well known, although the mass and the energy are preserved, other relevant quantities like the second order moment of the density or the L^p–norm, $p > 2$, have dispersive properties. We analyze the behaviour of such quantities in the context of a single quantum state modeled by the Schrödinger–Poisson system. However, our analysis can be easily extended to the mixed–state case. The study of the solutions to these systems has been done in several papers [29, 59]. Our main goal in Chapter 4 is to improve the results obtained in those works. Upper and lower estimates for the $\mathrm{L}^p(\mathbb{R}^3)$ norms of the solutions, with $2 < p < 6$, are obtained. These estimates describe, the behaviour of those quantities. Under appropriate hypothesis on the initial condition, it can be proved that the associated solution to the SP system verifies

$$\frac{C_1}{|t|^{\frac{3p-6}{2p}}} \le \|\psi(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \le \frac{C_2}{|t|^{\alpha(p)}}, \quad \forall\, |t| \ge \xi,\ \forall\, p \in [2,6]\,,$$

with C_i positive constants, $\xi > 0$ and

$$\alpha(p) = \begin{cases} 1 - \frac{2}{p}, & \text{if } p \in [2,3], \\ \frac{2}{3} - \frac{1}{p} & \text{if } p \in [3,6]\,. \end{cases}$$

See Theorem 4.1 (pag. 78) for more details. Upper time decay rates have been improved with respect to those obtained in [29, 59]. Also, the lower estimates are optimal. These estimates obtained from the dispersion equation standing for the VP solutions and an inequality due to P.L. Lions, which links the kinetic and potential energy with the L^3 norm of a solution.

The second quantum model considered here is the Scrödinger–Poisson–Slater (SPS) system defined by

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta_x\psi + V\psi - C_S n^{\frac{1}{3}}\psi, \qquad \lim_{|x|\to\infty}\psi(x,t) = 0, \tag{1.8}$$

$$\psi(x,t=0) = \phi(x), \tag{1.9}$$

$$\Delta_x V = -\,n, \qquad \lim_{|x|\to\infty} V(x,t) = 0\,. \tag{1.10}$$

This system coincides with the Schrödinger–Poisson (SP) system when the contribution of the last term (the Slater term) is not considered, i.e. $C_S = 0$. Here, C_S stands for the Slater constant. The repulsive effect of the Coulomb potential seems to be too strong when we compare the behaviour of the solutions to the SP system to simulations of superlattice structures (see [89, 111]). Some different approximations have been studied to overcome this problem. The SPS model appears as an appropriate adaptation of the Poisson potential (see [20] for more details).

As for the SP system, the solutions to the SPS system exhibit some conserved quantities as the charge (L^2 norm) or the energy, defined by

$$E[\psi] = \int_{\mathbb{R}^3}\left\{\frac{\hbar^2}{2m}|\nabla\psi(x,t)|^2 + \int_{\mathbb{R}^3}\frac{|\psi(x,t)|^2|\psi(x',t)|^2}{8\pi|x-x'|}dx' - \frac{3C_S}{4}|\psi(x,t)|^{\frac{8}{3}}\right\}dx\,.$$

The energy is constituted by the kinetic energy, the Coulomb potential energy and the potential energy term corresponding to the Slater correction.

The qualitative analysis of the solutions to the SPS system is determined by the balance between the potential terms. One important feature of the

SPS system is that its associated potential energy can reach negative values depending on the constants of the system (mass, initial energy or Slater constant). This fact implies some relevant properties of the SPS system in the repulsive case: 1) the minimum of the total energy operator is negative for some choices of the physical constants; 2) there are solutions (depending on the initial energy) that do not exhibit dispersive character; 3) there exist steady–state solutions, i.e. solutions with constant density; 4) there are solutions, even with positive energy, which preserve the L^p norm and do not decay with time. These properties show important qualitative differences between the SPS system and the SP system.

We now rouhly present our main results. Firstly we propose the variational problem

$$I_M = \inf\{E[\psi]\,;\ \psi \in \mathrm{H}^1(\mathbb{R}^3)\,,\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M\}. \tag{1.11}$$

Under some technical hypotheses we conclude the existence of a minimum for this problem (see Theorem 5.2 pag. 103). In this case, the energy functional is nonconvex and invariant by space translations. The minimizing problem is solved by considering two different techniques: concentration–compactness and nonzero weak compactness. The existence of minimizers allows us to obtain two interesting consequences.

We claim the existence of stationary solutions (time independent density) to the SPS, given by $\psi(x,t) = e^{-i\beta t}\psi(x)\,,\ \beta \in \mathbb{R}$. By combining this result with the Galilean invariance we can state the existence of solutions to the SPS system (even with positive energy) whose $\mathrm{L}^p(\mathbb{R}^3)$ norm remains constant along the time evolution for $p \in [8/3, 6]$. The qualitative behaviour of these solutions is clearly different to that of the SP solutions.

We also get optimal bounds for the kinetic energy of the solutions, similar to those obtained for the VP system. We prove that the kinetic energy of the solutions to the SPS system ranges between the values

$$E^{\pm}_{KIN} = -2I_M\left(1 - \frac{E_0}{2I_M} \pm \sqrt{1 - \frac{E_0}{I_M}}\right), \tag{1.12}$$

where M and E_0 respectively hold for the mass and the energy of the solutions (see Proposition 5.5, pag. 104).

The Galilean invariance of the solutions allows to deduce a criterium to distinguish those solutions whose L^p norms do not vanish from those which are dispersive in a statistical sense. Thus, for any SPS solution ψ with initial condition ϕ such that

$$E[\phi] < \frac{1}{2}\frac{|\langle x\rangle|^2}{\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}}\,,$$

there exists positive constants C, C' and C'' for which

$$\|\psi(t\cdot)\|_{\mathrm{L}^p(\mathbb{R}^3)} \geq C, \quad E_{POT}[\psi] \leq -C'\,, \quad \forall t \geq 0, \quad p \in [8/3, 6]\,.$$

Here, $\langle x \rangle := \int_{\mathbb{R}^3} x\phi\, dx$. If ϕ satisfies the reverse inequality

$$E[\phi] > \frac{1}{2} \frac{|\langle x \rangle|^2}{\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}}\,,$$

then we get the lower bound

$$\|\psi(\cdot, t)\|_{L^p(\mathbb{R}^3)} \geq \frac{C''}{t^{\frac{3p-6}{2p}}}, \quad \forall t > \xi > 0, \quad p \in [2, 6]\,.$$

Furthermore, dispersion effects are proved in a statistical sense:

$$\int_{\mathbb{R}^3} |(x - \langle x \rangle)|^2 n(x)\, dx = O(t^2)\,.$$

See Corollary 5.1 pag. 109 for more details. To recap we have shown that the Slater correction produces relevant changes in the qualitative behaviour of the solutions.

We observe that the X^α-approach to the SP system (see Chapter 5) is linked with the polytropic solutions to the VP equation by a minimization problem over the associated energy functionals subject to a finiteness constraint on some L^p norm. This gives rise to a Lagrange multiplier, which is precisely the X^α correction to the SP system.

Drift-Diffusion models

The last part of the thesis is concerned with two works based on a Discrete Drift–Diffusion system, which models charge transport in weakly coupled semiconductor superlattices. These SL are such that the barrier width is much larger than the reciprocal of the typical electron wave number inside the barrier. Nonlinear charge transport phenomena are observed in these devices due to the existence of field domains (domains in which the electric field achieves homogeneous values). The electrons constituting the total charge can be produced by doping or irradiating the SL with appropriate laser intensity. Depending on the charge density inside the SL we can observe different typical configurations. For any value of constant applied voltage, the typical response of the current in the device can be measured. The relation between voltage and current constitutes the current–voltage ($I - V$) diagram characteristic curve. When the electron density inside the SL is sufficiently low, the electric field is almost spatially uniform and the $I-V$ curve is smooth. Provided that the charge inside the SL is large enough, these configurations are unstable and a stationary field configuration having two electric field domains appears. In this case, the $I-V$ exhibits a sow–tooth like profile where different branches appear separated by discontinuities (See Chapter 6). The discontinuities between the branches are motivated by the displacement from one SL period to an adjacent one of the wall connecting the electric field domains. Finally, when intermediate values of the charge are adopted self–sustained oscillations are observed.

We now describe in some detail the Discrete Drift–Diffusion model. In such weakly coupled semiconductor SL, the dominant mechanism of charge transport is sequential resonant tunneling. The displacement of one electron from one well to the adjacent one can be split into three stages: scattering, relaxation and tunnelling. During the scattering time, an electron originally in an excited subband tends to lose energy and fall to the first subband. Afterwards, the electron stay in that subband during the relaxation time. Tunnelling is the mechanism employed by the electron to scape from one well to the next one. The model assumes that scattering times are shorter than escape times from quantum wells, the latter being shorter than dielectric relaxation times. Then, the dominant mechanism of vertical transport is sequential tunneling; only the first subband of each well is appreciably occupied and the tunneling current is quasistationary (the well-to-well tunnelling current density across a barrier is calculated assuming a constant value of the applied electric field and a constant electron density at the wells adjacent to the barrier). In the simplest situation, the center of each quantum well is n-doped and the thermal energy is large compared to the energy of the lowest miniband. Then, electronic transport in these devices can be described by a Discrete Drift-Diffusion model (see [1, 23, 22, 107]). In such a model, we consider an array of $N+1$ consecutive cells, which are well–barrier pairs, labelled by the index $i \in \{0, \ldots, +N\}$. The barrier separating the injecting contact from the first well of the SL is considered as the 0–th barrier, while the barrier of the N–th SP period separates the N-th well from the collector. The model assumes that the electrons are singularly concentrated on a two–dimensional region allocated in the center of the quantum well. The unknowns are the two–dimensional electron density n_i , $i = 1, \ldots, N$ (number of electrons per unit area of the superlattice cross section at the center of the i–th well) and the average electric field F_i in each cell, $i = 0, \ldots, N$. These quantities are related through the following discrete Poisson equation

$$F_i - F_{i-1} = \frac{e}{\varepsilon}(n_i - N_D^w), \quad i \in \{1, \ldots, N\}. \tag{1.13}$$

In (1.13), N_D^w stands for the two–dimensional doping in the wells, assumed to be constant, while $\overline{\varepsilon}$ is the average permittivity in the SL and $e = -q$ stands for the electron charge. Notice that the set of relations (1.13) involves as an additional unknown the electric field F_0 at the injecting contact. On the other hand, denoting by $eJ_{i\to i+1}$ the tunneling current density through the barrier separating the cells $\#i$ and $\#(i+1)$, the density in the i–th cell satisfies the following charge continuity equation

$$\frac{dn_i}{dt} = J_{i-1\to i} - J_{i\to i+1}, \quad i \in \{1, \ldots, N\}. \tag{1.14}$$

Consequently, differentiating (1.13) and using (1.14), we notice that the quantity

$$\frac{\overline{\varepsilon}}{e}\frac{dF_i}{dt} + J_{i\to i+1} = J(t), \quad i \in \{0, \ldots, N\}\,, \tag{1.15}$$

does not depend on the considered cell. This is the so–called Ampère's law, where $eJ(t)$ stands for the total current density through the SL which does not depend on the index i.

Then, the model is completed by a constitutive law which defines the current density $eJ_{i\to i+1}$ by means of the (n_k, F_k)'s. The tunneling current density depends on the electrochemical potentials at cells $\#i$ and $\#(i+1)$ and on the average electric field F_i [22, 107]. The electrochemical potentials that "drive" the tunneling current (a nonzero current is a consequence of unequal electrochemical potentials at cells $\#i$ and $\#(i+1)$) are functions of the electron densities and therefore we may consider that the tunneling current $eJ_{i\to i+1}$ depends on n_i, n_{i+1} and F_i [22, 107]. First–principles calculations of $eJ_{i\to i+1}$ are at best sketchy. In the literature, some formulae have been derived from quantum kinetic equations for the Green's functions [107] (assuming constant electric field across the superlattice, simplified hopping Hamiltonians and scattering) and from the transfer Hamiltonian formalism [1, 23, 22] (a many–body version of the WKB method originally proposed by Bardeen [9]). At high (room) temperature, all these formulae imply that the tunneling current is given by the difference of a drift term and a diffusion term as follows

$$J_{i\to i+1} = \frac{n_i v(F_i)}{\ell} - \frac{D(F_i)(n_{i+1} - n_i)}{\ell^2}, \quad i \in \{1, \ldots, N-1\}. \tag{1.16}$$

The drift velocity and the diffusion coefficient are defined through functions v and D of the electric field, which depend on the physical properties of the material used in the SL (see [22] for more details). The special nature of the three–dimensional emitter and collector layers (different from the essentially two–dimensional quantum wells that form the superlattice) is considered in the calculation of the boundary tunneling current. By using the transfer Hamiltonian formalism, the following approximate expressions can be derived [23]

$$J_{0\to -N} = j^{(e)}(F_{-N-1}) - \tfrac{n_{-N}W^{(b)}(F_{-N-1})}{\ell}, \tag{1.17}$$

$$J_{N\to N+1} = \tfrac{n_N W^{(f)}(F_N)}{\ell}. \tag{1.18}$$

These equations involve the emitter current density $ej^{(e)}$, the emitter backward velocity $W^{(b)}$ and the collector forward velocity $W^{(f)}$, which are given functions of the electric field. All the coefficients $v, D, W^{(b)}, W^{(f)}, j^{(e)}$ are supposed to be nonnegative and satisfy some regularity properties. Typical graphs for these functions can be found in Chapter 6.

We remark that one equation is still missing since we have one unknown more than equations. A realistic boundary condition is the so–called voltage bias condition: the total voltage across the superlattice,

$$\ell \sum_{i=1}^{N} F_i = V, \tag{1.19}$$

remains equal to a given quantity V.

Relations (1.13), (1.14) and (1.19) form a closed system of equations for n_i with $i \in \{1, \ldots, N\}$ and F_i with $i \in \{0, \ldots, N\}$, referred to in the sequel as the Discrete Drift–Diffusion (DDD) model.

The voltage V and the total current eJ are variables that can be measured in experiments. This allows us to compare the experimental evidence with the numerical simulations. Furthermore, there exist other indirect experiment measures (based on photoluminiscense measurements) that have confirmed the existence of field domains.

The problem studied in Chapter 6 was motivated by recent experimental evidence obtained in relocation experiments [92, 93]. As we mentioned above, highly doped weakly coupled semiconductor superlattices typically exhibit a $I-V$ diagram with many sharp branches due to formation of static electric field domains. The field domains are connected by an intermediate wall which is an accumulation layer, typically alocated in one well. The discontinuities in the $I-V$ curve are motivated by the displacement of the wall from one well to other. The relocation experiments consist in the measuring of the time delay of the system to reach a new stable field configuration at voltage $V_1 = V_0 + \Delta V$ when the voltage is suddenly increased from V_0. If V_0 and V_1 are alocated in separated branches, the domain wall has to relocate so that a stable field configuration appropriate to the new voltage is reached [80]. In [80] it was claimed that when V_0 and V_1 are in adjacent branches the time delay depends on the distance between V_1 and the $I - V$ discontinuity. The relocation time is bigger as V_1 is closer to the jump between the branches. Other experiments have shown that the relocation time for up jumps ($\Delta V > 0$) close to the discontinuity in the I-V characteristic is random and have also investigated its probability distribution function [92, 93]. In Chapter 6 we shall present a stochastic theory of domain relocation in highly doped SL explaining these experiments. The stochastic model has been derived from the DDD model, where we take into account shot noise effects which arise in semiconductor devices by the quantization of the charge [19]. We have tested numerically the model by using numerical methods for stochastic differential equations. The numerical results are in qualitative agreement with those obtained in experiments, concluding that the fluctuations observed in relocation experiments are due to shot effects.

The problem we deal with in Chapter 7 is focussed on SL where the charge density inside the device reaches intermediate values. In this case, stationary responses and self–sustained oscillations are observed depending on the values of the applied voltage. The DDD model captures this situation. Indeed, the (hyperbolic) continuum limit has been proposed in the literature to explain self–sustained oscillations. The electric field inside the device depends on the applied voltage. Low biased SL present low values of the field. In Chapter 7 we rigorously study the continuum limit of the DDD model in a low–field regime. We have proved that in this regime the solutions can be aproximated by those of the system

$$\begin{cases} \partial_t n + \partial_x J(F,n) = 0, \\ J(F,n) = v(F)n - D(F)\partial_x n\,, \\ \partial_x F = n - N_D\,, \\ \int_X F = V\,, \\ J(F,n)(X) = W^{(f)}(F)n(X)\,, \\ J(F,n)(-X) = (j^{(e)}(F) - W^{(b)}(F)n)(-X)\,. \end{cases} \tag{1.20}$$

See Theorem 7.3 pag. 154 for more details. The rigorous treatment of this limit exhibits several difficulties. The discrete nature of the solutions (steep–wise functions) to the DDD model forces to consider functional spaces in which derivatives are measures. The special consideration of the current densities in the contacts needs a particular analysis of the limit in both contacts. Finally, we remark that the bias condition has to be replaced in a first approach by an artificial Dirichlet type condition on the electric field in the emitter, in order to get appropriate *a priori* estimates. Then, we recover the bias condition by a simple argument.

Chapter 2

Asymptotic behaviour for the Vlasov-Poisson System in the stellar dynamics case

Introduction

The purpose of this chapter is to study the asymptotic behaviour of the solutions of the Vlasov–Poisson system (VP) in the gravitational case

$$\begin{cases} \partial_t f + v \cdot \nabla_x f - \nabla_x \phi \cdot \nabla_v f = 0 \ , \\ \\ f(t=0,x,v) = f_0(x,v) \ , \\ \\ \Delta_x \phi = 4\pi\gamma\rho \ , \quad \lim_{|x|\to\infty} \phi(t,x) = 0 \ , \end{cases}$$

by the mean of an associated variational problem.

We first obtain optimal upper and lower bounds of the kinetic and potential energies in terms of the mass and of the minimum of the total energy functional (Theorem 2.1). These estimates are optimal in the sense that they coincide in the case of one of the so-called *polytropic gas spheres* solutions (Theorem 2.2; see [15] for a study of these solutions by means of the associated characteristics system). We reduce the problem to the proof that the minimum of the energy is realized in a class of bounded functions (see below). In Section 2, we completely characterize the minimizers, which in turn gives an optimal constant for an interesting inequality (see Appendix B), and also proves a nonlinear stability result (Theorem 2.3).

The dispersive character of the solutions of the VP system in the plasma physical case has been proved by using L^p-estimates of the mass density. As was pointed out in [58], a different qualitative behaviour can be expected for the gravitational case, due to the existence of stationary solutions. Section 2 of this paper is devoted to the study of this case. In terms of the orientation of an inequality which relates the value of the energy, the mass and the momentum of the initial data, we distinguish two situations: either we can derive positive lower bounds for the potential and a norm of the mass density, or we prove that the variance of the density function is of order t^2 as in the plasma physics case. For that purpose, we extensively use the *Galilean invariance* of the VP system, and also the *pseudo-conformal law* as in the dispersive case.

There is a general interest in understanding the large time behaviour of time dependent solutions of the VP system, which has given rise to various approaches in the literature, ranging from the study of the stability of certain solutions [11, 48, 50] to the analysis of the time evolution of integral quantities (moments, L^p-norms, ...), see *e.g.* [13]. Our dispersion results extend the estimates of J. Batt in [13] to the non spherically symmetric case.

The solutions corresponding to polytropic gas spheres are radial and take the special form

$$f(x,v) = c(E_0 - |v|^2/2 - \phi(x))_+^\mu \, |x \times v|^{2k}$$

(see [15, 16, 48] for details). In [48] (see [50, 90] for more recent results) some of these solutions (the ones corresponding to $0 < \mu < \frac{3}{2} + k$, $c > 0$, $k > -1$) were obtained as minima of a so-called Energy-Casimir functional. Here, we extend these results and the compactness arguments to the limit case which formally corresponds to $\mu = 0$ and $k = 0$. Considerations on the total energy functional are fruitless at a first sight, since this functional is not bounded from below in the functional spaces proposed in [48]. This motivates an extra restriction (a uniform bound), which is stable under the evolution of the VP system and corresponds to the standard framework for solving the Cauchy problem.

We face different kinds of difficulties: lack of compactness due to translation invariance, and possibility of *dichotomy* in the large-time dispersive regime due to the invariance under Galilean translations. The possible regimes are much richer in the gravitational case than in the plasma physics case (see for instance [67] for the construction of time-periodic solutions). This also makes the analysis, for instance of the dispersive regime, much harder than in the plasma physics case [58, 85, 30].

Optimal bounds for the kinetic and potential energies

The goal of this section is to determine an optimal interval for the kinetic and potential energies in terms of the total energy, the total mass being fixed. We reduce the question to a minimization problem and prove that it is achieved.

Let $f(t,x,v)$ be a solution of the VP system and define the total energy associated to f by

$$E(f) := E_{KIN}(f) - \gamma\, E_{POT}(f)$$

where the kinetic and the potential energies are defined respectively by

$$E_{KIN}(f) = \frac{1}{2}\int_{\mathbb{R}^6} |v|^2\, f(t,x,v)\; dx\, dv \quad \text{and} \quad E_{POT}(f) = \frac{1}{8\pi}\int_{\mathbb{R}^3} |\nabla\phi|^2\; dx\ .$$

In the last expression the potential ϕ associated to f is given by

$$\phi = -\frac{\gamma}{|\cdot|} * \int_{\mathbb{R}^3} f(\cdot, v)\, dv\ . \tag{2.1}$$

For a smooth solution the total energy remains constant along the time evolution of the solution as well as the total mass which is defined by

$$\|f(t,\cdot,\cdot)\|_{\mathrm{L}^1(\mathbb{R}^6)} = \int_{\mathbb{R}^6} f(t,x,v)\; dx\, dv$$

(see [57, 85]). The transport of the distribution function also preserves uniform bounds:

$$\|f(t,\cdot,\cdot)\|_{\mathrm{L}^\infty(\mathbb{R}^6)} \le \|f(0,\cdot,\cdot)\|_{\mathrm{L}^\infty(\mathbb{R}^6)}\ .$$

For these reasons, it is natural to consider the functional space $\mathrm{L}^1\cap\mathrm{L}^\infty(\mathbb{R}^6)$. Our main result relates $E(f)$, $E_{KIN}(f)$ and $E_{POT}(f)$ in this functional space. It is by the way independent of the VP system itself but of course applies to any of its solutions. Before, we need some further notations and definitions. For any $M > 0$, let

$$\Gamma_M = \{f \in \mathrm{L}^1\cap\mathrm{L}^\infty(\mathbb{R}^6)\ :\ f(x,v) \ge 0\,,\ \|f\|_{\mathrm{L}^1(\mathbb{R}^6)} = M\,,\ \|f\|_{\mathrm{L}^\infty(\mathbb{R}^6)} \le 1\}$$

and consider

$$E_M := \inf\{E(f)\ :\ f\in\Gamma_M\}\ . \tag{2.2}$$

In the rest of this paper, we will assume without further notice that $\gamma = 1$ (gravitational case). For any $E \geq E_M$, define

$$K_\pm(E,M) = -2E_M \left(1 - \frac{E}{2E_M} \pm \sqrt{1 - \frac{E}{E_M}}\right)$$

$$P_\pm(E,M) = -2E_M \left(1 \pm \sqrt{1 - \frac{E}{E_M}}\right) .$$

Theorem 2.1. E_M is negative, bounded from below and for any $f \in \Gamma_M$, with $E = E(f)$, the following properties hold:

(i) $E_{KIN}(f) \in \Big[\ K_-(E,M),\ K_+(E,M)\ \Big]$

(ii) $E_{POT}(f) \in \Big[\ \max\{0, P_-(E,M)\},\ P_+(E,M)\ \Big]$

(iii) $E_{POT}(f) \in \Big[\ 0,\ \sqrt{-4E_M E_{KIN}(f)}\ \Big]$

Moreover, there exist functions which minimize (2.2) and these are stationary solutions to the VP system for which $E = E_M$ and

$$K_\pm(E,M) = E_{KIN}(f) = \frac{1}{2}\, E_{POT}(f) = P_\pm(E,M) .$$

The rest of this section is devoted to the proof of Theorem 2.1, apart the fact that minimizers are solutions of the VP system, which is going to be an easy consequence of the explicit form of the minimizers (see Theorem 2.2 in Section 2).

A potential energy estimate

Lemma 2.1. There exists a positive constant C such that for any nonnegative function f in $\mathrm{L}^1 \cap \mathrm{L}^\infty(\mathbb{R}^6)$ with $|v|^2 f \in L^1(\mathbb{R}^6)$ and ϕ given by 2.1,

$$\int_{\mathbb{R}^3} |\nabla\phi|^2\, dx \leq C\, \|f\|^{7/6}_{\mathrm{L}^1(\mathbb{R}^6)}\, \|f\|^{1/3}_{\mathrm{L}^\infty(\mathbb{R}^6)} \left(\int_{\mathbb{R}^6} |v|^2 f(x,v)\, dx\, dv\right)^{1/2} . \qquad (2.3)$$

In the rest of this paper, we shall denote by $\mathcal{C}$ the best constant in Inequality 2.3 (see Appendix B for more details).

Proof. From the definition of ϕ we have

$$\int_{\mathbb{R}^3} |\nabla\phi|^2\, dx = \int_{\mathbb{R}^3} (-\Delta\phi)\, \phi\, dx = 4\,\pi \int_{\mathbb{R}^6} \frac{\rho(y)\rho(x)}{|x-y|}\, dx\, dy$$

with $\rho(x) = \int_{\mathbb{R}^3} f(x,v)\,dv$. According to the Hardy-Littlewood-Sobolev inequalities,

$$\int_{\mathbb{R}^3} |\nabla\phi|^2\, dx \le 4\pi\,\Sigma\,\|\rho\|^2_{\mathrm{L}^{\frac{6}{5}}(\mathbb{R}^3)}$$

for some constant $\Sigma > 0$. Because of Hölder's inequality,

$$\|\rho\|_{\mathrm{L}^{6/5}(\mathbb{R}^3)} \le \|\rho\|^{7/12}_{\mathrm{L}^1(\mathbb{R}^3)} \|\rho\|^{5/12}_{\mathrm{L}^{5/3}(\mathbb{R}^3)} \,.$$

The $\mathrm{L}^{5/3}$-norm of ρ can be estimated by the standard interpolation inequality

$$\int_{\mathbb{R}^3} |\rho|^{5/3}\, dx \le C\,\|f\|^{2/3}_{\mathrm{L}^\infty(\mathbb{R}^6)} \int_{\mathbb{R}^6} |v|^2\, f(x,v)\; dx\, dv \,.$$

□

An equivalent minimization problem

Define

$$J(f) = \frac{\frac{1}{2}\int_{\mathbb{R}^6} |v|^2\, f\; dx\, dv}{\left(\frac{1}{8\pi}\int_{\mathbb{R}^6} |\nabla\phi|^2\, dx\right)^2} \equiv \frac{E_{KIN}(f)}{(E_{POT}(f))^2}$$

and consider the minimization problem

$$J_M = \inf\{J(f)\ :\ f \in \Gamma_M\} \,.$$

The strict positive character of J_M is a trivial consequence of the Inequality (2.3). A simple scaling argument proves that the constraint $\|f\|_{\mathrm{L}^\infty(\mathbb{R}^6)} \le 1$ has to be saturated.

Lemma 2.2. The minimization problems $E(f) = E_M$ and $J(f) = J_M$ over the set Γ_M are equivalent in the following sense.

(i) Their respective minima satisfy

$$4\, J_M\, E_M = -1 \,.$$

(ii) If $f_M \in \Gamma_M$ is a minimizer of the functional E, then it is also a minimizer of the functional J. On the other hand, if $J(g_M) = J_M$ for some $g_M \in \Gamma_M$, then $E(g_M^\sigma) = E_M$ where $g_M^\sigma(x,v) := g_M(\sigma x, v/\sigma)$ and $\sigma = \frac{E_{POT}(g_M)}{2E_{KIN}(g_M)}$.

Proof. The set Γ_M is stable under the action of the scaling $f \mapsto f^\sigma(x,v) = f(\sigma x, v/\sigma)$ for any $\sigma > 0$. Since for every $f \in \Gamma_M$,

$$E(f^\sigma) = \sigma^2 E_{KIN}(f) - \sigma\, E_{POT}(f)\ , \tag{2.4}$$

we can select the value of the parameter σ for which the total energy reaches the minimum over the uniparametric family of functions $\{f^\sigma\ :\ \sigma \in \mathbb{R}^+\}$. Let

$$\sigma = \sigma_{min} = \frac{E_{POT}(f)}{2\, E_{KIN}(f)}\ .$$

In that case,

$$E(f) \geq E(f^{\sigma_{min}}) = -\frac{1}{4}\frac{(E_{POT}(f))^2}{E_{KIN}(f)} = -\frac{1}{4\, J(f)}\ . \tag{2.5}$$

Note that $E(f^{\sigma_{min}}) < 0$. Since $-\frac{1}{4J(f)} \geq -\frac{1}{4J_M}$, this proves that $E_M \geq -\frac{1}{4\, J_M}$. On the other hand, the functional J is invariant under scalings. so we may rewrite 2.5 as

$$J(f) = J(f^{\sigma_{min}}) = -\frac{1}{4E(f^{\sigma_{min}})}\ . \tag{2.6}$$

Again $-\frac{1}{4E(f^{\sigma_{min}})} \geq -\frac{1}{4E_M}$ proves the inequality: $J_M \geq -\frac{1}{4E_M}$, so that $E_M \leq -\frac{1}{4\, J_M}$ because $E_M < 0$. Assertions concerning the minimizers directly follow from 2.5 and 2.6.

□

The fact that E_M is negative, bounded from below, is a straightforward consequence of Lemma 2.1 and Lemma 2.2. We can now prove Assertions (i)-(iii) of Theorem 2.1. By definition of $E(f)$ and $J(f)$, we have

$$E := E(f) = E_{KIN} - E_{POT} \quad \text{and} \quad \frac{E_{KIN}(f)}{(E_{POT}(f))^2} = J(f) \geq -\frac{1}{4\, E_M}\ .$$

This proves Assertion (iii): $(E_{POT}(f))^2 \leq -\,4\, E_M\, E_{KIN}(f)$, and

$$-\frac{E_{POT}(f))^2}{4\, E_M} - E_{POT}(f) \leq E\ , \quad (E_{KIN} - E)^2 \leq -\,4\, E_M\, E_{KIN}\ ,$$

from which (i) and (ii) easily follow, using the positivity of $E_{POT}(f)$. Note that $K_-(E,M)$ is nonnegative, which is the case for $P_-(E,M)$ only if $E < 0$.

The rest of this section is devoted to the proof of the existence of minimizers.

Corollary 2.1. Let f_M be a minimizing function for the functional E on Γ_M. Then

$$E_{POT}(f_M) = 2\, E_{KIN}(f_M) = -2\, E_M \;. \tag{2.7}$$

Proof. (2.7) is a trivial consequence of the scaling argument 2.4: derive the identity with respect to σ at $\sigma = 1$. Note that

$$E_M = -E_{KIN}(f_M) = -\frac{1}{2}\, E_{POT}(f_M) < 0 \;.$$

□

Remark. *Property 2.7 is shared by any stationary solution f of the VP system:*

$$E_{POT}(f) = 2\, E_{KIN}(f) = -2\, E(f) \;.$$

For a proof, see identity 2.23.

Spherical symmetry and regularity of the potential

We first prove by symmetric nonincreasing rearrangements (see Appendix A) that when minimizing the functional E on Γ_M, we can consider minimizing sequences having radial nonincreasing mass densities, which provides further regularity properties of the associated potentials.

Lemma 2.3. Let $M > 0$. There exists a minimizing sequence $(f_n)_{n\in\mathbb{N}} \in \Gamma_M^{\mathbb{N}}$ of the functional E such that for any $n \in \mathbb{N}$ the mass density $\rho_n(x) = \int_{\mathbb{R}^3} f_n(x,v)\,dv$ is a radial nonincreasing function.

Proof. Let $(f_n)_{n\in\mathbb{N}} \in \Gamma_M^{\mathbb{N}}$ be an arbitrary minimizing sequence of the functional E. The symmetric nonincreasing rearrangement $f_n^{*x} \in \Gamma_M$ (see Appendix A) of f_n (with respect to the x variable only) also belongs to Γ_M for any $n \in \mathbb{N}$, because of (2.27)-(2.28). Using Riesz' theorem (see Theorem 2.4 in Appendix A for a statement) we get

$$\begin{aligned}
\int_{\mathbb{R}^3} |\nabla\phi|^2\,dx &= 4\,\pi \int_{(\mathbb{R}^3)^4} \frac{f(x,v)\,f(x',v')}{|x-x'|}\,dx\,dx'\,dv\,dv' \\
&\leq 4\,\pi \int_{(\mathbb{R}^3)^4} \frac{f^{*x}(x,v)\,f^{*x}(x',v')}{|x-x'|}\,dx\,dx'\,dv\,dv' \\
&\leq \int_{\mathbb{R}^3} |\nabla\phi_*|^2\,dx
\end{aligned}$$

where $\phi = |\cdot|^{-1} * \int_{\mathbb{R}^3} f(\cdot,v)\,dv$ and $\phi_* = |\cdot|^{-1} * \int_{\mathbb{R}^3} f^{*x}(\cdot,v)\,dv$. This and (2.29) prove that f_n^{*x} is a minimizing sequence. Properties (2.30)-(2.31) provide the spherically symmetric and nonincreasing character of the sequence of mass densities associated to f_n^{*x}. □

The spherically symmetric character of the mass density implies regularity properties of the potential function ϕ (see Lemma 2 of [48] for a proof) which go beyond the estimate of Lemma 2.1.

Lemma 2.4. Let $\rho \in \mathrm{L}^1(\mathbb{R}^3) \cap \mathrm{L}^{5/3}(\mathbb{R}^3)$ be a nonnegative and spherically symmetric function with $\|\rho\|_{\mathrm{L}^1(\mathbb{R}^3)} = M > 0$ and define $\phi = -|\cdot|^{-1} * \rho$. Then ϕ belongs to $W^{2,5/3}_{\mathrm{loc}}(\mathbb{R}^3)$ and there exists a $\eta > 0$ such that for any $R > 0$ we have

$$\int_{|x|<R} |\nabla\phi|^{2+\eta}\, dx \leq C(M,R) \left(\int_{|x|<R} \rho^{5/3}\, dx + 1 \right)$$

for some $C = C(M,R) > 0$ which does not depend on ρ.

A priori estimates, scalings and tools of the concentration-compactness method

Several of the results of this paragraph are basic tools of the concentration-compactness method (see [77, 90] for more details in this direction). We start with a very elementary computation which will be usefull later.

Lemma 2.5. Let ρ be a radial L^1 nonnegative nontrivial function on $\mathbb{R}^3$ and consider the corresponding potential ϕ given by the Poisson equation

$$\Delta\phi = 4\,\pi\,\rho\,, \qquad \lim_{|x|\to+\infty} \phi(x) = 0\ .$$

Then ϕ is radial, nondecreasing and strictly increasing in the interior of the support of ρ. With the notation $\int_{\mathbb{R}^3} \rho(x)\, dx =: M > 0$ and the standard abuse of notations: $r = |x|$, $\rho(x) = \rho(r)$, $\phi(x) = \phi(r)$ for any $x \in \mathbb{R}^3$ and $M = \int_{\mathbb{R}^3} \rho(x)\, dx = 4\pi \int_0^\infty r^2 \rho(r)$, the two following estimates hold:

(i) For any $r > 0$,

$$\phi'(r) \leq \frac{M}{r^2} \quad \text{and} \quad -\frac{M}{r} \leq \phi(r) \leq 0\ .$$

(ii) For any $R > 0$,

$$\int_{|x|\geq R} |\nabla\phi(x)|^2\, dx \leq 4\,\pi\,\frac{M^2}{R}\ .$$

Proof. The Poisson equation written in radial coordinates is

$$\frac{1}{r^2}\left(r^2\phi'\right)' = 4\,\pi\,\rho$$

which gives after one integration

$$\phi'(r) = \frac{4\,\pi}{r^2}\int_0^r s^2\,\rho(s)\,ds \le \frac{M}{r^2}\ .$$

An integration from $R > 0$ to $+\infty$ gives (i) while (ii) is obtained by writing

$$\int_{|x|\ge R} |\nabla\phi(x)|^2\,dx \le 4\,\pi\int_R^{+\infty} r^2\,\left(\phi'(r)\right)^2\,dr \le 4\,\pi\int_R^{+\infty}\frac{M^2}{r^2}\,dr\ .$$

The bound on ϕ readily follows from the expression of ϕ'. □

Our next result is based on a scaling argument.

Lemma 2.6. Let M be a positive real number. Then, the identity

$$E_M = M^{7/3}\,E_1 \tag{2.8}$$

holds.

Proof. Let $f \in \Gamma_1$. We scale this function as $\bar f(x,v) = f(M^{1/3}x, M^{-2/3}v)$, obtaining

$$\|\bar f\|_{L^1(\mathbb{R}^6)} = M\ ,\quad \|\bar f\|_{L^\infty(\mathbb{R}^6)} \le 1\ ,\quad E(\bar f) = M^{7/3}\,E(f)\ .$$

This scaling trivially implies (2.8). □

The following result is a splitting estimate (see [48] for similar estimates).

Lemma 2.7. Let $f \in \Gamma_M$ be a function such that the mass density $\rho(x) = \int_{\mathbb{R}^3} f(x,v)\,dv$ is spherically symmetric. Given $R > 0$, we can write

$$M - \lambda = \int_{|x|<R}\int_{\mathbb{R}^3} f(x,v)\,dv\,dx\ ,$$

for some $\lambda \in [0, M]$. Then

$$E(f) - E_M \ge -\left(\frac{7}{3}\,\frac{E_M}{M^2} + \frac{1}{4\,\pi\,R}\right)\,(M-\lambda)\,\lambda\ . \tag{2.9}$$

Proof. Let χ_{B_R} be the characteristic function of $B_R := \{x \in \mathbb{R}^3\ :\ |x| < R\}$. We split the potential function in two parts $\phi = \phi_1 + \phi_2$, where ϕ_1 and ϕ_2 are defined by

$$\Delta\phi_1(x) = \int_{\mathbb{R}^3}\chi_{B_R}(x)\,f(x,v)\,dv\ ,\qquad \Delta\phi_2(x) = \int_{\mathbb{R}^3}(1-\chi_{B_R}(x))\,f(x,v)\,dv\ .$$

In the same line we write $E(f)$ as

$$\begin{aligned} E(f) &= E_{KIN}(\chi_{B_R} f) + E_{KIN}((1-\chi_{B_R})f) \\ &\quad -\frac{1}{8\pi}\int_{\mathbb{R}^3} |\nabla\phi_1|^2\, dx - \frac{1}{8\pi}\int_{\mathbb{R}^3} |\nabla\phi_2|^2\, dx - \frac{1}{4\pi}\int_{\mathbb{R}^3} \nabla\phi_1\cdot\nabla\phi_2\, dx \\ &= E(\chi_{B_R} f) + E((1-\chi_{B_R})f) - \frac{1}{4\pi}\int_{\mathbb{R}^3} \nabla\phi_1\cdot\nabla\phi_2\, dx \\ &\geq E_{M-\lambda} + E_\lambda + \frac{1}{4\pi}\int_{\mathbb{R}^3} \phi_2\,\Delta\phi_1\, dx\ . \end{aligned}$$

Using (2.8) we find

$$E(f) - E_M \geq \left[\left(1-\frac{\lambda}{M}\right)^{\frac{7}{3}} + \left(\frac{\lambda}{M}\right)^{\frac{7}{3}} - 1\right] E_M + \frac{1}{4\pi}\int_{\mathbb{R}^3} \phi_2\,\Delta\phi_1\, dx\ . \quad (2.10)$$

In order to bound the first term on the right hand side of (2.10) we take advantage of the negative value of E_M and use the identity

$$(1-x)^{7/3} + x^{7/3} - 1 \leq -\frac{7}{3}\, x\,(1-x)\ ,$$

which is valid for all x in $[0,1]$. The second term of the right hand side of (2.10) is nonpositive and bounded by

$$\left|\frac{1}{4\pi}\int_{\mathbb{R}^3} \phi_2\,\Delta\phi_1\, dx\right| \leq \|\phi_2\|_{\mathrm{L}^\infty(\mathbb{R}^3)} \int_{\mathbb{R}^6} \chi_{B_R}\, f\, dx\, dv = \|\phi_2\|_{\mathrm{L}^\infty(\mathbb{R}^3)}\,(M-\lambda)\ ,$$

where $\|\phi_2\|_{\mathrm{L}^\infty(\mathbb{R}^3)}$ can be calculated by using the spherically symmetric character of the mass density $\rho = \int_{\mathbb{R}^3} f\, dv$:

$$\phi_2'(r) = \frac{4\pi}{r^2}\int_0^r s^2\,\rho(s)\,(1-\chi_{B_R}(s))\, ds \geq 0\ ,$$

so that $\phi_2'(r) \equiv 0$ on $(0,R)$, which implies that

$$\|\phi_2\|_{\mathrm{L}^\infty(\mathbb{R}^3)} = |\phi_2(0)| = |\phi_2(R)| \leq \frac{\lambda}{4\,\pi\, R}$$

according to Lemma 2.5. Combining the above estimates we obtain 2.9. □
In the next lemma we prove that no vanishing of mass occurs.

Lemma 2.8. Let $R_0 > \frac{3\,M^2}{28\,\pi\,|E_M|}$ and consider a minimizing sequence $(f_n)_{n\in\mathbb{N}} \in \Gamma_M^{\mathbb{N}}$ for the functional E. Assume moreover that $(f_n)_{n\in\mathbb{N}}$ is given as in Lemma 2.3. Then

$$\limsup_{n\to\infty}\int_{|x|\geq R_0}\int_{\mathbb{R}^3} f_n\, dv\, dx = 0\ .$$

Proof. If the statement was not true, there would exist a $\lambda \in (0, M]$ and a subsequence (we keep the same notation for the sake of simplicity) such that

$$\lim_{n\to\infty} \int_{|x|\geq R_0} \int_{\mathbb{R}^3} f_n \, dv \, dx = \lambda \, .$$

In this case, for every f_n, there would exist $R(n) > R_0$ such that

$$\frac{\lambda}{2} = \int_{|x|\geq R(n)} \int_{\mathbb{R}^3} f_n \, dv \, dx \, .$$

Apply now Lemma 2.7 to each f_n with $R = R(n)$:

$$\begin{aligned} E(f_n) - E_M &\geq -\left(\frac{7\,E_M}{3\,M^2} + \frac{1}{4\pi R(n)}\right)\left(M - \frac{\lambda}{2}\right)\frac{\lambda}{2} \\ &\geq -\left(\frac{7\,E_M}{3\,M^2} + \frac{1}{4\pi R_0}\right)\left(M - \frac{\lambda}{2}\right)\frac{\lambda}{2} > 0 \, . \end{aligned}$$

This would clearly be in contradiction with the assumption that the sequence is a minimizing sequence for the functional E. □

Convergence of a minimizing sequence

Proposition 2.1. Let $(f_n)_{n\in\mathbb{N}} \in \Gamma_M^{\mathbb{N}}$ be a minimizing sequence for the functional E, with radial nonincreasing mass densities. Up to a subsequence, the sequence converges to a minimizer $f_M \in \Gamma_M$ such that $E_M = E(f_M)$, $\text{supp}\,(f_M) \subset B_{R_0} \times \mathbb{R}^3$ where $R_0 = \frac{3\,M^2}{28\,\pi\,|E_M|}$.

Proof. At each step of the proof, we may extract subsequences that we still index by n, for simplicity. From Lemma 2.1, it is clear that both $E_{KIN}(f_n)$ and $E_{POT}(f_n)$ are bounded sequences. Thanks to Lemma 2.8, $\lim_{n\to\infty} \int_{B_{R_0}} \int_{\mathbb{R}^3} f_n \, dv \, dx = M$. The sequence $(f_n)_{n\in\mathbb{N}}$ verifies the hypothesis of the Dunford-Pettis theorem:

(i) [boundedness] $(f_n)_{n\in\mathbb{N}}$ is bounded in $\mathrm{L}^1(\mathbb{R}^6)$,

(ii) [no concentration] for any measurable set A,

$$\int_A f_n \, dx \, dv \;\leq\; \|f_n\|_{\mathrm{L}^\infty(\mathbb{R}^6)} \, |A| \;\leq\; |A| \, ,$$

(iii) [no vanishing] for any K_1, K_2, either $K_1 < R_0$ and

$$\int_{|x|>K_1} \int_{|v|>K_2} f_n \, dx \, dv \leq \int_{\mathbb{R}^3} \int_{|v|>K_2} f_n \, dx \, dv \leq \frac{1}{K_2^2} \, E_{KIN}(f_n) \, ,$$

or $K_1 \geq R_0$ and

$$\lim_{n\to\infty} \int_{|x|>K_1} \int_{|v|>K_2} f_n \; dx\, dv \leq \lim_{n\to\infty} \int_{|x|\geq R_0} \int_{\mathbb{R}^3} f_n \; dx\, dv = 0 \; .$$

As a consequence, there exists a function $f \in \mathrm{L}^1(\mathbb{R}^6)$ and a subsequence which weakly converges in $\mathrm{L}^1(\mathbb{R}^6)$ to f. As a consequence, $\|f\|_{\mathrm{L}^1(\mathbb{R}^6)} = M$ (see [77, 48] for more details). Moreover, f is nonnegative a.e. as a weak limit of nonnegative functions. The sequence $(f_n)_{n\in\mathbb{N}}$ is bounded in $\mathrm{L}^\infty(\mathbb{R}^3)$ and thus also converges to f w.r.t. the *-weak L^∞ topology, up to the extraction of a further subsequence, so that $\|f\|_{\mathrm{L}^\infty(\mathbb{R}^3)} \leq 1$. Thus f belongs to Γ_M. The weak convergence in $\mathrm{L}^1(\mathbb{R}^6)$ implies

$$\int_{\mathbb{R}^6} |v|^2 f \; dx\, dv \leq \liminf_{n\to\infty} \int_{\mathbb{R}^6} |v|^2 f_n \; dx\, dv \; .$$

Let ϕ_n and ϕ be the solutions to the Poisson equation with mass densities associated with f_n and f respectively. The proof that $\lim_{n\to\infty} \|\nabla\phi_n - \nabla\phi\|_{\mathrm{L}^2(\mathbb{R}^3)} = 0$ up to the extraction of a subsequence follows from the splitting

$$\int_{\mathbb{R}^3} |\nabla\phi_n - \nabla\phi|^2 \; dx \leq \int_{B_R} |\nabla\phi_n - \nabla\phi|^2 \; dx + 4\,\pi\,\frac{M^2}{R}\,, \tag{2.11}$$

which is itself a consequence of Lemma 2.5. Here $B_R := \{x \in \mathbb{R}^3 \;:\; |x| < R\}$. From Lemma 2.4 and the Sobolev compact inclusion $W^{2,5/3}(B_R) \hookrightarrow W^{1,\frac{15}{4}}(B_R)$, we obtain the convergence by choosing R large enough in (2.11). This proves that $E(f) = E_M$. □

Solutions of the VP system with minimal energy and nonlinear stability

We characterize the functions with minimal energy and prove that they are solutions of the VP system. For that purpose, we characterize the mass density of a minimizer, as was proposed in [90].

Theorem 2.2. Let f_M be a minimizing function for the functional E on Γ_M, with radial mass density. Then f_M is defined almost everywhere by

$$f_M(x,v) = \begin{cases} 1 & \text{if} \quad \frac{1}{2}\,|v|^2 + \phi_{f_M}(x) < \frac{7}{3}\frac{E(f_M)}{M}\;, \\ 0 & \text{otherwise}\;, \end{cases}$$

where ϕ_{f_M} is the unique radial solution on $\mathbb{R}^3$ of

$$\Delta\phi_{f_M} = \frac{1}{3}\,(4\pi)^2\left[2\left(\frac{7}{3}\frac{E_M}{M} - \phi_{f_M}\right)_+\right]^{3/2} .$$

It is the unique minimizer with radial mass density and it is also a steady-state solution to the VP system. Moreover, if f is another minimizing function, then

$$f(x,v) = f_M(x-\bar{x},v) \quad \forall\ (x,v)\in\mathbb{R}^6 ,$$

where $\bar{x} = \frac{1}{M}\int_{\mathbb{R}^6} x\, f(x,v)\,dx\,dv$.

Here w_+ denotes the positive part of w. The existence of a minimum implies by translation in space the existence of other ones. The fact f_M is a solution to the VP system is a straightforward consequence of the fact that f_M is a function of the *microscopic energy:* $\frac{1}{2}\,|v|^2+\phi_{f_M}(x)$, namely

$$f_M(x,v) = \chi_{\frac{1}{2}\,|v|^2+\phi_{f_M}(x)<\frac{7}{3}\frac{E(f_M)}{M}}(x,v) .$$

In this section, we first prove Theorem 2.2 and then state a nonlinear stability result for the solutions of the VP system.

Explicit form of the minimizers

For convenience, we split the proof of Theorem 2.2 into three intermediate results.

Lemma 2.9. Let f_M be a minimizing function for the functional E on Γ_M. Then

$$f_M(x,v) = \begin{cases} 1 & \text{for } (x,v) \text{ such that } |v| \le \left(\frac{3}{4\pi}\,\rho_M(x)\right)^{1/3} \text{ a.e. ,} \\ 0 & \text{otherwise .} \end{cases} \tag{2.12}$$

Note that we do not assume that f_M has a radial mass density.

Proof. We are going to split the proof of (2.12) into several steeps. First, we observe that

$$\|f_M\|_{L^\infty(\mathbb{R}^6)} = 1 .$$

If this is not the case, consider the scaling $\bar{f}(x,v) = \kappa f(\kappa^{2/3}x,\kappa^{-1/3}v)$, which gives

$$\|\bar{f}\|_{L^1(\mathbb{R}^6)} = \|f\|_{L^1(\mathbb{R}^6)} , \quad \|\bar{f}\|_{L^\infty(\mathbb{R}^6)} = \kappa\,\|f\|_{L^\infty(\mathbb{R}^6)} , \quad E(\bar{f}) = \kappa^{2/3}\,E(f) .$$

By applying this scaling to $f = f_M$ with $\kappa = \|f_M\|^{-1}_{\mathrm{L}^\infty(\mathbb{R}^6)} > 1$, we would get $E(\bar f) = \kappa^{\frac{2}{3}} E_M < E_M$ (remind that $E_M < 0$), a contradiction.

Using the Euler-Lagrange multipliers method, we are now going to prove that

$$f_M \equiv 1 \text{ a.e. on } \mathrm{supp}\,(f_M)\ .$$

Let $\epsilon \in (0,1)$ be a fixed real number. Let $g(x,v) \in \mathrm{L}^1(\mathbb{R}^6) \cap \mathrm{L}^\infty(\mathbb{R}^6)$ be a test function such that $g \geq 0$ a.e. in $\mathbb{R}^6 \setminus \mathrm{supp}\,(f_M)$, with compact support contained inside

$$(\mathrm{supp}\,(f_M) \setminus S_\epsilon)^c \equiv \Big(\mathbb{R}^6 \setminus \mathrm{supp}\,(f_M)\Big) \cup S_\epsilon\ ,$$

where

$$S_\epsilon = \{(x,v) \in \mathbb{R}^6\ :\ \epsilon \leq f_M(x,v) \leq 1-\epsilon\}\ .$$

With $T := M\,\epsilon\,\Big(M\|g\|_{\mathrm{L}^\infty(\mathbb{R}^6)} + \|g\|_{\mathrm{L}^1(\mathbb{R}^6)}\Big)^{-1}$, we have that

$$g(t) = M\,\frac{tg + f_M}{\|tg+f_M\|_{\mathrm{L}^1(\mathbb{R}^6)}} \in \Gamma_M \quad \forall\, t \in [0,T]\ . \tag{2.13}$$

The function g depends on t, x and v. However, to emphasize the dependence in t, we will write it $g(t)$. Identity 2.13 follows from a detailed analysis of the function $tg + f_M$:

$$\begin{array}{llll} 0 \leq -T\|g\|_{\mathrm{L}^\infty(\mathbb{R}^6)} + \epsilon \leq tg + f_M & \text{in } S_\epsilon\,, \\ 0 \leq \qquad f_M \qquad = tg + f_M & \text{in } \mathrm{supp}\,(f_M) \setminus S_\epsilon\,, \\ 0 \leq \qquad tg \qquad = tg + f_M & \text{in } \mathbb{R}^6 \setminus \mathrm{supp}\,(f_M)\,, \end{array}$$

gives the positivity of $g(t)$ and implies

$$M(1-\epsilon) \leq \|tg + f_M\|_{\mathrm{L}^1(\mathbb{R}^6)} = t\int_{\mathbb{R}^6} g\ dx\,dv + M \leq M(1+\epsilon)\ .$$

It is clear that $\|g(t)\|_{\mathrm{L}^1(\mathbb{R}^6)} = M$ and the estimate

$$\|g(t)\|_{\mathrm{L}^\infty(S_\epsilon)} \leq M\frac{T\|g\|_{L^\infty(\mathbb{R}^6)} + 1 - \epsilon}{M - T\|g\|_{L^1(\mathbb{R}^6)}} = 1$$

ends the proof of 2.13.

To prove that S_ϵ is a set of measure 0 for any $\epsilon > 0$, we compute $E(g(t)) - E_M = E(g(t)) - E(f_M)$ and then derive it with respect to t at $t = 0_+$. Deriving $g(t)$ with respect to t, we get

$$\begin{aligned} \frac{g'(t)}{M} &= \frac{g}{\|tg+f_M\|_{\mathrm{L}^1(\mathbb{R}^6)}} - \frac{(tg+f_M)\int_{\mathbb{R}^6} g\ dx\,dv}{\|tg+f_M\|^2_{\mathrm{L}^1(\mathbb{R}^6)}}\ , \\ \frac{g''(t)}{M} &= -2\,\frac{g\int_{\mathbb{R}^6} g\ dx\,dv}{\|tg+f_M\|^2_{\mathrm{L}^1(\mathbb{R}^6)}} + 2\,\frac{(tg+f_M)\left[\int_{\mathbb{R}^6} g\ dx\,dv\right]^2}{\|tg+f_M\|^3_{\mathrm{L}^1(\mathbb{R}^6)}}\ . \end{aligned}$$

By a Taylor expansion at $t=0_+$, there exists a $\theta\in(0,t)$ such that

$$g(t)-f_M=t\,g'(0)+\frac{t^2}{2}\,g''(\theta)=t\left(g-\frac{1}{M}\left[\int_{\mathbb{R}^6}g\;dx\,dv\right]f_M\right)+\frac{t^2}{2}\,g''(\theta)\;,$$

where

$$|g''(\theta)|\le C\,(|f_M|+|g|)$$

for some constant $C>0$ which depends only on f_M and g. Using the decomposition $E(g(t))-E_M=\frac{1}{2}\,\mathcal{K}(t)-\frac{1}{8\pi}\,\mathcal{P}(t)$ with

$$\begin{aligned}\mathcal{K}(t)&=\int_{\mathbb{R}^6}|v|^2\Big[g(t)-f_M\Big]\,dx\,dv\\ \mathcal{P}(t)&=8\pi\int_{\mathbb{R}^6}\phi_{f_M}\Big[g(t)-f_M\Big]\,dx\,dv-\int_{\mathbb{R}^3}\Big[\,\Big|\nabla\phi_{g(t)}-\nabla\phi_{f_M}\Big|^2\,\Big]\,dx\end{aligned}$$

we have therefore the following estimates:

$$\left|\int_{\mathbb{R}^6}|v|^2\Big[g(t)-f_M-t\,g'(0)\Big]dxdv\right|\le C\,t^2\int_{\mathbb{R}^6}|v|^2\Big[|g|+f_M\Big]dxdv=O(t^2)\;,$$

$$\left|\int_{\mathbb{R}^6}\phi_{f_M}\Big[g(t)-f_M-t\,g'(0)\Big]dxdv\right|\le C\,t^2\int_{\mathbb{R}^6}\phi_{f_M}\Big[|g|+f_M\Big]dxdv=O(t^2)\;,$$

$$\int_{\mathbb{R}^3}\Big|\nabla\phi_{g(t)}-\nabla\phi_{f_M}\Big|^2dx=\int_{\mathbb{R}^3}|\nabla\phi_{g(t)-f_M}|^2dx=t^2\|\nabla\phi_{g'(0)}\|^2_{\mathrm{L}^2(\mathbb{R}^3)}+O(t^2)=O(t^2)\;.$$

From (2.7) and the above estimates we deduce

$$\begin{aligned}E(g(t))-E_M&=t\int_{\mathbb{R}^6}\left(\frac{1}{2}\,|v|^2+\phi_{f_M}\right)g'(0)\;dx\,dv+O(t^2)\\ &=t\int_{\mathbb{R}^6}\left(\frac{1}{2}\,|v|^2+\phi_{f_M}\right)\left(g-\left[\frac{\int_{\mathbb{R}^6}g\;dx\,dv}{M}\right]f_M\right)\,dx\,dv+O(t^2)\\ &=t\int_{\mathbb{R}^6}\left(\frac{1}{2}\,|v|^2+\phi_{f_M}-\frac{3E_M}{M}\right)g\;dx\,dv+O(t^2)\,.\end{aligned}$$

Since f_M minimizes $E(\cdot)-E_M$ on Γ_M, we have that $E(g(t))-E_M\ge 0$ for any $t\in[0,T]$ and consequently

$$\int_{\mathbb{R}^6}\left(\frac{1}{2}\,|v|^2+\phi_{f_M}-\frac{3E_M}{M}\right)g\;dx\,dv\ge 0$$

for every g and ϵ. There are two relevant consequences of this inequality:

(i) From the nonnegative character of g on $\mathbb{R}^6\setminus\mathrm{supp}\,(f_M)$ we have

$$\frac{1}{2}\,|v|^2+\phi_{f_M}(x)\ge\frac{3E_M}{M}\quad\forall\;(x,v)\in\mathbb{R}^6\setminus\mathrm{supp}\,(f_M)\;,$$

or equivalently

$$\left\{(x,v)\in\mathbb{R}^6\;:\;\frac{1}{2}\,|v|^2+\phi_{f_M}(x)\le\frac{3E_M}{M}\right\}\subset\mathrm{supp}\,(f_M)\;.$$

(ii) On the other hand, g has no determined sign on S_ϵ. This implies that

$$\frac{1}{2}\,|v|^2 + \phi_{f_M}(x) = \frac{3E_M}{M} \quad \forall\,(x,v) \in S_\epsilon \cap \mathrm{supp}\,(f_M)\ .$$

The Lebesgue measure of the set defined by the above identity is zero. The set S_ϵ also has zero Lebesgue measure for any $\epsilon \in (0,1)$.

We conclude that $f_M \equiv 1$ on $\mathrm{supp}\,(f_M)$.

It remains to check that (2.12) holds. Since f_M minimizes the total energy functional, it also minimizes $\{E(f)\ :\ f \in \gamma_M\}$ where

$$\gamma_M = \left\{ f \in \Gamma_M\ :\ f \equiv 1 \text{ a.e. on } \mathrm{supp}(f)\,,\ \int_{\mathbb{R}^3} f(x,v)\,dv = \rho_M(x) \quad \forall\, x \in \mathbb{R}^3 \right\}\ .$$

Since all $f \in \gamma_M$ have the same potential energy, $E_{POT}(f) = E_{POT}(f_M)$. The problem is therefore reduced to the minimization of $\{E_{KIN}(f)\ :\ f \in \gamma_M\}$. Using radial nonincreasing rearrangements with respect to v, for fixed $x \in \mathbb{R}^3$ (use 2.32 but exchange the roles of x and v), we get

$$\int_{\mathbb{R}^3} |v|^2\, f^{*_v}\ dv \le \int_{\mathbb{R}^3} |v|^2\, f\ dv$$

with a strict inequality unless $f \equiv f^{*_v}$ a.e. Thus

$$f_M \equiv \chi_{|v| \le \left(\frac{3}{4\pi}\rho_M(x)\right)^{1/3}} \quad \text{in } \mathbb{R}^3 \times \mathbb{R}^3 \text{ a.e.}$$

since, at least in the distributions sense,

$$\rho_M(x) = \int_{\mathbb{R}^3} f_M(x,v)\ dv = \int_{\mathbb{R}^3} f_M^{*_v}(x,v)\ dv = \frac{4\pi}{3}\,|\,\mathrm{supp}\,(f_M)(x,\cdot)\,|^3\ .$$

This conclude the proof of (2.12). □

We have now to use the fact that f_M is a minimizer to understand the properties of ρ_M.

Lemma 2.10. Let f_M be a minimizing function for the functional E on Γ_M with radial mass density. Then $\rho_M = \int_{\mathbb{R}^3} f_M(\cdot,v)\,dv$ and $\phi_{f_M} = |\cdot|^{-1} * \rho_M$ are related by

$$\rho_M(x) = \begin{cases} \frac{4\pi}{3}\left[2\left(\frac{7}{3}\,\frac{E_M}{M} - \phi_{f_M}(x)\right)\right]^{3/2} & \text{if} \quad \phi_{f_M}(x) \le \frac{7}{3}\frac{E_M}{M}\ , \\ 0 & \text{otherwise}\ . \end{cases} \tag{2.14}$$

Proof. Let $\rho(x) \in \mathrm{L}^1(\mathbb{R}^3) \cap \mathrm{L}^{5/3}(\mathbb{R}^3)$ be a nonnegative function such that $\|\rho\|_{\mathrm{L}^1(\mathbb{R}^3)} = M$. We define

$$f_\rho(x,v) = \begin{cases} 1 & \text{for } (x,v) \in \mathbb{R}^6 \text{ such that } |v| \le \left(\frac{3}{4\pi}\,\rho(x)\right)^{1/3} \text{ a.e.}\,, \\ \\ 0 & \text{in other case}\,. \end{cases}$$

We observe that $f_\rho \in \Gamma_M$. Since f_M minimizes E on Γ_M and verifies (2.3) and (2.12), it also minimizes the problem

$$\min\{E(f_\rho)\ :\ \rho \in \tilde{\Gamma}_M\}\,, \tag{2.15}$$

where

$$\tilde{\Gamma}_M := \{\rho \in \mathrm{L}^1(\mathbb{R}^3) \cap \mathrm{L}^{5/3}(\mathbb{R}^3)\ :\ \rho(x) \ge 0,\ \|\rho\|_{\mathrm{L}^1(\mathbb{R}^3)} = M\}\,.$$

Easy computations provide

$$\begin{aligned} E_{POT}(f_\rho) &= \frac{1}{2}\int_{\mathbb{R}^6} \frac{\rho(y)\,\rho(x)}{|x-y|}\,dx\,dy\,, \\ E_{KIN}(f_\rho) &= \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} |v|^2 f_\rho(x,v)\,dv\,dx = \frac{3^{5/3}}{10\,(4\pi)^{2/3}}\int_{\mathbb{R}^3}\Big[\rho(x)\Big]^{5/3} dx\,, \end{aligned}$$

which implies that (2.15) can be rewritten as

$$\min\Big\{F(\rho)\ :\ \rho(x) \in \tilde{\Gamma}_M\Big\} \tag{2.16}$$

where

$$F(\rho) := \frac{3^{5/3}}{10\,(4\pi)^{2/3}}\int_{\mathbb{R}^3}\Big[\rho(x)\Big]^{5/3} dx - \frac{1}{2}\int_{\mathbb{R}^6}\frac{\rho(y)\,\rho(x)}{|x-y|}\,dx\,dy\,.$$

The density ρ_M is a minimizer of 2.16 and therefore obeys to the corresponding Euler-Lagrange equations:

$$\frac{1}{2}\left[\frac{3}{4\pi}\,\rho_M(x)\right]^{2/3} - \int_{\mathbb{R}3}\frac{\rho_M(y)}{|x-y|}\,dy\ -\ \chi = \mu \tag{2.17}$$

where μ is a real-valued Lagrange multiplier associated to the constraint $\|\rho\|_{\mathrm{L}^1(\mathbb{R}^3)} = M$, and

$$\begin{cases} \chi = 0 & \text{if } \rho_M(x) > 0\,, \\ \chi \ge 0 & \text{if } \rho_M(x) = 0\,. \end{cases}$$

Multiplying 2.17 by ρ_M, integrating and using (2.7), we can obtain the value of μ:

$$\begin{aligned}\mu\, M &= \frac{1}{2}\left(\frac{3}{4\pi}\right)^{2/3}\int_{\mathbb{R}^3}\Big[\rho_M(x)\Big]^{5/3}\,dx - \int_{\mathbb{R}6}\frac{\rho_M(y)\,\rho_M(x)}{|x-y|}\,dx\,dy\ ,\\ &= \frac{5}{3}\,E_{KIN}(f_M) - 2\,E_{POT}(f_M) = \frac{7}{3}\,E_M\ ,\end{aligned}$$

which implies that

$$\mu = \frac{7}{3}\,\frac{E_M}{M}\ .$$

Equation 2.17 now reads

$$\frac{1}{2}\left[\frac{3}{4\pi}\,\rho_M(x)\right]^{2/3} + \phi_{f_M}(x) = \mu \quad \text{on supp}\,(\rho_M)$$

and the condition $\rho_M \geq 0$ is now equivalent to $\phi_{f_M} \leq \mu$. Note that according to Lemma 2.5, ϕ_{f_M} is nondecreasing: as a consequence, ρ_M is monotone decreasing (as a radial function) on its support and ϕ_{f_M} is monotone increasing. □

Lemma 2.11. With the notations of Lemma 2.10, ϕ_{f_M} is unique and continuously differentiable. Furthermore, if f is another minimum of E on Γ_M, then there exists $y \in \mathbb{R}^3$ such that

$$\int_{\mathbb{R}^3} f(x,v)\,dv = \rho_M(x-y) \quad a.e.\ x \in \mathbb{R}^3\ .$$

Proof. Let us rewrite the Poisson equation for ϕ_{f_M} using (2.14) and (2.17):

$$\Delta\phi_{f_M} = 4\pi\rho_M(x) = \begin{cases} \frac{1}{3}\,(4\pi)^2\left[2\left(\frac{7}{3}\frac{E_M}{M} - \phi_{f_M}\right)\right]^{3/2} & \text{if } \phi_{f_M}(x) \leq \frac{7}{3}\frac{E_M}{M}\ ,\\ 0 & \text{otherwise}\ .\end{cases}$$

Since ϕ_{f_M} is radially symmetric, this equation can be rewritten for

$$w(r) = \frac{7}{3}\,\frac{E_M}{M} - \phi_{f_M}(r/\sqrt{c})$$

as

$$(r^2 w'(r))' + r^2 w_+^{3/2}(r) = 0$$

with $r = |x|$ and $c = \frac{1}{3}\,32\sqrt{2}\,\pi^2$. Let $R = \frac{3M^2}{7|E_M|}\,\sqrt{c}$. According to Lemma 2.5 (see the proof: $\phi_{f_M}(r) = -\frac{M}{r}$ for any $r \geq R/\sqrt{c}$),

$$0 = w(R) = \frac{7}{3}\frac{E_M}{M} + \frac{M\sqrt{c}}{R} \quad \text{and} \quad w'(R) = -\frac{1}{\sqrt{c}}\,\phi'_{f_M}\left(\frac{R}{\sqrt{c}}\right) = -\frac{M\sqrt{c}}{R^2}\ .$$

The uniqueness and the regularity of w follow by standard ODE results.

The expression of non radial minimizers is a consequence of (2.12), the fact that the associated mass densities minimize (2.16), the conservation of the L^p-norm by radial nonincreasing rearrangements and Riesz' theorem (see Theorem 2.4 in Appendix A). □

This also concludes the proof of Theorem 2.2. Note that the minimizer with radial symmetric density was previously found as a solution of the VP system in [15], but in a different context.

Nonlinear stability for the evolution problem

Using the conservation of mass and energy, we obtain on Γ_M a nonlinear stability result of the minimal energy solution for the evolution problem. We follow the strategy of Guo in [48]. Consider for any g, $h \in \Gamma_M$ the distance d defined by

$$d(g,h) = E(g) - E(h) + \frac{1}{4\pi}\,\|\nabla\phi_g - \nabla\phi_h\|^2_{L^2(\mathbb{R}^3)}$$

where ϕ_g and ϕ_h are solutions of the Poisson equation with mass densities associated to g and h respectively.

Theorem 2.3. For every $\epsilon > 0$, there exists a $\delta > 0$ such that the following property holds. If f is a solution of the VP system with an initial condition $f_0 \in \Gamma_M$, then

$$d(f_0, f_M) \leq \delta \quad \Longrightarrow \quad d(f^*(t), f_M) \leq \epsilon \quad \forall\, t \geq 0\ .$$

Proof. The result is easily achieved by contradiction since $E(f^*(t)) - E(f_M) \leq E(f_0) - E(f_M) \searrow 0$ implies $\|\nabla\phi_{f^*(t)} - \nabla\phi_{f_M}\|_{L^2(\mathbb{R}^3)} \searrow 0$. □

Large time behaviour

The Galilean invariance of a classical solution f to the VP system with initial data $f_0(x,v)$ means that for any $u \in \mathbb{R}^3$, the solution with initial data $f_0^u(x,v) = f_0(x, v-u)$ is given by

$$f^u(t,x,v) = f(t, x-tu, v-u) \quad \forall\, (t,x,v) \in (0,+\infty) \times \mathbb{R}^3 \times \mathbb{R}^3\ .$$

Galilean invariance and asymptotic behaviour

The Galilean translations give rise to a family of solutions with same L^p-norm and potential energy for every $t \geq 0$, parametrized by $u \in \mathbb{R}^3$. Nevertheless, other quantities like the total momentum

$$\langle v\rangle(f^u) := \int_{\mathbb{R}^6} v f^u(t,x,v)\, dx\, dv = \langle v\rangle(f) + u \, \|f(t)\|_{\mathrm{L}^1(\mathbb{R}^6)}$$

and the total energy

$$E(f^u) = E(f) + u \cdot \langle v\rangle(f) + \frac{1}{2}\, |u|^2 \, \|f\|_{\mathrm{L}^1(\mathbb{R}^6)} \, . \tag{2.18}$$

are not invariant under Galilean translations. Note that

$$\langle v\rangle^2(f) \leq 2 \, \|f\|_{\mathrm{L}^1(\mathbb{R}^6)} \, E_{KIN}(f)$$

and among the family $(f^u)_{u\in\mathbb{R}^3}$, the minimum of $E_{KIN}(f^u)$ is reached by

$$E_{KIN}(f^{\bar{u}}) = \; E_{KIN}(f) - \frac{\langle v\rangle^2(f)}{2\, \|f\|_{\mathrm{L}^1(\mathbb{R}^6)}} \quad \text{for } \bar{u} = -\frac{\langle v\rangle(f)}{\|f\|_{\mathrm{L}^1(\mathbb{R}^6)}} \, .$$

Also note that $u = \bar{u}$ is the unique value of the parameter for which

$$\langle v\rangle(f^u) = 0 \, .$$

This can be summarized by the following statement.

Lemma 2.12. Let $f \in \mathrm{L}^1(\mathbb{R}^6)$ be a distribution function with finite mass and energy. If

$$E(f) < \frac{1}{2} \, \frac{\langle v\rangle^2(f)}{\|f\|_{\mathrm{L}^1(\mathbb{R}^6)}} \, , \tag{2.19}$$

then, with the above notations, the function $f^{\bar{u}}$ reaches a negative total energy value. Otherwise, every element of the parametric family of the Galilean translation has non-negative energy. In any case, the minimal energy solution of the parametric family has null momentum.

Since the quantities involved in (2.18) are all time independent, the result also holds for any t for the solution $f(t,\cdot,\cdot)$ to the VP system with initial data f_0.

Proposition 2.2. Let $f_0 \in \mathrm{L}^1 \cap \mathrm{L}^\infty(\mathbb{R}^6)$ be a nonnegative distribution function with finite mass and energy and verifying (2.19). Then there exists three constants C_1, C_2, $C_3 > 0$ such that the solution f of the VP system with initial data f_0 verifies for any $t \geq 0$

$$C_1 \leq E_{POT}(f(t,\cdot,\cdot)) \leq C_2 \, , \tag{2.20}$$

$$\|\rho_f(t,\cdot)\|_{\mathrm{L}^{5/3}(\mathbb{R}^3)} \geq C_3 \, . \tag{2.21}$$

Proof. According to Lemma 2.1, 2.3,

$$8\,\pi\, E_{POT}(f(t)) \leq \mathcal{C}\, \|f_0\|^{7/6}_{L^1(\mathbb{R}^6)}\, \|f_0\|^{1/3}_{L^\infty(\mathbb{R}^6)}\, (2E_{KIN})^{1/2}(f(t))$$

with the notation $f(t) = f(t,\cdot,\cdot))$, so that, if $E(f_0) < 0$, then

$$0 \geq E(f_0) \geq C\ E^2_{POT}(f(t)) - E_{POT}(f(t))$$

with $C = \frac{1}{2}\left(\frac{8\,\pi}{\mathcal{C}}\right)^2 \|f_0\|^{-7/3}_{L^1(\mathbb{R}^6)}\, \|f_0\|^{-2/3}_{L^\infty(\mathbb{R}^6)}$. This means that

$$E_{POT}(f(t)) \in \left[\frac{1}{2\,C}\Big(1 - \sqrt{1 + 4\,E(f_0)\,C}\Big),\ \frac{1}{2\,C}\Big(1 + \sqrt{1 + 4\,E(f_0)\,C}\Big)\right]\ .$$

Estimate (2.20) holds because there exists a function in the family of the Galilean translations associated to f_0 with negative total energy: it is therefore not restrictive to take $E(f_0) < 0$ to evaluate $E_{POT}(f(t))$. On the other hand (2.21) is a direct consequence of the Hardy-Littlewood-Sobolev inequalities (see the proof of Lemma 2.1) with $C_3 = \frac{8\pi\, C_1}{\sqrt{\Sigma}}$.

□

Variance and dispersion estimates

The solutions to the VP system in the gravitational case have a qualitative behaviour which strongly differs from the behaviour in the plasma physics case since, for instance, stationary solutions exist. The rest of this section is devoted to solutions in the gravitational case for which Condition (2.19) is violated. Our goal is to prove some dispersion estimates. For that purpose, consider the dispersion operators in space and in velocity defined by

$$<(\Delta x)^2> \quad := \int_{\mathbb{R}^6} |x|^2 f(t,x,v)\; dx\, dv - \left(\int_{\mathbb{R}^6} x f(t,x,v)\; dx\, dv\right)^2\ ,$$

and

$$<(\Delta v)^2> \quad := \int_{\mathbb{R}^6} |v|^2 f(t,x,v)\; dx\, dv - \left(\int_{\mathbb{R}^6} v f(t,x,v)\; dx\, dv\right)^2\ .$$

Up to a mass normalization, the dispersion operator in space coincides with the statistical variance of the density mass function and, consequently, it is a measure of the dispersion of such a distribution. If f is a solution of the VP system, the time evolution of both quantities are related with the total energy and the momentum by the dispersion equation. Since this property is also valid for the VP system in plasma physics we will consider both situations.

Lemma 2.13. Let f be a classical solution of VP with finite mass, energy and space dispersion. Then, it verifies

$$\frac{1}{2}\,\frac{d^2}{dt^2} <(\Delta x)^2> \;=\; E(f) + \frac{1}{2} <(\Delta v)^2> -\frac{1}{2}\,\langle v\rangle^2(f)\,. \tag{2.22}$$

Proof. A straightforward calculation using the VP system gives

$$\begin{aligned}
\frac{1}{2}\,\frac{d^2}{dt^2}\int_{\mathbb{R}^6} |x|^2 f(t,x,v)\,dx\,dv &= \frac{1}{2}\,\frac{d}{dt}\int_{\mathbb{R}^6} |x|^2\left(-v\cdot\nabla_x f + \nabla_x\phi\cdot\nabla_v f\right)\,dx\,dv \\
&= \int_{\mathbb{R}^6} (v\cdot x)\,\left(-v\cdot\nabla_x f + \nabla_x\phi\cdot\nabla_v f\right)\,dx\,dv \\
&= \int_{\mathbb{R}^6} |v|^2\,f\,\,dx\,dv - \frac{1}{4\gamma\pi}\int_{\mathbb{R}^3} (x\cdot\nabla_x\phi)\,\Delta\phi\,\,dx \\
&= \int_{\mathbb{R}^6} |v|^2\,f\,\,dx\,dv - \frac{1}{8\gamma\pi}\int_{\mathbb{R}^3} |\nabla\phi|^2\,\,dx \\
&= E(f) + \frac{1}{2}\int_{\mathbb{R}^6} |v|^2 f\,\,dx\,dv
\end{aligned} \tag{2.23}$$

which is equivalent to 2.22. □

Equation (2.22) is equivalent to a formula proposed by R. Illner and G. Rein in [58], and B. Perthame in [85]. As a straightforward consequence, the following *pseudo-conformal law* holds.

Lemma 2.14. [58, 85] Let $f_0 \in \mathrm{L}^1 \cap \mathrm{L}^\infty(\mathbb{R}^6)$ be a nonnegative initial data with finite mass, energy and space dispersion. Then a classical solution f to the VP system with initial data f_0 satisfies the following identity:

$$\frac{d}{dt}\left(\int_{\mathbb{R}^6} |x-tv|^2 f(t,x,v)\,dx\,dv - \frac{t^2}{4\pi\gamma}\int_{\mathbb{R}^3} |\nabla\phi|^2\,\,dx\right) = -\frac{t}{4\pi\gamma}\int_{\mathbb{R}^3} |\nabla\phi|^2\,\,dx\,. \tag{2.24}$$

Proof. For completion, let us give a proof of this identity.

$$\int_{\mathbb{R}^6} |x-t\,v|^2 f dx dv = \int_{\mathbb{R}^6} |x|^2 f\,\,dx dv + t^2\int_{\mathbb{R}^6} |v|^2 f dx dv - t\,\frac{d}{dt}\left(\int_{\mathbb{R}^6} |x|^2 f dx dv\right)$$

Then, the left hand side term of (2.24) can be written as

$$\begin{aligned}
&\frac{d}{dt}\left[\int_{\mathbb{R}^6}|x|^2 f dx dv - t\,\frac{d}{dt}\left(\int_{\mathbb{R}^6}|x|^2 f dx dv\right) + t^2\int_{\mathbb{R}^6}|v|^2 f dx dv - \frac{t^2}{4\pi\gamma}\int_{\mathbb{R}^3}|\nabla\phi|^2 dx\right] \\
&\qquad = \frac{d}{dt}\left[\int_{\mathbb{R}^6}|x|^2 f\,\,dx\,dv - t\,\frac{d}{dt}\left(\int_{\mathbb{R}^6}|x|^2 f\,\,dx\,dv\right) + 2t^2 E(f)\right] \\
&\qquad = -t\frac{d^2}{dt^2}\int_{\mathbb{R}^6}|x|^2 f\,\,dx\,dv + 4tE(f) = -\frac{t}{4\pi\gamma}\int_{\mathbb{R}^3}|\nabla\phi|^2\,\,dx
\end{aligned}$$

where in the last equality we have used 2.23. □

Consider now the solutions with positive energy, in the case $\gamma = +1$.

Proposition 2.3. Let f be a solution of the VP system in the gravitational case with positive energy corresponding to a nonnegative initial datum $f_0 \in \mathrm{L}^1(\mathbb{R}^6) \cap \mathrm{L}^\infty(\mathbb{R}^6)$ with finite mass, energy and space dispersion. Then, there exists positive constants C, C_1, C_2 such that for some $t_0 > 0$,

$$C_1\, t^2 \leq \int_{\mathbb{R}^6} |x|^2 f(t,x,v)\; dx\, dv \leq C_2\, t^2 \quad \forall\, t \geq t_0 > 0\;, \tag{2.25}$$

and, for any $p \in [1,\infty)$,

$$\|\rho(t,x)\|_{\mathrm{L}^p(\mathbb{R}^3)} \geq \frac{C}{t^{3(p-1)/p}}, \quad \forall\, t > t_0\;,$$

where C_i depend on $E(f)$, $\|f_0\|_{\mathrm{L}^1(\mathbb{R}^6)}$, $\|f_0\|_{\mathrm{L}^\infty(\mathbb{R}^6)}$ and C also depends on p.

Proof. We can rewrite 2.23 as

$$\frac{1}{2}\,\frac{d^2}{dt^2}\left(\int_{\mathbb{R}^6} |x|^2\, f(t,x,v)\; dx\, dv\right) = 2E(f) + E_{POT}(f)\;.$$

Combining this and the estimate of Theorem 2.1, we find

$$2E(f) \leq \frac{1}{2}\,\frac{d^2}{dt^2}\int_{\mathbb{R}^6} |x|^2\, f(t,x,v)\; dx\, dv \leq 2E(f) + C\;,$$

where C depends on $E(f)$, $\|f_0\|_{\mathrm{L}^1(\mathbb{R}^6)}$, $\|f_0\|_{\mathrm{L}^\infty(\mathbb{R}^6)}$. This estimate proves (2.25) by integrating twice in time. As for the estimate on ρ, we may write

$$\begin{aligned}
\int_{\mathbb{R}^6} f(t,x,v)\; dx\, dv \;&\leq\; \int_{\mathbb{R}^3}\int_{|x|\leq R} f(t,x,v)\; dx\, dv + \int_{\mathbb{R}^3}\int_{|x|>R} f(t,x,v)\; dx\, dv \\
&\leq \left(\frac{4\,\pi}{3}\,R^3\right)^{(p-1)/p} \|\rho(t,\cdot)\|_{\mathrm{L}^p(\mathbb{R}^3)} + \frac{1}{R^2}\int_{\mathbb{R}^6} |x|^2 f(t,x,v)\; dx\, dv \\
&\leq C\,\|\rho(t,x)\|_{\mathrm{L}^p(\mathbb{R}^3)}^{\frac{2p}{5p-3}} \left(\int_{\mathbb{R}^6} |x|^2 f(t,x,v)\; dx\, dv\right)^{\frac{3p-3}{5p-3}}
\end{aligned}$$

where in the last line we optimized on $R > 0$. The conclusion holds because of the time preservation of the $\mathrm{L}^1(\mathbb{R}^6)$-norm and Estimate (2.25). □

This argument can be used for solutions of the VP system in the plasma physical case and provides the same type of results: see [30] (with a different approach). Observe furthermore that Proposition 2.3 does not imply any dispersion property in the usual sense, as can be shown by considering a Galilean translation of a stationary solution with positive energy (*i.e.* for $|u|$ big enough). This motivates the last result of the paper.

Proposition 2.4. Let f be a solution of the VP system in the gravitational case with positive energy corresponding to a nonnegative initial datum $f_0 \in \mathrm{L}^1(\mathbb{R}^6) \cap \mathrm{L}^\infty(\mathbb{R}^6)$ with mass $\|f_0\|_{\mathrm{L}^1(\mathbb{R}^6)} = 1$, and finite energy and space dispersion. Assume that

$$E(f_0) > \frac{1}{2} \left| \int_{\mathbb{R}^6} v\, f_0(x,v)\; dx\, dv \right|^2 . \tag{2.26}$$

Then, there exists a $t_0 > 0$ and two positive constants C_1, C_2 such that

$$C_1\, t^2 \quad \le \quad <(\Delta x)^2> \quad \le \quad C_2\, t^2 \quad \forall\, t \ge t_0\,,$$

where C_i depend on $E(f)$, $\|f_0\|_{\mathrm{L}^1(\mathbb{R}^6)}$ and $\|f_0\|_{\mathrm{L}^\infty(\mathbb{R}^6)}$.

Proof. The space dispersion operator is invariant under Galilean translations

$$<(\Delta x)^2>\,(f^u) \quad = \quad <(\Delta x)^2>\,(f) \quad \forall\, u \in \mathbb{R}^3\ .$$

With the notations of the beginning of this section, consider the Galilean translation of f with minimal energy and null momentum. The dispersion equation (2.22) applied to this function $f^{\bar u}$ reads as

$$\frac{1}{2}\,\frac{d^2}{dt^2} <(\Delta x)^2> \quad = \quad E(f^{\bar u}) + \frac{1}{2} <(\Delta v)^2>\,,$$

where

$$E(f^{\bar u}) = E(f_0) - \frac{1}{2}\,|\bar u|^2\ , \quad \bar u = \langle v\rangle(f_0) = -\int_{\mathbb{R}^6} v\, f_0(x,v)\; dx\, dv\ ,$$

so that $E(f^{\bar u})$ is positive by (2.26). Since $<(\Delta v)^2>$ is positive and bounded by Lemma 2.3, we deduce

$$E(f) \quad < \quad \frac{1}{2}\,\frac{d^2}{dt^2} <(\Delta x)^2> \quad < \quad E(f) + C\ ,$$

where C is controlled in terms of $E(f)$ by Theorem 2.1. This ends the proof by integrating twice in time. □

Appendix A – Symmetric nonincreasing rearrangements

This appendix is devoted to the statement of basic properties of symmetric nonincreasing rearrangements of nonnegative functions. Such a tool has been widely used in open quantum problems (see for example [97, 70]). As a special case, we consider functions of the variables x and v, which are rearranged with respect to the x variable only (see [74]).

The symmetric rearrangement A^* of the set A in $\mathbb{R}^n$, $n \geq 1$, is the open ball in $\mathbb{R}^n$ centered at the origin whose volume is that of A. The symmetric nonincreasing rearrangement of the characteristic function χ_A of A is then defined by

$$\chi_A^* := \chi_{A^*} = \begin{cases} 1 & \text{if } \frac{1}{n}\,|S^{n-1}|\,|x|^n \leq \|\chi_A\|_{\mathrm{L}^1(\mathbb{R}^n)} \\ 0 & \text{otherwise.} \end{cases}$$

Let $h : \mathbb{R}^n \to \mathbb{C}$ be a Borel measurable function such that $\|\chi_{\{|h|>t\}}\|_{\mathrm{L}^1(\mathbb{R}^n)}$ is finite for all t. Here we denote by $\{|h| > t\}$ the set $\{x \in \mathbb{R}^n \ : \ |h(x)| > t\}$. Then

$$|h(x)| = \int_0^\infty \chi_{\{|h|>t\}}(x)\ dt$$

holds and we can define the nonincreasing rearrangement of h by

$$h^*(x) := \int_0^\infty \chi^*_{\{|h|>t\}}(x)\ dt\ .$$

The symmetric nonincreasing rearrangement of a function $(x, v) \mapsto g(x, v) \geq 0$ with respect to the x variable only (*i.e.* for fixed v) is then defined as

$$g^{*_x}(x, v) := \int_0^\infty \chi^*_{\{x\in\mathbb{R}^n\ :\ g(x,v)>t\}}\ dt\ .$$

Thanks to the Fubini's theorem we can easily adapt to the case of the symmetric nonincreasing rearrangement with fixed v the standard properties of the usual symmetric nonincreasing rearrangements:

$$\int_{\mathbb{R}^{2n}} g^{*_x}(x, v)\ dx\, dv = \int_{\mathbb{R}^{2n}} g(x, v)\ dx\, dv\ , \tag{2.27}$$

$$\|g^{*_x}\|_{\mathrm{L}^\infty(\mathbb{R}^{2n})} = \|g\|_{\mathrm{L}^\infty(\mathbb{R}^{2n})}\ , \tag{2.28}$$

$$\int_{\mathbb{R}^{2n}} |v|^2 g^{*_x}(x, v)\ dx\, dv = \int_{\mathbb{R}^{2n}} |v|^2 g(x, v)\ dx\, dv\ , \tag{2.29}$$

$$\int_{\mathbb{R}^n} g^{*_x}(x, v)\, dv = \int_{\mathbb{R}^n} g(x', v)\, dv \quad \text{if } |x| = |x'|\ , \tag{2.30}$$

$$\int_{\mathbb{R}^n} g^{*_x}(|x|, v)\, dv \geq \int_{\mathbb{R}^n} g^{*_x}(|y|, v)\, dv \quad \text{if } |x| \leq |y|\ , \tag{2.31}$$

$$\int_{\mathbb{R}^n} \psi(|x|)\, g^{*_x}(|x|, v)\, dv \leq \int_{\mathbb{R}^n} \psi(|x|)\, g(x, v)\, dv\ , \tag{2.32}$$

where in the last inequality the function $r \mapsto \psi(r)$ is nondecreasing. If moreover ψ is (strictly) increasing on $\mathbb{R}^+$, then the inequality in 2.32 is strict almost everywhere in $v \in \mathbb{R}^n$ unless $g^{*x} \equiv g$ almost everywhere on $\mathbb{R}^n \times \mathbb{R}^n$.

For completion, let us state Riesz' theorem (see [74]):

Theorem 2.4. Let f, g and h be three nonnegative functions on $\mathbb{R}^n$. Then

$$\int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f(x)\, g(x-y)\, h(y)\, dx\, dy =: I(f,g,h) \leq I(f^*, g^*, h^*)\ , \tag{2.33}$$

with the convention that $I(f^*, g^*, h^*) = \infty$ if $I(f,g,h) = \infty$. If g is radially symmetric and strictly decreasing, *i.e.* if $g(x) > g(y)$ for any x, y such that $|x| < |y|$, equality in (2.33) holds only if $f(x) = f^*(x-y)$ and $h(x) = h^*(x-y)$ for some $y \in \mathbb{R}^n$.

Appendix B: Explicit form of the optimal constant

Let w be the solution of the ODE

$$\begin{cases} (r^2 w')' + r^2 w_+^{3/2} = 0 \quad r \in [0, +\infty) \\ \\ w(0) = 1\ , \quad w'(0) = 0 \end{cases} \tag{2.34}$$

Note that $w' \leq 0$ as long as $w \geq 0$. Let u be given by $w(r) = u(-\log r)/r^4$. Then it solves the equation: $u'' + 7u' + 12u + u_+^{3/2} = 0$. A phase diagram analysis of (u, u'), shows that w has to change sign. Denote by σ its first positive zero and define the quantities

$$A := \int_0^\sigma r^2\, w^{5/2}\, dr\ ,$$

$$B := \int_0^\sigma r^2\, w^{3/2}\, dr\ .$$

The best constant $\mathcal{C}$ in Inequality 2.3 of Lemma 2.1 is defined as

$$\mathcal{C}^{-1} = \inf \left[\|f\|_{\mathrm{L}^1(\mathbb{R}^6)}^{7/6}\, \|f\|_{\mathrm{L}^\infty(\mathbb{R}^6)}^{1/3}\, \frac{\left(\int_{\mathbb{R}^6} |v|^2 f(x,v)\, dx\, dv\right)^{1/2}}{\int_{\mathbb{R}^3} |\nabla \phi|^2\, dx} \right]$$

where the infimum is taken over the set of the functions $f \in \mathrm{L}^1 \cap \mathrm{L}^\infty(\mathbb{R}^6)$ such that $f \geq 0$, $|v|^2 f \in \mathrm{L}^1(\mathbb{R}^6)$, $f \not\equiv 0$.

Proposition 2.5. With the above notations,

$$\mathcal{C} = 8\pi M^{-7/6}\,(2J_M)^{-1/2} = 8\pi\,\frac{(2\,|E_M|)^{1/2}}{M^{7/6}}$$

is independent of $M > 0$ and takes the value:

$$\mathcal{C} = 32\,\pi^2\sqrt{\frac{2^{5/2}\,a^{7/4}\,A}{5\,c^{3/2}}}\ ,$$

where $a = \frac{c^2}{4}\left(\frac{3}{(4\pi)^2\,B}\right)^{4/3}$ and $c = \frac{1}{3}\,32\,\sqrt{2}\,\pi^2$.

Proof. The independence in M is a consequence of the scaling invariance (see Lemma 2.6) and the fact that according to Lemma 2.2, $\mathcal{C}$ is achieved by the minima of the functional E on Γ_M. Without restriction, we can assume that $M = 1$. Let $f = f_1$, $\rho = \rho_1$ and $\phi = \phi_{f_1}$ be the corresponding mass density and potential. From Theorem 2.2, we get

$$\Delta\phi = 4\pi\,\rho = \frac{1}{3}\,(4\pi)^2\left[2\left(-\frac{7}{6}\left(\frac{\mathcal{C}}{8\pi}\right)^2 - \phi\right)_+\right]^{3/2}\ .$$

On the other hand, by the proof of Lemma 2.9 and Corollary 2.1, we get

$$\int_{\mathbb{R}^6}|v|^2\,f\;dx\,dv = \frac{4\pi}{5}\int_{\mathbb{R}^3}\left(\frac{3}{4\pi}\,\rho\right)^{5/3}dx = \frac{1}{8\pi}\int_{\mathbb{R}^3}|\nabla\phi|^2\;dx = 2\,|E_M|\ .$$

Thus we obtain

$$\mathcal{C} = \sqrt{8\pi}\,\left(\int_{\mathbb{R}^3}|\nabla\phi|^2\;dx\right)^{1/2}\ .$$

With the notations of the proof of Lemma 2.11, $w_a(r) = -\frac{7}{6}\,\left(\frac{\mathcal{C}}{8\pi}\right)^2 - \phi_{f_M}\left(r/\sqrt{c}\right)$ is a solution of

$$\left\{\begin{array}{l}(r^2 w_a'(r))' + r^2 (w_a)_+^{3/2}(r) = 0\\[2ex] w_a(0) = a\ ,\quad w_a'(0) = 0\end{array}\right.$$

where $a > 0$ has to be determined in order that

$$1 = \int_{\mathbb{R}^3}\rho\;dx = \frac{1}{3}\,(4\pi)^2\int_0^{\sigma(a)/\sqrt{c}} r^2\,\left(2\,w_a\!\left(\sqrt{c}\,r\right)\right)^{3/2}\;dr\ .$$

Here $\sigma(a)$ denotes the smallest zero of w_a. Note that $\rho(r) = \frac{1}{3}\,4\pi\,[2\,w_a(\sqrt{c}\,r)]^{3/2}$ for $r \le \sigma(a)/\sqrt{c}$. The scaling invariance

$$w_a(r) = a\,w_1(a^{1/4}\,r)$$

reduces the computation to the case $a = 1$, $w = w_1$ given by 2.34: on $(0, \sigma(a)/\sqrt{c})$, $\rho(r) = \frac{1}{3}\, 4\pi\, [2a\, w(a^{1/4}\sqrt{c}\, r)]^{3/2}$, so that

$$1 = \frac{1}{3}\,(4\pi)^2 \left(\frac{2}{c}\right)^{3/2} a^{3/4} \int_0^\sigma r^2\, w^{3/2}\, dr = \frac{1}{3}\,(4\pi)^2 \left(\frac{2}{c}\right)^{3/2} a^{3/4}\, B\;,$$

where $\sigma = \sigma(1)$, and allows to express a in terms of B:

$$a = \frac{c^2}{4} \left(\frac{3}{(4\pi)^2\, B}\right)^{4/3}\;.$$

Similarly, we compute

$$\int_{\mathbb{R}^3} |\nabla\phi|^2\, dx = \frac{1}{5}\, 32\,\pi^2 \int_{\mathbb{R}^3} \left(\frac{3}{4\pi}\,\rho\right)^{5/3} dx = \frac{1}{5}\, 32\,\pi^2\, 4\pi\, 2^{5/2}\, a^{7/4}\, c^{-3/2}\, A\;.$$

This gives the expression of $\mathcal{C}$ simply by collecting the estimates. □

Remark. *The expression given in Proposition 2.5 is not easy to use. A numerical computation provides $\mathcal{C} \approx 54.62...$. Going back to Lemma 2.1, we may wonder if the estimate given in the proof is optimal. This is actually not the case. Let Σ be the optimal constant in the Hardy-Littlewood-Sobolev inequality*

$$\int_{\mathbb{R}^3} |\nabla\phi|^2\, dx = 4\pi \int_{\mathbb{R}^3} \frac{\rho(x)\,\rho(y)}{|x-y|}\, dx\, dy \le 4\pi\, \Sigma\, \|\rho\|^2_{\mathrm{L}^{6/5}(\mathbb{R}^3)}\;,$$

which, according to [71], is $\Sigma = \frac{4}{3}\left(\frac{4}{\sqrt{\pi}}\right)^{2/3}$. Keeping track of the constants in the interpolation identity, we get the following estimate :

$$\mathcal{C} \le 4\pi\, \Sigma\, \left(\frac{5}{3}\,(2\pi)^{2/5}\right)^{5/6} = \frac{16\,\pi}{3} \left(\frac{20}{3}\right)^{5/6} \approx 81.42...$$

Chapter 3

Orbital stability for polytropic galaxies

Introduction and main results

This chapter relies on the analysis of stability properties of stationary solutions, called polytropic spheres, to the VP system in the gravitational case

$$\partial_t f + v\nabla_x f - \nabla_x \phi \nabla_v f = 0\,, \tag{3.1}$$

$$f(t=0,x,v) = f^0(x,v), \tag{3.2}$$

$$\Delta_x \phi = 4\pi\gamma\rho, \quad \lim_{|x|\to\infty} \phi(t,x) = 0\,. \tag{3.3}$$

This topic is of particular interest in stellar dynamics for the understanding of galaxies and clusters.

The existence of families of stationary solutions to the gravitational VP system has been previously analyzed in several works, e. g. [15, 56]. Here, we focus our attention on a particular family, the so called polytropic spherical systems [56], which are defined by

$$\nu_\mu = \nu(x,v) = c\left(E_0 - |v|^2/2 - \phi(|x|)\right)_+^\mu, \tag{3.4}$$

where $(f)_+$ denotes the positive part of f, $\alpha < E_0 < 0$, $-1 < \mu$ and $c > 0$. ϕ is coupled with ν by the Poisson equation (3.3) and satisfies $\lim_{|x|\to 0}\phi(|x|) = E_0 - \alpha$. The family (3.4) involves four different parameters. However, the Coulombian constraint implies the existence of a unique polytrope for any admissible values of μ, c and α. Typically, these solutions are indexed by the exponent μ. The functions represented by (3.4) can be seen as a particular case of the family of generalized polytropic solutions [15, 56]. The existence of these and other families of solutions were proved in [15] by means of the associated characteristic system.

A wide literature could be mentioned from the 60's about the stability properties of these solutions. In [4, 5] Antonov studied the linear stability of polytropic solutions with $0 < \mu < 7/2$. Later, in [12, 56] the stability for other values of μ was analyzed from a numerical point of view. Several works develop nonlinear dynamical stability criteria Chapter 2, [48, 49, 110] for *some* of these solutions via variational arguments based on the Energy–Casimir or the Energy functionals. In this direction, in [48, 110] the polytropes defined by $0 < \mu < \frac{3}{2}$, $c = 1$ and $\int_{\mathbb{R}^3} \nu_\mu \, dx = M > 0$ were deduced as the minimizers of the Energy–Casimir functionals

$$Q_{\mu,k}(f) = \frac{\mu}{\mu+1} \int_{\mathbb{R}^6} f^{1+1/\mu} L^{-k/\mu} \, dxdv + E(f) \,, \tag{3.5}$$

where $L = |x \times v|^2$ and the Total Energy functional $E(f)$ is defined by

$$E(f) \equiv E_{KIN}(f) - E_{POT}(f) = \frac{1}{2} \int_{\mathbb{R}^6} |v|^2 f(t,x,v) \, dx \, dv - \frac{1}{8\pi\gamma} \int_{\mathbb{R}^3} |\nabla\phi|^2 \, dx \,. \tag{3.6}$$

Here, the first term in the right–hand side is the kinetic energy and (minus) the second term is the potential energy. This result was also proved for generalized polytropic solutions under the additional assumption that f is also spherically symmetric. The restriction $\mu < 3/2$ was removed in [49] by minimizing the energy functional in the space

$$\Lambda_M^\mu = \left\{ f : \mathbb{R}^6 \to \mathbb{R}_0^+ \, ; \; \frac{\mu}{\mu+1} \|f\|^{1+1/\mu}_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} + \left(\frac{7}{2} - \mu\right) \|f\|_{\mathrm{L}^1(\mathbb{R}^6)} = M \right\} .$$

However, these results do not determine exactly neither the spherical polytrope minimizer nor the set of minimizers. In Chapter 2, the polytrope corresponding to $\mu = 0, \; c = 1 \,, \int_{\mathbb{R}^3} \nu_0 \, dx = M$ was obtained as the minimizer of

$$\inf \left\{ E(f) \, ; \; f \in \mathrm{L}^1_+(\mathbb{R}^6, M) \cap \mathrm{L}^\infty_+(\mathbb{R}^6, 1) \right\} , \tag{3.7}$$

where

$$\mathrm{L}^p_+(\mathbb{R}^n, F) := \{ g \in \mathrm{L}^p(\mathbb{R}^n) \, ; \; g : \mathbb{R}^n \to \mathbb{R}_0^+ \, , \; \|g\|_{\mathrm{L}^p(\mathbb{R}^n)} = F \} \, .$$

The dynamical stability criteria developed in Chapter 2 and [48, 49, 110] are established in terms of the functionals

$$d(f,h) = O(f) - O(h) + \frac{1}{4\pi} \|\nabla\phi_f - \nabla\phi_h\|^2_{\mathrm{L}^2(\mathbb{R}^3)} \,, \tag{3.8}$$

where O denotes the functional to minimize, i.e. the Energy–Casimir or Energy functionals, depending on the variational problem under consideration with respect to μ for functions in the space $\mathrm{L}^1_+(\mathbb{R}^6, M)$, Λ^μ_M or

$L^1_+(\mathbb{R}^6, M) \cap L^\infty_+(\mathbb{R}^6, 1)$, respectively. Also, ϕ_f denotes the solution to the Poisson equation $\Delta_x \phi_f = 4\pi\gamma\rho_f$. If ν_μ is a minimizer, the dynamical stability criteria stablish that for f^0 as initial condition in the above spaces and "close to" ν_μ, the solution remains close to the set of minimizers, always in terms of the distance d. Due to the time invariance of the functional O for the solutions of the VP system, these criteria establish stability for the potential energies instead of for the solutions (cf. (3.8)). An alternative stability criterium was obtained in [108] in terms of the $L^2(\mathbb{R}^6)$ norm of the distribution, although it only covers the case $\mu = 1$.

The dynamics of the solutions to the VP system is much richer and the above criteria give only a partial answer to the stability problem in terms of the potential. The aim of this work is to extend these stability criteria to a stronger picture: *the orbital stability.* This concept has been widely analyzed in other contexts such as bound states and traveling wave solutions to nonlinear PDE's, for instance Klein–Gordon and Schrödinger equations (see [28, 27, 46]). Usually, the solutions of these systems exhibit some invariance properties up to some non–compact group of symmetries. This gives rise to the concept of orbit of a solution. The solutions to the VP system are invariant by space translations. Thus, the orbit of the solution f is described by $\{f(t, x + k, v)\ ; k \in \mathbb{R}^3\}$. The main idea of orbital stability relies on the fact that a stationary solution f_S is orbitally stable if small perturbations of f_S remain close to the orbit of f_S along the evolution (in some sense to be specified). Furthermore, the criterium is optimal as shown the following application of the Galilean invariance property: If ν_μ is a solution to the VP system, then for all $u \in \mathbb{R}^3$ we have that $\nu^u_\mu(x, v) = \nu_\mu(x - tu, v - u)$ is also a solution with initial condition $\nu_\mu(x, v - u)$ (see Chapter 2). By choosing u small enough (in norm) we obtain initial conditions close to ν_μ, meanwhile the corresponding solution only travels close (in some distance defined in terms of the minimization problem) to the orbit and not pointwise.

The total energy, as well as the norms $\|f\|_{L^p(\mathbb{R}^6)}$ with $p \in [1, \infty]$, remain constant along the time evolution for regular solutions. In case of $p = 1$, we actually have mass conservation. Literature concerning the stability of such solutions is based on these conserved properties. For instance, only spherical polytropes with $-1/2 \le \nu \le 7/2$ have finite mass, and if $\nu < 7/2$ they also have compact support.

Technically all these minimizing problems exhibit the same difficulty, say the functional under consideration is invariant under space translations. This clearly motivates a lack of compactness of any minimizing sequence.

In this work we deal with the variational problem

$$I^\mu_{M,J} := \inf \left\{ E(f)\ ;\ f \in \Gamma^\mu_{M,J} \right\} \tag{3.9}$$

where $\Gamma^\mu_{M,J} = \mathrm{L}^1_+(\mathbb{R}^6, M) \cap \mathrm{L}^{1+1/\mu}_+(\mathbb{R}^6, J)$. We will prove that the polytropic gas sphere solutions are orbitally stable in the following sense:

Theorem 3.1 (Orbital Stability). Let $\mu \in [0, 7/2)$ and $\epsilon > 0$. Also, let ν_μ be a spherical polytropic solution given by (3.4) with $\|\nu_\mu\|_{\mathrm{L}^1(\mathbb{R}^6)} = M$ and $\|\nu_\mu\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} = J$. Then, there exists $\delta = \delta(\epsilon) > 0$ such that for every initial condition f^0 satisfying

i) $E(f_0) - E(\nu_\mu) \leq \delta$,

ii) $f_0 \in \Gamma^\mu_{M,J} \cap C^1_0(\mathbb{R}^6)$,

the associated solution f to (3.1)–(3.3) verifies

$$\inf_{k\in\mathbb{R}^3} \|f(t,\cdot,\cdot) - \nu_\mu(\cdot - k, \cdot)\|_{\mathrm{L}^1(\mathbb{R}^6)} \leq \epsilon\,, \quad \forall t \in (0, \infty). \tag{3.10}$$

If $\mu \neq 0$ we also have

$$\inf_{k\in\mathbb{R}^3} \|f(t,\cdot,\cdot) - \nu_\mu(\cdot - k, \cdot)\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} \leq \epsilon\,, \quad \forall t \in (0, \infty)\,.$$

One of the main improvements of this result with respect to previous dynamical criteria for the solutions of the VP system is that the stability for the solutions is established in terms of the $\mathrm{L}^1(\mathbb{R}^6)$ norm, which is the natural in the VP context. This approach allows to cover the range of polytropes with $\mu \in [0, 7/2)$ Now, the stability criteria are perfectly established for any polytrope ν_μ in terms of its mass and $\mathrm{L}^{1+1/\mu}$ norm.

Several approaches have been developed in other contexts to study orbital stability properties. We first refer to [27], where variational techniques valid for Schrödinger–type equations were considered. To prove Theorem 3.1, in this work we follow the argumental scheme of [27] sketched below:

i) *The system of equations is well–posed in a particular functional framework and the solutions satisfy some conservation laws.*

ii) *Stationary solutions minimize the variational problem*

$$\inf\{O(u)\,; u \in X,\ R(u) = M\}\,, \tag{3.11}$$

where the functional O as well as the constraints given by R are conserved quantities of the solutions. We remark that if the functionals O and R are invariant by a noncompact group of symmetries, then the set of minimizers of (3.11) is a noncompact set.

iii) *All minimizing sequences for (3.11) are relatively compact up to symmetries.* In our case, this means that for any minimizing sequence f_n, there exists $y_n \in \mathbb{R}^3$ such that the sequence $f_n(\cdot - y_n, \cdot)$ is relatively compact in L^1.

Since assumption *i)* is verified by ν_μ, $\mu \in [0, 7/2)$, we shall focus our attention on proving that *ii)* and *iii)* are also satisfied. In this direction we have the following result.

Theorem 3.2. For every $0 \leq \mu < 7/2$, $M > 0$ and $J > 0$ there exists a minimum of (3.9). Furthermore, this minimum is reached in the orbit of the spheric polytrope ν_μ verifying $\|\nu_\mu\|_{\mathrm{L}^1(\mathbb{R}^6)} = M$ and $\|\nu_\mu\|_{\mathrm{L}^{1+1\mu}(\mathbb{R}^6)} = J$. More precisely, every minimizing sequence f_n is relatively compact in $\mathrm{L}^1(\mathbb{R}^6)$ up to spatial translations, i.e., there exists $y_n \in \mathbb{R}^3$ such that $f_n(\cdot - y_n, \cdot)$ is relatively compact in $\mathrm{L}^1(\mathbb{R}^6)$. In the case $\mu \in (0, 7/2)$, $f_n(\cdot - y_n, \cdot)$ is also relatively compact in $\mathrm{L}^{1+\frac{1}{\mu}}(\mathbb{R}^6)$.

Once we have proved that *i)–iii)* holds, it is a simple matter to show that the solutions ν_μ are orbitally stable.

Proof of Theorem 3.1. If the thesis of Theorem 3.1 is not true, there would exist ϵ_0, f_n^0 and t_n such that:

$$\begin{cases} f_n^0 \in \Gamma^\mu_{M,J} \cap C^1_0(\mathbb{R}^6)\,, \\ E(f_n^0) \longrightarrow E(\nu_\mu),\ n \to \infty\,, \\ \forall k \in \mathbb{R}^3 \begin{cases} \|f_n(t_n, \cdot, \cdot) - \nu_\mu(\cdot - k, \cdot)\|_{\mathrm{L}^1(\mathbb{R}^6)} > \epsilon_0 \\ \text{or} \\ \|f_n(t_n, \cdot, \cdot) - \nu_\mu(\cdot - k, \cdot)\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} > \epsilon_0\,, \end{cases} \end{cases} \tag{3.12}$$

for $\mu \in (0, 7/2)$, and

$$\begin{cases} f_n^0 \in \Gamma^0_{M,J}, \\ E(f_n^0) \longrightarrow E(\nu_0),\ n \to \infty\,, \\ \forall k \in \mathbb{R}^3\ \|f_n(t_n, \cdot, \cdot) - \nu_0(\cdot - k, \cdot)\|_{\mathrm{L}^1(\mathbb{R}^6)} > \epsilon_0\,, \end{cases} \tag{3.13}$$

for $\mu = 0$. Now, we use the conservation of the mass and of the L^p norms to deduce that $\{f_n(t_n, \cdot, \cdot)\}$ is a minimizer for (3.9), since

$$f_n(t_n, \cdot, \cdot) \in \Gamma^\mu_{M,J}\,, \qquad E(f_n^0(\cdot, \cdot)) = E(f_n(t_n, \cdot, \cdot)) \longrightarrow E(\nu_\mu)\,.$$

Then, (3.12) or (3.13) are clearly in contradiction with Theorem 3.2 as we can extract a subsequence from $\{f_n(t_n, \cdot, \cdot)\}$ which is relatively compact up to translations. □

Theorem 3.1 establishes the concept of orbital stability for kinetic equations. The techniques used in [46, 47] to deal with the orbital stability of stationary solutions to nonlinear wave equations are strongly based on the analysis of the linearized operators. These arguments mainly consist in considering an abstract Hamiltonian system which is invariant under a group of operators and then studying the effects of these invariances on the stability of solitary waves.

The rest of the chapter is devoted to prove Theorem 3.2. The minimization problems (3.9) present several difficulties. First, the energy is a nonconvex functional. Also, it is invariant by space translations which implies a lack of relative compactness of any minimizing sequence. The space proposed for the minimization problem, $\Gamma^{\mu}_{M,J} = \mathrm{L}^1_+(\mathbb{R}^6, M) \cap \mathrm{L}^{1+1/\mu}_+(\mathbb{R}^6, J)$, has two constraints. Our minimizing argument is based into overcome the above difficulties through a series of equivalent reduced problems. Section 3 explores the relation between the variational problems (3.9) and the proposed equivalent problems for the densities. In fact, we prove that beyond this equivalence there is a deeper concept which implies that the minimizing sequences are even connected. This interesting relation between the different minimization problems allows us to give a new minimizing argument for (3.9). In Section 3 we minimize the reduced problem obtained in the previous section. The argument developed at this point is related to those used in [90]. The results obtained for the reduced problem lead to the proof of Theorem 3.2 in Section 3. Finally, in an Appendix the connection between the minimization problems associated to the Casimir energies, to the Energy with mass-Casimir constraint and (3.9) are analyzed.

Let us finally notice that the concept of solution considered in this work assumes that the sufficient conditions necessary to claim the well–posedness (existence and uniqueness) of the problem hold, see for example [14, 79] for a review.

The results of this chapter are collected in [100].

Equivalent reduced problem

As we pointed out in the introduction, we now propose a variational approach related to the problems stated in (3.9) in order to prove the orbital stability of spherical polytropes with $0 \leq \mu < 7/2$. We actually show the relative compactness in L^p of any minimizing sequence and that the minimum value is achieved in a particular polytropic solution (up to translations in both cases). The method proposed in this work tries to minimize the difficulties by considering a sequence of equivalent reduced problems. The equivalence relations rely on the fact that between the functions $f \in \Gamma^{\mu}_{M,J}$ *with the same density* $\rho(x) = \int_{\mathbb{R}^3} f(x,v)\,dv$ there are special functions $\tilde{f}$ whose energy is as small as possible. Besides, $\tilde{f}$ can be expressed in terms of ρ and J by

$$\tilde{f}(x,v) = J\left(\frac{1}{2}\left(\frac{3\rho(x)}{4\pi J}\right)^{\frac{2}{3}} - \frac{|v|^2}{2}\right)^{0}_{+} \equiv \begin{cases} J & \text{if } |v| \leq \left(\frac{3\rho(x)}{4\pi J}\right)^{\frac{1}{3}} \\ 0 & \text{elsewhere} \end{cases}, \tag{3.14}$$

when $\mu = 0$, and

$$\tilde{f}(x,v) = \left(\left(\frac{2\mu+5}{2(\mu+1)} C \rho^{\frac{2}{2\mu+3}}(x) - \frac{3}{2(\mu+1)} C^{\frac{2\mu+3}{3}} \frac{1}{K_{1,1}} \frac{|v|^2}{2}\right)_{+}\right)^{\mu} \tag{3.15}$$

for $\mu > 0$. Here,

$$C = \frac{J^{1+1/\mu}}{\int_{\mathbb{R}^3} \rho(x)^{\frac{2\mu+5}{2\mu+3}}\,dx}$$

and $K_{1,1}$ is a positive constant (to be determined) depending only on μ. The total energy for such a function is given by

$$E(\tilde{f}) = E^{\mu}_{J}(\rho) := K \frac{\left(\int_{\mathbb{R}^3} \rho(x)^{\frac{2\mu+5}{2\mu+3}}\,dx\right)^{\frac{2\mu+3}{3}}}{J^{\frac{2(\mu+1)}{3}}} - \frac{1}{2}\int_{\mathbb{R}^6} \frac{\rho(x)\rho(y)}{|x-y|}\,dxdy\,,$$

where $K = \frac{3^{\frac{5}{3}}}{10(4\pi)^{\frac{2}{3}}}$ for $\mu = 0$ and $K = K_{1,1}$ for $\mu > 0$. We can now establish the equivalence between (3.9) and the following reduced problems for the densities:

$$\inf\left\{E^{\mu}_{J}(\rho)\ ;\ \ \|\rho\|_{L^1(\mathbb{R}^3)} = M,\ \rho(x) \geq 0\right\}.$$

The idea of finding an equivalent problem was proposed by G. Rein in [90] in the context of the Energy-Casimir minimization problem. Our argument is summarized in the next theorem.

Theorem 3.3. The variational problems

$$R^{\mu}_{J,M} := \inf\left\{E^{\mu}_{J}(\rho)\,;\ \rho \in L^1_+(\mathbb{R}^3, M) \cap L^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)\right\} \tag{3.16}$$

and (3.9) are equivalent in the following sense:

i) Their infima values coincide: $R^{\mu}_{J,M} = I^{\mu}_{J,M}$.

ii) Let $\{f_n\}$ be a minimizing sequence for any problem (3.9). Then, $\rho_n(x) = \int_{\mathbb{R}^3} f_n(x,v)dv$ is a minimizing sequence for the corresponding problem (3.16). Moreover, if ρ_n is a minimizing sequence for any problem (3.16), then the sequence of functions $\tilde{f}_n$ defined by (3.14) or (3.15) with associated densities ρ_n is a minimizing sequence for the corresponding problem (3.9).

iii) (3.9) has a minimum if and only if (3.16) also has a minimum. In that case, the corresponding minimizers verify ii).

The proof of this theorem is an immediate consequence of the following

Proposition 3.1. Let $M > 0$, $J > 0$ and $\mu \in [0, \frac{7}{2})$. Consider $f \in \Gamma^{\mu}_{M,J}$ such that $E(f) < \infty$. Then, there exists a positive function $\tilde{f}$ verifying

i) f and $\tilde{f}$ have the same mass density ρ,

ii) $\|f\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} = \|\tilde{f}\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} = J$,

iii) $E(\tilde{f}) \leq E(f)$.

Moreover, $\tilde{f}$ is defined by (3.14) or (3.15) in terms of ρ and J. We also have

$$E_{KIN}(\tilde{f}) = \frac{3^{\frac{5}{3}}}{10(4\pi J)^{\frac{2}{3}}} \int_{\mathbb{R}^3} \rho(x)^{\frac{5}{3}}\, dx \tag{3.17}$$

for $\mu = 0$ and

$$\int_{\mathbb{R}^3} \tilde{f}^{1+1/\mu}(x,v)\, dv = C\rho(x)^{\frac{2\mu+5}{2\mu+3}}\,, \qquad E_{KIN}(\tilde{f}) = \frac{\left(\int_{\mathbb{R}^3} \rho(x)^{\frac{2\mu+5}{2\mu+3}}\, dx\right)^{\frac{2\mu+3}{3}}}{J^{\frac{2(\mu+1)}{3}}} K_{1,1} \tag{3.18}$$

for $\mu \in (0, \frac{7}{2})$. Here, $C = \frac{J^{1+1/\mu}}{\int_{\mathbb{R}^3} \rho(x)^{\frac{2\mu+5}{2\mu+3}}\, dx}$ and $K_{1,1}$ is a positive constant depending only on μ.

Remark. Proposition 3.1 admits a reverse reading. Let us consider a function $\rho \in \mathrm{L}^1_+(\mathbb{R}^3, M) \cap \mathrm{L}^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)$. Then, the function $\tilde{f}$ defined by (3.14) or (3.15), with associated density function ρ, satisfies:

i) $\tilde{f} \in \mathrm{L}^1_+(\mathbb{R}^6, M) \cap \mathrm{L}^{1+1/\mu}_+(\mathbb{R}^6, J)\,,$

ii) $\tilde{f}$ verifies (3.17)–(3.18),

iii) $E(\tilde f) \le E(f)\,, \quad \forall f \in \mathrm{L}^{1+1/\mu}_+(\mathbb{R}^6, J)$ such that $\int_{\mathbb{R}^3} f\,dv = \int_{\mathbb{R}^3} \tilde f\,dv = \rho$.

Proposition 3.1 requires the study of an auxiliary problem, defined in the following

Lemma 3.1. The minimization problem

$$K_{G,H} = \inf\left\{\frac{1}{2}\int_{\mathbb{R}^3} |v|^2 z(v)\,dv\,;\ z \in \mathrm{L}^1_+(\mathbb{R}^3, G) \cap \mathrm{L}^{1+1/\mu}_+(\mathbb{R}^3, H)\right\} \qquad (3.19)$$

has a minimum for $0 \le \mu < 7/2$. $K_{G,H}$ verifies

$$K_{G,H} = \frac{G^{\frac{2\mu+5}{3}}}{H^{\frac{2\mu+2}{3}}}\,K_{1,1}\ ,\ \text{for } \mu > 0$$

and

$$K_{G,H} = \frac{(3G)^{\frac{5}{3}}}{10(4\pi H)^{\frac{2}{3}}}\,,\ \text{for } \mu = 0\,,$$

where $K_{1,1}$ is defined by (3.19) with $G = H = 1$. This minimum is reached by a unique function $z_{G,H}$. If $\mu > 0$ and G, $H > 0$, then $z_{G,H}$ is explicitly given by

$$z_{G,H}(v) = \left(\left(\frac{2\mu+5}{2(\mu+1)}\frac{H^{\frac{\mu+1}{\mu}}}{G} - \frac{3}{2(\mu+1)}\frac{H^{\frac{\mu+1}{\mu}\frac{2\mu+3}{3}}}{G^{\frac{2\mu+5}{3}}}\frac{1}{K_{1,1}}\frac{|v|^2}{2}\right)_+\right)^{\mu}. \qquad (3.20)$$

In the case $\mu = 0$, $z_{G,H}$ is defined by

$$z_{G,H}(v) = \begin{cases} H & \text{if } |v| \le \left(\frac{3G}{4\pi H}\right)^{\frac{1}{3}}\,, \\ 0 & \text{elsewhere}\,. \end{cases} \qquad (3.21)$$

If $G = H = 0$, (3.19) trivially implies $K_{0,0} = 0$ and $z_{0,0} \equiv 0$.

The rest of this section is devoted to prove the last two results.

Proof of Proposition 3.1. Integrals involved in (3.17) and (3.18) are well defined in virtue of the following inequalities

$$\int_{\mathbb{R}^3} |\rho|^{\frac{2\mu+5}{2\mu+3}}\,dx \quad \le \quad C\|f\|^{\frac{2\mu+2}{2\mu+3}}_{\mathrm{L}^{1+\frac{1}{\mu}}(\mathbb{R}^6)}\left(\int_{\mathbb{R}^6} |v|^2|f(x,v)|\,dv\,dx\right)^{\frac{3}{2\mu+3}}\,, \quad (3.22)$$

which can be proved by usual arguments thanks to the nonnegativity of f.

A function $\tilde{f}$ verifying *i)*, *ii)* and *iii)* minimizes the problem

$$\inf\left\{E(l)\ ;\ l \in \Theta\right\},$$

where $\Theta = \left\{l \in \mathrm{L}_+^{1+1/\mu}(\mathbb{R}^6, J)\,,\ \int_{\mathbb{R}^3} l(x,v)\,dv = \rho(x)\ \ a.e.\ x \in \mathbb{R}^3\right\}$. This problem is equivalent to study

$$\inf\left\{E_{KIN}(l)\ ;\ l \in \Theta\right\} \tag{3.23}$$

because the potential energy only depends on the function ρ.

Let us first consider the case $\mu > 0$. We define the sets

$$\Theta_{\rho,h} = \left\{\ l : \mathbb{R}^6 \to \mathbb{R}_0^+\ ;\ \int_{\mathbb{R}^3} l\,dv = \rho(x)\,,\ \int_{\mathbb{R}^3} l^{1+1/\mu}\,dv = h(x)\,,\ a.e.\ x \in \mathbb{R}^3\right\}$$

and

$$\Theta_\rho = \left\{h \in \mathrm{L}_+^1(\mathbb{R}^3, J^{1+1/\mu})\,;\ Supp(\rho) = Supp(h)\right\}.$$

Then, $\Theta = \bigcup_{h\in\Theta_\rho} \Theta_{\rho,h}$. This simple idea provides the equivalence between (3.23) and the problem

$$\inf\left\{\ \inf\{E_{KIN}(l)\ ; l \in \Theta_{\rho,h}\}\,; h \in \Theta_\rho\right\}. \tag{3.24}$$

In order to solve (3.24) we first analyze

$$\inf\{E_{KIN}(l)\ ; l \in \Theta_{\rho,h}\} \tag{3.25}$$

for any fixed but arbitrary $h \in \Theta_\rho$. The constraints defining $\Theta_{\rho,h}$ are fixed for any $x \in \mathbb{R}^3$. Then, we propose to study (3.25) by considering the problem

$$\begin{aligned} P_x = \inf\Bigg\{\frac{1}{2}\int_{\mathbb{R}^3} |v|^2 l(x,v)\,dv\ ;\\ l \geq 0,\ \int_{\mathbb{R}^3} l(x,v)\,dv = \rho(x)\,,\ \int_{\mathbb{R}^3} l(x,v)^{1+1/\mu}\,dv = h(x)\Bigg\} \end{aligned} \tag{3.26}$$

for almost everywhere $x \in \mathbb{R}^3$ fixed but arbitrary. Our argument is founded on the following basic idea: If (3.26) has a minimum P_x a.e. $x \in \mathbb{R}^3$ and this minimum is achieved by a function $l_x(v)$, then (3.25) has also a minimum $\int_{\mathbb{R}^3} P_x\,dx$ and it is achieved by the function $l(x,v) = l_x(v)$.

We can control the dependence with respect to x in (3.26) because this problem obeys the general profile of (3.19), where we identify $l(x,\cdot) = z(\cdot)$, $G = \rho(x)$ and $H^{1+1/\mu} = h(x)$. Let us observe that the dependence with respect to x is entirely concentrated on the value of the *constants* G and H. Lemma 3.1 gives the existence of a minimizer for (3.26), where $z_{G,H}$ depends on G and H. The detailed analysis of this dependence done in the proof of Lemma 3.1 is motivated by the fact that we have to define $h_x(\cdot) = z_{G,H}(\cdot)$ for $G = \rho(x)$ and $H^{1+1/\mu} = h(x)$. Therefore, we have analogous results for the problem (3.26): If $x \in Supp(\rho) = Supp(h)$, then (3.26) has a minimum

$$P_x = \frac{\rho(x)^{\frac{2\mu+5}{3}}}{h(x)^{\frac{2\mu}{3}}} K_{1,1} \,. \tag{3.27}$$

This minimum is achieved by

$$l(x,v) = l_x(v) = \left(\left(\frac{2\mu+5}{2(\mu+1)} \frac{h(x)}{\rho(x)} - \frac{3}{2(\mu+1)} \frac{h(x)^{\frac{2\mu+3}{3}}}{\rho(x)^{\frac{2\mu+5}{3}}} \frac{1}{K_{1,1}} \frac{|v|^2}{2} \right)_+ \right)^{\mu} .$$

If $x \in \mathbb{R}^3 - Supp(\rho)$, then $P_x = 0$. Now, using (3.27), we can rewrite (3.24) as

$$\inf \left\{ \int_{\mathbb{R}^3} \frac{\rho(x)^{\frac{2\mu+5}{3}}}{h(x)^{\frac{2\mu}{3}}} K_{1,1}\, dx \,;\ h \in \Theta_\rho \right\} . \tag{3.28}$$

which is directly solvable by using Hölder's inequality in the following way

$$\int_{\mathbb{R}^3} \rho(x)^{\frac{2\mu+5}{2\mu+3}}\, dx \le \left(\int_{\mathbb{R}^3} \frac{\rho(x)^{\frac{2\mu+5}{3}}}{h(x)^{\frac{2\mu}{3}}}\, dx \right)^{\frac{3}{2\mu+3}} \cdot \left(\int_{\mathbb{R}^3} h(x)\, dx \right)^{\frac{2\mu}{2\mu+3}} ,$$

or equivalently

$$\frac{\left(\int_{\mathbb{R}^3} \rho(x)^{\frac{2\mu+5}{2\mu+3}}\, dx \right)^{\frac{2\mu+3}{3}}}{\left(\int_{\mathbb{R}^3} h(x)\, dx \right)^{\frac{2\mu}{3}}} \le \int_{\mathbb{R}^3} \frac{\rho(x)^{\frac{2\mu+5}{3}}}{h(x)^{\frac{2\mu}{3}}}\, dx \,.$$

Furthermore, the equality holds if and only if h is proportional to $\rho^{\frac{2\mu+5}{2\mu+3}}$. As consequence, the mimimun of (3.28) is

$$\frac{\left(\int_{\mathbb{R}^3} \rho(x)^{\frac{2\mu+5}{2\mu+3}}\, dx \right)^{\frac{2\mu+3}{3}}}{J^{\frac{2(\mu+1)}{3}}} K_{1,1}$$

and it is reached when $h = C\rho^{\frac{2\mu+5}{2\mu+3}}$, where

$$C = \frac{J^{1+1/\mu}}{\int_{\mathbb{R}^3} \rho(x)^{\frac{2\mu+5}{2\mu+3}}\, dx}.$$

We conclude that the infimum of (3.23) is achieved by $\tilde{f}$, defined as

$$\tilde{f}(x,v) = \left(\left(\frac{2\mu+5}{2(\mu+1)} C \rho^{\frac{2}{2\mu+3}} - \frac{3}{2(\mu+1)} C^{\frac{2\mu+3}{3}} \frac{1}{K_{1,1}} \frac{|v|^2}{2} \right)_+ \right)^{\mu},$$

and the infimum value is

$$E_{KIN}(\tilde{f}) = \frac{\left(\int_{\mathbb{R}^3} \rho(x)^{\frac{2\mu+5}{2\mu+3}}\, dx \right)^{\frac{2\mu+3}{3}}}{J^{\frac{2(\mu+1)}{3}}} K_{1,1}\,.$$

In the case $\mu = 0$ our argument becomes easier because both conditions defining Θ are local in space. By using the previous arguments we deduce in this case

$$\tilde{f}(x,v) = l_x(v) = J \left(\frac{1}{2} \left(\frac{3\rho(x)}{4\pi J} \right)^{\frac{2}{3}} - \frac{|v|^2}{2} \right)_+^0$$

and

$$E_{KIN}(\tilde{f}) = \frac{3^{\frac{5}{3}}}{10(4\pi J)^{\frac{2}{3}}} \int_{\mathbb{R}^3} \rho(x)^{\frac{5}{3}}\, dx\,,$$

which concludes the proof of Proposition 3.1. □

We now prove Lemma 3.1.

Proof of Lemma 3.1. Set $S_\mu(z) = \frac{1}{2} \int_{\mathbb{R}^3} |v|^2 z(v)\, dv$ and consider $K_{G,H}$ defined by (3.19).
The positivity of $K_{G,H}$ is deduced from the inequality

$$\|g\|_{\mathrm{L}^1(\mathbb{R}^3)}^{\frac{2\mu+5}{3}} \leq C \|g\|_{\mathrm{L}^{1+\frac{1}{\mu}}(\mathbb{R}^3)}^{\frac{2\mu+2}{3}} \int_{\mathbb{R}^3} |x|^2 g(x)\, dx\,,$$

which holds for any positive function g. By using the scaling $\bar{z}(x) = az(bx)$, where $a = \frac{H^{\mu+1}}{G^\mu}$ and $b = (H/G)^{\frac{\mu+1}{3}}$, we find

$$K_{G,H} = \frac{G^{\frac{2\mu+5}{3}}}{H^{\frac{2\mu+2}{3}}} K_{1,1}\,.$$

Also, the minimizers for a pair $G = 1,\ H = 1$ are related to the minimizers for G', H' by the same scaling. Thus, we can rewrite (3.19) as

$$\inf \left\{ \frac{1}{2} \int_{\mathbb{R}^3} |v|^2 z(v)\, dv\,;\ z \in \mathrm{L}^1_+(\mathbb{R}^3, G),\ \|z\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^3)} \leq H \right\} \tag{3.29}$$

since both problems have the same minimum and minimizers (any minimizer $z_{G,H}$ for (3.29) verifies $\|z_{G,H}\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^3)} = H$).

Let $\{z_n\}$ be a minimizing sequence for (3.29). We have that $\|z_n\|_{\mathrm{L}^{1+\frac{1}{\mu}}(\mathbb{R}^3)}$ and $\int_{\mathbb{R}^3} |v|^2 z_n(v)\,dv$ are uniformly bounded. Therefore, $\{z_n\}$ is under the hypotheses of the Dunford–Pettis theorem:

i) is bounded in $\mathrm{L}^1(\mathbb{R}^3)$, because $\|z_n\|_{\mathrm{L}^1(\mathbb{R}^3)} = G$;

ii) there is no concentration in any measurable set A, since

$$\int_A z_n(v)\,dv \le \|z_n\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^3)} |A|^{\mu+1}\,;$$

iii) and there is no vanishing, since $\int_{|v|\ge R} z_n(v)dv \le \frac{1}{R^2}\int_{\mathbb{R}^3} |v|^2 z_n(v)dv\,.$

Thus, we can extract a subsequence verifying $z_n \rightharpoonup z_{G,H}$ weakly in $\mathrm{L}^1(\mathbb{R}^3)$ and

$$\begin{cases} z_n \rightharpoonup z_{G,H} \text{ weakly in } \mathrm{L}^{1+1/\mu}(\mathbb{R}^3)\,, & \text{for } \mu \in (0, 7/2)\,, \\ z_n \rightharpoonup z_{G,H} \text{ in the weak-* } \mathrm{L}^\infty(\mathbb{R}^3) \text{ topology} & \text{for } \mu = 0\,. \end{cases}$$

Also $z_{G,H} \in \mathrm{L}^1(\mathbb{R}^3) \cap \mathrm{L}^{1+1/\mu}(\mathbb{R}^3)$ and is nonegative because it is obtained as a weak limit of nonnegative functions. Using the inequalities

$$\begin{aligned} \int_{\mathbb{R}^3} |v|^2 z_{G,H}(v)\,dv &= \lim_{R\to\infty}\int_{|v|\le R} |v|^2 z_{G,H}(v)\,dv = \lim_{R\to\infty}\lim_{n\to\infty}\int_{|v|\le R} |v|^2 z_n(v)\,dv \\ &\le \lim_{R\to\infty}\lim_{n\to\infty}\int_{\mathbb{R}^3} |v|^2 z_n(v)\,dv = \lim_{n\to\infty}\int_{\mathbb{R}^3} |v|^2 z_n(v)\,dv\,, \\ \|z_{G,H}\|_{\mathrm{L}^{1+\frac{1}{\mu}}(\mathbb{R}^3)} &\le \liminf_{n\to\infty} \|z_n\|_{\mathrm{L}^{1+\frac{1}{\mu}}(\mathbb{R}^3)} \le H \end{aligned}$$

and

$$\|z_{G,H}\|_{\mathrm{L}^1(\mathbb{R}^3)} \le \liminf_{n\to\infty} \|z_n\|_{\mathrm{L}^1(\mathbb{R}^3)} = G\,, \tag{3.30}$$

we have that $z_{G,H}$ verifies $S_\mu(z_{G,H}) \le \liminf_{n\to\infty} S_\mu(z_n) = K_{G,H}$. To conclude that $z_{G,H}$ is a minimizer for (3.29), we have to check that $\|z_G\|_{\mathrm{L}^1(\mathbb{R}^3)} = G$. Let ϵ be a positive constant. Then, there exists R (depending only on ϵ) such that

$$\begin{aligned} \int_{B_R} z_{G,H} &= lim_{n\to\infty}\int_{B_R} z_n = G - lim_{n\to\infty}\int_{\mathbb{R}^3 - B_R} z_n \\ &\ge G - lim_{n\to\infty}\frac{1}{R^2}\int_{\mathbb{R}^3} |v|^2 z_n \ge G - \epsilon\,. \end{aligned} \tag{3.31}$$

Thus, by using (3.30) and (3.31) we deduce that $\|z_{G,H}\|_{\mathrm{L}^1(\mathbb{R}^3)} = G$.

Once we know that a minimum of (3.29) (equivalent of (3.19)) exists, we study some of the properties of the minimizers. Let us prove that $z_{G,H}$ is a nonincreasing function. For radial nonincreasing rearrangements z^* of z (see [74]) we have

$$\int_{\mathbb{R}^3} |v|^2 z^*(v) dv \leq \int_{\mathbb{R}^3} |v|^2 z(v) dv \,,$$

with strict inequality unless $z \equiv z^*$. Then, $z_{G,H}$ coincides with its rearranged function and consequently it is a symmetric nonincreasing function.

The expression of these functions is obtained from the Euler–Lagrange equation, which for $\mu > 0$ reads

$$\frac{1}{2}|v|^2 + \lambda z_{G,H}^{\frac{1}{\mu}} + \beta\chi = \gamma \,, \tag{3.32}$$

where λ, β, γ are the Lagrange multipliers and the function χ is defined by

$$\chi(v) = \begin{cases} 0 & \text{if } z_{G,H}(v) > 0 \,, \\ \geq 0 & \text{if } z_{G,H}(v) = 0 \,. \end{cases}$$

We first note that $\lambda \neq 0$ since otherwise $Supp(z_{G,H}) \subset \{v \in \mathbb{R}^3 \,; \frac{1}{2}|v|^2 = \gamma\}$, which is a set of null measure. Then, we have

$$z_{G,H}(v) = \frac{1}{\lambda^\mu}\left(\gamma - \frac{1}{2}|v|^2\right)^\mu \,, \text{ for } v \in Supp(z_{G,H}) \,.$$

This expression combined with the nonincreasing and nonnegative character of $z_{G,H}$ implies that $\lambda > 0$ and $Supp(z_{G,H}) \subset \{v \in \mathbb{R}^3 \,; \frac{1}{2}|v|^2 \leq \gamma\}$. On the other hand, we have

$$\gamma - \frac{1}{2}|v|^2 = \beta\chi(v) \,, \text{ for } v \in \mathbb{R}^3 - Supp(z_{G,H}) \,.$$

Then, $\beta < 0$ (since $z_{G,H}$ is nonincreasing) and

$$z_{G,H}(v) = \frac{1}{\lambda^\mu}\left(\gamma - \frac{1}{2}|v|^2\right)_+^\mu \,. \tag{3.33}$$

By using (3.33) we can compute λ and γ. Multiplying (3.32) by $z_{G,H}$ and integrating over $\mathbb{R}^3$ we find

$$K_{G,H} + \lambda H^{1+1/\mu} = \gamma G \,.$$

The use of radial coordinates leads to the following equality

$$\begin{aligned} K_{G,H} &= \frac{1}{2}\int_{\mathbb{R}^3} |v|^2 z_{G,H}(v) dv = \frac{1}{2}\frac{4\pi}{\lambda^\mu}\int_0^{\sqrt{2\beta}} r^4(\beta - \frac{1}{2}r^2)^\mu \, dr \\ &= \frac{1}{2}\frac{4\pi}{\lambda^\mu}\frac{3}{\mu+1}\int_0^{\sqrt{2\gamma}} r^2(\beta - \frac{1}{2}r^2)^{\mu+1} \, dr = \frac{1}{2}\frac{3\lambda}{\mu+1}\int_{\mathbb{R}^3} z_{G,H}^{1+1/\mu} \, dv \\ &= \frac{3\lambda}{2(\mu+1)} H^{1+1/\mu}. \end{aligned}$$

From these equations and Lemma 3.1 we have

$$\lambda = \frac{2(\mu+1)}{3} G^{\frac{2\mu+5}{3}} H^{-(\mu+1)(\frac{1}{\mu}+\frac{2}{3})} K_{1,1} \quad \text{and} \quad \gamma = \frac{2\mu+5}{3} G^{\frac{2\mu+2}{3}} H^{-\frac{(2\mu+2)}{3}} K_{1,1}\,,$$

which proves (3.20).

In the case $\mu = 0$ the corresponding Euler–Lagrange equation reads

$$\frac{1}{2}|v|^2 + \lambda\varphi + \beta\chi = \gamma, \tag{3.34}$$

where λ, β, γ are the Lagrange multipliers and the functions φ and χ are defined by

$$\varphi(v) = \begin{cases} 0 & \text{if } z_{G,H}(v) < H\,, \\ \geq 0 & \text{if } z_{G,H}(v) = H\,, \end{cases} \qquad \chi(v) = \begin{cases} 0 & \text{if } z_{G,H}(v) > 0\,, \\ \geq 0 & \text{if } z_{G,H}(v) = 0\,. \end{cases}$$

Then, (3.34) implies that $\{v \in \mathbb{R}^3 \ ; \ 0 < z_{G,H}(v) < H\}$ has null measure in $\mathbb{R}^3$, therefore $z_{G,H} = H \quad a.e. \quad Supp(z_{G,H})$. We finally need to determine $Supp(z_G)$ in order to give an explicit expression for this function. The symmetric nonincreasing character of $z_{G,H}$ determines that $Supp(z_{G,H})$ must coincide with the ball in $\mathbb{R}^3$ with radius $\left(\frac{3G}{4\pi H}\right)^{1/3}$, concluding (3.21). □

Analysis of the reduced problem

In this section we study the minimization problem (3.16). We adapt the techniques employed in [90] to deal with reduced equivalent problems to those concerning the Energy–Casimir functional. These ideas are based on concentration–compactness arguments, where scaling techniques are relevant for proving that loss of mass at infinity does not occur. In our case we are able to prove an equivalent minimization and compactness result, although the scaling arguments with respect to the parameter M are not appropriate at first sight in (3.16). We have

Theorem 3.4. Let us consider $M > 0$, $J > 0$ and $\mu \in [0, 7/2)$. Let $\{\rho_n\}$ be a minimizing sequence for the problem (3.16) determined by μ, M and J. Then, there exists a sequence of shift vectors $\{a_n\} \in \mathbb{R}^3$ and a subsequence of $\{\rho_n\}$, again denoted by $\{\rho_n\}$, such that for any $\epsilon > 0$ there exists $R > 0$ such that

$$\int_{a_n+B_R} \rho_n(x)\,dx \geq M - \epsilon, \quad n \in \mathbb{N},$$

$$\rho_n(\cdot + a_n) \to \rho_0 \text{ strongly in } \mathrm{L}^{1+\frac{2}{2\mu+3}}(\mathbb{R}^3), \quad n \to \infty,$$

and
$$\int_{B_R} \rho_0 \geq M - \epsilon\,.$$
Finally,
$$\nabla \phi_{T\rho_n} \to \nabla \phi_{\rho_0} \quad \text{strongly in } \mathrm{L}^2(\mathbb{R}^3), \quad n \to \infty, \tag{3.35}$$
and ρ_0 is a minimizer for (3.16). The set of minimizers is determined by $\{\rho_0(\cdot - y)\,;\; y \in \mathbb{R}^3\}$, where ρ_0 is the unique spherically symmetric minimizer. Any minimizer verifies
$$\rho_0(x)^{\frac{2}{2\mu+3}} = \frac{3}{2\mu+5} \frac{J^{\frac{2(\mu+1)}{2\mu+3}}}{K^{\frac{3}{2\mu+3}}} (-R^{\mu}_{M,J})^{\frac{-2\mu}{2\mu+3}} \left(\frac{7-2\mu}{3} \frac{R^{\mu}_{M,J}}{M} - \phi_{\rho_0}(x) \right)_+ \tag{3.36}$$
and
$$\int_{\mathbb{R}^3} \rho_0(x)^{\frac{2\mu+5}{2\mu+3}}\, dx = \frac{(-R^{\mu}_{M,J})^{\frac{3}{2\mu+3}} J^{\frac{2\mu+2}{2\mu+3}}}{K^{\frac{3}{2\mu+3}}}\,. \tag{3.37}$$

The proof of Theorem 3.4 is a consequence of several intermediate results. The following lemma provides some properties of $R^{\mu}_{M,J}$. Let us remark that using Corollary 3.3 these properties are also satisfied by $I^{\mu}_{M,J}$.

Lemma 3.2. Let $\mu \in [0, 7/2)$ and M, J be positive constants. Then, the infimum values of (3.9) and (3.16) verify

i) $I^{\mu}_{M,J} = R^{\mu}_{M,J} = M^{\frac{7}{3} - \frac{2\mu}{3}} J^{\frac{2(\mu+1)}{3}} I^{\mu}_{1,1}$,

ii) $-\infty < I^{\mu}_{M,J} = R^{\mu}_{M,J} < 0\,.$

Furthermore, if f_μ is a minimizer for $I^{\mu}_{1,1}$ then $I^{\mu}_{M,J}$ is achieved by $\bar{f}_\mu(x,v) := af_\mu(bx, cv)$, where $a = J^{\mu+1}/M^{\mu}$, $b = J^{\frac{2(\mu+1)}{3}}/M^{\frac{2\mu-1}{3}}$ and $c = M^{\frac{\mu-2}{3}}/J^{\frac{\mu+1}{3}}$. The relation between the minimizers is also satisfied for $R^{\mu}_{M,J}$.

Proof. The proof of *i)* is based on the scaling $\bar{f}(x,v) := af(bx, cv)$. If a, b and c are defined as in Lemma 3.2, then $E(\bar{f}) = M^{\frac{7}{3} - \frac{2\mu}{3}} J^{\frac{2(\mu+1)}{3}} E(f)$, $\|\bar{f}\|_{\mathrm{L}^1(\mathbb{R}^6)} = M \|f\|_{\mathrm{L}^1(\mathbb{R}^6)}$ and $\|\bar{f}\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} = J \|f\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)}$. *i)* is deduced from simple arguments.

To prove *ii)*, let $\rho \in \mathrm{L}^1(\mathbb{R}^3) \cap \mathrm{L}^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)$. By the Hölder and Hardy–Littlewood–Sobolev inequalities we have
$$\|\rho\|_{\mathrm{L}^{\frac{6}{5}}(\mathbb{R}^3)} \leq \|\rho\|^{\frac{7-2\mu}{12}}_{\mathrm{L}^1(\mathbb{R}^3)} \|\rho\|^{\frac{2\mu+5}{12}}_{\mathrm{L}^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)}$$
and
$$\frac{1}{2} \int_{\mathbb{R}^6} \frac{\rho(x)\rho(y)}{|x-y|}\, dxdy \leq C \|\rho\|^2_{\mathrm{L}^{\frac{6}{5}}(\mathbb{R}^3)}\,. \tag{3.38}$$

Combining both estimates we find

$$\frac{K}{J^{\frac{2(\mu+1)}{3}} M^{\frac{7-2\mu}{3}}} \|\rho\|^4_{\mathrm{L}^{\frac{6}{5}}(\mathbb{R}^3)} - \frac{1}{2C}\|\rho\|^2_{\mathrm{L}^{\frac{6}{5}}(\mathbb{R}^3)} \leq E^{\mu}_{M,J}(\rho) \tag{3.39}$$

for any function $\rho \in \mathrm{L}^1_+(\mathbb{R}^3, M) \cap \mathrm{L}^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)$ defined in problem (3.16). Thus, we obtain $R^{\mu}_{M,J} > -\infty$ because the left–hand side of (3.39) can be seen as a second degree polynomial in the variable $\|\rho\|^2_{\mathrm{L}^{\frac{6}{5}}(\mathbb{R}^3)}$. To conclude, we have to prove $R^{\mu}_{M,J} < 0$. Consider the scaled function $\bar{\rho}(x) = b^3\rho(bx)$, where b is a positive constant. Clearly, $\bar{\rho}$ verifies $\|\bar{\rho}\|_{\mathrm{L}^1(\mathbb{R}^3)} = \|\rho\|_{\mathrm{L}^1(\mathbb{R}^3)} = M$ and

$$E^{\mu}_J(\bar{\rho}) = b^2 K \frac{\left(\int_{\mathbb{R}^3} \rho(x)^{\frac{2\mu+5}{2\mu+3}}\,dx\right)^{\frac{2\mu+3}{3}}}{J^{\frac{2(\mu+1)}{3}}} - \frac{1}{2} b \int_{\mathbb{R}^6} \frac{\rho(x)\rho(y)}{|x-y|}\,dxdy\,.$$

By choosing b small enough we find a scaled function such that $E^{\mu}_J(\bar{\rho}) < 0$, which implies $R^{\mu}_{M,J} < 0$. This ends the proof. □

The boundedness of any minimizing sequence will be relevant for the miniminization argument. This is what we state in the following result.

Corollary 3.1. Any minimizing sequence for (3.16) is uniformly bounded in $\mathrm{L}^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)$.

Proof. Let $\{\rho_n\}$ be a minimizing sequence. (3.39) implies that any minimizing sequence is uniformly bounded in $\mathrm{L}^{\frac{6}{5}}(\mathbb{R}^3)$. Then, by using (3.38) we also deduce that

$$\frac{1}{2}\int_{\mathbb{R}^6} \frac{\rho_n(x)\rho_n(y)}{|x-y|}\,dxdy$$

is uniformly bounded. Finally, the definition of E^{μ}_J allows to conclude the proof. □

The proof of Theorem 3.4 is also based on the fact that the minimizing sequence cannot vanish, as well as on the well–known compactness properties of the solution of the Poisson equation. Our next result shows an estimate which will confirm that the minimizing sequence does not vanish. Also, Lemma 3.4 concerns the compactness properties of the solution of the Poisson equation. Although, these results were already proved in [90], we write them here again for self–consistency (see [90] for more details).

Lemma 3.3. Let $\rho \in L^1_+(\mathbb{R}^3, M) \cap L^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)$. Then, for all $R > 1$ the inequality

$$\sup\left\{\int_{B(a,R)} \rho(x)\,dx\,;\; a \in \mathbb{R}^3\right\} \;\geq\; \frac{1}{RM}\left(\int_{\mathbb{R}^6} \frac{\rho(x)\rho(y)}{|x-y|}\,dx\,dy - \frac{M^2}{R} - C\frac{\|\rho\|^2_{L^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)}}{R^{\frac{(7-2\mu)}{(2\mu+5)}}}\right)$$

holds, where C is a constant and $B(a,R)$ denotes the ball centered in a with radius R.

Corollary 3.2. Let ρ_n be a minimizing sequence for (3.16). Then, there exist δ_0, R_0, $n_0 \in \mathbb{N}$ and a sequence of shift vectors $a_n \in \mathbb{R}^3$ such that

$$\int_{B_{(a_n,R)}} \rho_n(x)\,dx \geq \delta_0, \quad n > n_0,\; R > R_0\,.$$

Lemma 3.4. Let $\{\rho_n\}$ be a bounded sequence in $L^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)$ such that

$$\rho_n \rightharpoonup \rho \text{ weakly in } L^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)\,.$$

We have

i) For any $R > 0$,

$$\nabla\phi_{\chi_{B_{(0,R)}}\rho_n} \to \phi_{\chi_{B_{(0,R)}}\rho} \text{ strongly in } L(\mathbb{R}^3)\,.$$

Here, $\chi_{B_{(0,R)}}$ denotes the characteristic function in the ball $B_{(0,R)}$.

ii) If in addition $\{\rho_n\}$ is bounded in $L^1(\mathbb{R}^3)$, $\rho \in L^1(\mathbb{R}^3)$, and for any $\epsilon > 0$ there exist $R > 0$ and $n_0 \in \mathbb{N}$ such that

$$\int_{|x|>R} |\rho_n(x)|\,dx \leq \epsilon, \quad \forall n \geq n_0\,,$$

then

$$\nabla\phi_{\rho_n} \to \phi_\rho \text{ strongly in } L^2(\mathbb{R}^3)\,.$$

Proof of Theorem 3.4. We first deal with the existence of a minimimum. The main idea is to prove that any minimizing sequence $\{\rho_n\}$ for (3.16) has a subsequence (up to translations) which is under the hypotheses of Lemma 3.4.

The boundedness of ρ_n is deduced from Corollary 3.1. Now, we prove that for all ϵ there exist R and $a_n \in \mathbb{R}^3$, $\forall n \in \mathbb{N}$, such that

$$\int_{\mathbb{R}^3 - B(a_n,R)} \rho_n(x)\,dx \leq \epsilon\,. \tag{3.40}$$

Let $\rho \in \mathrm{L}^1_+(\mathbb{R}^3, M) \cap \mathrm{L}^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)$. Define ρ_i $i = 1, 2, 3$ as

$$\rho = \chi_{B(0,R_1)}\rho + \chi_{B(0,R_2)-B(0,R_1)}\rho + \chi_{\mathbb{R}^3-B(0,R_2)}\rho = \rho_1 + \rho_2 + \rho_3\,,$$

where χ_Ω is the characteristic function of the set Ω. Setting

$$\alpha_i = \frac{\int_{\mathbb{R}^3} \rho_i(x)^{\frac{2\mu+5}{2\mu+3}}\,dx}{\int_{\mathbb{R}^3} \rho(x)^{\frac{2\mu+5}{2\mu+3}}\,dx}\,, \quad \beta_i = \frac{\int_{\mathbb{R}^3} \rho_i(x)\,dx}{\int_{\mathbb{R}^3} \rho(x)\,dx} \quad \text{and} \quad F_{i,j} = \int_{\mathbb{R}^6} \frac{\rho_i(x)\rho_j(y)}{|x-y|}\,dxdy$$

for $i, j = 1,\ 2,\ 3$, we have

$$\begin{aligned} E^\mu_J(\rho) &= \sum_{i=1}^3 K \frac{\left(\int_{\mathbb{R}^3} \rho_i(x)^{\frac{2\mu+5}{2\mu+3}}\,dx\right)^{\frac{2\mu+3}{3}}}{\left(\alpha_i^{\frac{\mu}{\mu+1}} J\right)^{\frac{2(\mu+1)}{3}}} + 2F_{i,i} - F_{1,2} - F_{2,3} - F_{1,3} \\ &= \sum_{i=1}^3 E^\mu_{\alpha_i^{\frac{\mu}{\mu+1}} J}(\rho_i) - F_{1,2} - F_{2,3} - F_{1,3} \\ &\geq \sum_{i=1}^3 R^\mu_{\beta_i M, \alpha_i^{\frac{\mu}{\mu+1}} J} - F_{1,2} - F_{2,3} - F_{1,3}. \end{aligned}$$

Now, from Lemma 3.2

$$\begin{aligned} E^\mu_J(\rho) &\geq \left(\sum_{i=1}^3 (\beta_i M)^{\frac{7}{3}-\frac{2\mu}{3}} \left(\alpha_i^{\frac{\mu}{\mu+1}} J\right)^{\frac{2(\mu+1)}{3}} I^\mu_{1,1}\right) - F_{1,2} - F_{2,3} - F_{1,3} \\ &\geq M^{\frac{7}{3}-\frac{2\mu}{3}} J^{\frac{2(\mu+1)}{3}} I^\mu_{1,1} \left(\sum_{i=1}^3 (\beta_i^{\frac{7}{3}})^{1-\frac{2\mu}{7}} \alpha_i^{\frac{2\mu}{3}}\right) - F_{1,2} - F_{2,3} - F_{1,3}\,. \end{aligned}$$

By Jensen's inequality we have

$$\begin{aligned} E^\mu_J(\rho) &\geq R^\mu_{M,J} \left(\sum_{i=1}^3 \alpha_i\right)^{\frac{2\mu}{3}} \left(\sum_{i=1}^3 \beta_i^{\frac{7}{3}}\right)^{1-\frac{2\mu}{7}} - F_{1,2} - F_{2,3} - F_{1,3} \\ &\geq R^\mu_{M,J} \left(\sum_{i=1}^3 \beta_i^{\frac{7}{3}}\right)^{1-\frac{2\mu}{7}} - F_{1,2} - F_{2,3} - F_{1,3} \end{aligned}$$

and the estimate
$$\sum_{i=1}^{3} \beta_i^{\frac{7}{3}} \leq 1 - \frac{7}{3}(\beta_1 + \beta_2)\beta_3 \,.$$
Therefore,
$$E_J^\mu(\rho) \geq R_{M,J}^\mu \left(1 - \frac{7}{3}(\beta_1 + \beta_2)\beta_3\right)^{1-\frac{2\mu}{7}} - F_{1,2} - F_{2,3} - F_{1,3}. \tag{3.41}$$
(3.41) and Lemma 3.2 now yield
$$R_{(M,J)}^\mu - E_J^\mu(\rho) \leq R_{M,J}^\mu \left(1 - \left(1 - \frac{7}{3}(\beta_1 + \beta_2)\beta_3\right)^{1-\frac{2\mu}{7}}\right) + F_{1,2} + F_{2,3} + F_{1,3} \,.$$
The first term in the right–hand side of this expression is estimated by using the inequality
$$b^\alpha - a^\alpha \geq \alpha\, b^{\alpha-1}(b-a),$$
valid for any $a,\ b > 0$ and $0 < \alpha < 1$ ([52] Th. 41). In the same way, as proposed in [90], for $R_2 > 2R_1$ we can estimate $F_{1,3}$ as follows
$$F_{1,3} \leq C/R_2.$$
We also have
$$F_{1,2} + F_{2,3} \leq C\|\rho\|_{\mathrm{L}^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)}^{\frac{2\mu+5}{6}} \|\nabla\phi_{\rho_2}\|_{\mathrm{L}^2(\mathbb{R}^3)} \leq C\|\nabla\phi_{\rho_2}\|_{\mathrm{L}^2(\mathbb{R}^3)} \,.$$
Thus, ρ verifies
$$R_{M,J}^\mu - E_J^\mu(\rho) \leq R_{M,J}^\mu \left(\frac{7}{3} - \frac{2\mu}{3}\right)(\beta_1 + \beta_2)\beta_3 + \frac{C}{R_2} + C\|\nabla\phi_{\rho_2}\|_{\mathrm{L}^2(\mathbb{R}^3)} \,. \tag{3.42}$$
Corollary 3.2 claims the existence of a sequence of shift vectors $a_n \in \mathbb{R}^3$ such that
$$\int_{B_{(0,R)}} \rho_n(x - a_n)\, dx \geq \delta_0, \quad n > n_0,\ R > R_0 \,,$$
for some $\delta_0,\ R_0,\ n_0 \in \mathbb{N}$. The sequence $\tilde{\rho}_n(\cdot) = \rho_n(\cdot - a_n)$ also minimizes (3.16) due to the translation invariance of E_J^μ. From the boundedness of that sequence in $\mathrm{L}^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)$, we get the existence of a weakly convergent subsequence
$$\tilde{\rho}_n(\cdot) = \rho_n(\cdot - a_n) \rightharpoonup \rho_0 \text{ weakly in } \mathrm{L}^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3) \,. \tag{3.43}$$

Let $\epsilon > 0$. Now we apply (3.42) to any $\tilde{\rho}_n$ with $R_1 > R_0$ and find

$$-R^{\mu}_{M,J}\frac{7-2\mu}{3}\frac{\delta_0}{M}\beta_3 \leq \frac{C}{R_2} + C\|\nabla\phi_{\tilde{\rho}_{n,2}}\|_{\mathrm{L}^2(\mathbb{R}^3)} + E^{\mu}_J(\tilde{\rho}_n) - R^{\mu}_{M,J}\,, \qquad (3.44)$$

for all $n > n_0$. (3.43) and Lemma 3.4 *i)* allow to choose R_1 sufficiently large to obtain $C\|\nabla\phi_{\tilde{\rho}_{n,2}}\|_{\mathrm{L}^2(\mathbb{R}^3)} \leq \epsilon/4$, $\forall n > n_1 > n_0$. Now, we fix R_1 such that $R_2 > 2R_1$ and $R_2 > 4C/\epsilon$. Finally, from the minimizing character of $\tilde{\rho}_n$, there exists $n_2 \in \mathbb{N}$, $n_2 \geq n_1$, such that $E^{\mu}_J(\tilde{\rho}_n) - R^{\mu}_{(M,J)} \leq \epsilon/4\,, \quad \forall n > n_2$. Hence, we conclude that

$$\frac{7-2\mu}{3}\frac{\delta_0}{M}\beta_3 \leq \epsilon \quad \forall n > n_2\,,$$

which ends the proof of (3.40). The boundedness of $\tilde{\rho}_n$ in $\mathrm{L}^1(\mathbb{R}^3)$ and Lemma 3.4 *ii)* lead to

$$\nabla\phi_{\tilde{\rho}_n} \to \phi_{\rho_0} \text{ strongly in } \mathrm{L}^2(\mathbb{R}^3)\,.$$

This convergence property joint with (3.43) and the minimizing character of $\tilde{\rho}_n$ give that $\|\tilde{\rho}_n\|_{\mathrm{L}^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)}$ decreases towards $\|\rho_0\|_{\mathrm{L}^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)}$ as $n \to \infty$. Then, $\tilde{\rho}_n$ converges strongly in $\mathrm{L}^{\frac{2\mu+5}{2\mu+3}}(\mathbb{R}^3)$ to ρ and this function is a minimizer.

Once we have the existence of a minimum we analyze the properties of the minimizers. By scaling arguments we deduce

$$R^{\mu}_{M,J} = E^{\mu}_J(\bar{\rho}_0) = -K\frac{\left(\int_{\mathbb{R}^3}\rho_0(x)^{\frac{2\mu+5}{2\mu+3}}\,dx\right)^{\frac{2\mu+3}{3}}}{J^{\frac{2(\mu+1)}{3}}} = \int_{\mathbb{R}^6}\frac{\rho_0(x)\rho_0(y)}{|x-y|}\,dxdy\,, \qquad (3.45)$$

which proves (3.37). Let $\bar{\rho_0}(x) = b^3\rho_0(bx)$, where b is a positive constant. Then, $\bar{\rho_0} \in \mathrm{L}^1_+(\mathbb{R}^3, M)$ and

$$E^{\mu}_J(\bar{\rho_0}) = b^2K\frac{\left(\int_{\mathbb{R}^3}\rho_0(x)^{\frac{2\mu+5}{2\mu+3}}\,dx\right)^{\frac{2\mu+3}{3}}}{J^{\frac{2(\mu+1)}{3}}} - b\frac{1}{2}\int_{\mathbb{R}^6}\frac{\rho_0(x)\rho_0(y)}{|x-y|}\,dxdy\,.$$

Since ρ_0 is a minimizer, (3.45) holds.

The Euler–Lagrange equation for any minimizer ρ_0 is given by

$$\frac{2\mu+5}{3}\frac{K}{J^{\frac{2\mu+2}{3}}}\left(\int_{\mathbb{R}^3}\rho_0(x)^{\frac{2\mu+5}{2\mu+3}}\,dx\right)^{\frac{2\mu}{3}}\rho_0(x)^{\frac{2}{2\mu+3}} + \phi_{\rho_0} + \lambda\chi = \beta\,, \qquad (3.46)$$

where λ and β are the Lagrange multipliers corresponding to the positivity and the mass constraints respectively, and where

$$\chi(x) = \begin{cases} 0 & \text{if } \rho_0(x) > 0 \\ \geq 0 & \text{if } \rho_0(x) = 0\,. \end{cases}$$

By multiplying (3.46) by ρ_0 and integrating we find

$$\left(\int_{\mathbb{R}^3} \rho_n(x)^{\frac{2\mu+5}{2\mu+3}}\, dx\right)^{\frac{2\mu+3}{3}} + \int_{\mathbb{R}^6} \frac{\rho_0(x)\rho_0(y)}{|x-y|}\, dxdy = \beta M\,. \tag{3.47}$$

Combining (3.47) and (3.45) we deduce that $\beta = \left(\frac{7-2\mu}{3}\right)\frac{R^{\mu}_{M,J}}{M} < 0$. (3.46) and the fact that $\lim_{|x|\to\infty}\phi_{\rho_0^*} = 0$ imply that $Supp(\rho_0) = \{x\,;\beta - \phi_{\rho_0} \geq 0\}$. As consequence, we deduce (3.36).

Now we will determine the set of minimimizers of (3.16). Riesz's Theorem (see [74], Theorem 3.7) applies to guarantee that the symmetric rearrangement ρ_0^* of any minimizer ρ_0 is also a minimizer. Now, we prove that there exists a unique spherically symmetric minimizer for (3.16). By Lemma 3.2, we can equivalently write (3.36) as

$$\rho_0^*(r := |x|) = a\Big(b - \phi_{\rho_0^*}(r)\Big)_+^{\mu+3/2},$$

where

$$a = \left(\frac{3}{2\mu+5}\right)^{\frac{2\mu+3}{2}} J^{\frac{(\mu+1)(2\mu+3)}{3}} M^{\frac{2\mu(7-2\mu)}{3(2\mu+3)}} K^{-1}(-I^{\mu}_{1,1})^{\mu}$$

and

$$b = \left(\frac{7-2\mu}{3}\right) J^{\frac{2(\mu+1)}{3}} M^{\frac{4-2\mu}{3}} I^{\mu}_{1,J}\,.$$

Note that $\phi_{\rho_0^*}$ is radial since ρ_0^* is radial. Then, $\phi_{\rho_0^*}$ is a solution to the Poisson equation (3.3) in radial coordinates

$$\frac{1}{r^2}(r^2\phi_{\rho_0^*}(r)')' = a\Big(b - \phi_{\rho_0^*}(r)\Big)_+^{\mu+3/2}.$$

Equivalently, by setting $y(r) = (b - \phi_{\rho_0^*}(a^{\frac{-1}{2}}r))$ we obtain

$$(r^2 y(r)')' = -r^2 (y(r))_+^{\mu+3/2}.$$

Thus, $y(r)$ is the positive part of the solution to the Emden–Folder equation. The existence and uniqueness of solutions of the initial value problem associated with this equation are well known. Actually, it is clear that

$$y(r) = \beta^{\frac{2}{\mu+1/2}}\varphi(\beta r)\,,$$

where β is defined by the initial condition $\lim_{r\to 0} y(r) = \alpha$. In our case, β is determined by the mass constraint since

$$M = 4\pi\int_r \rho_0^*(r)\, dr = 4\pi\int_r \Big(b - \phi_{\rho_0^*}(r)\Big)_+^{\mu+3/2} dr = 4\pi a^{\frac{-1}{2}}\int_r \Big(y(r)\Big)_+^{\mu+3/2} dr\,.$$

In particular, uniqueness enssures that ρ_0^* is unique. Therefore, the set of minimizers of (3.16) is the orbit of the unique spherical symmetric minimizer because E_J^μ is invariant by translations. This concludes the proof of Theorem 3.4. □

Minimizing argument: relative compactness

In this section we propose a new minimizing argument for the problems set in (3.9) which allows to establish that any minimizing sequence is relatively compact in $\mathrm{L}^1(\mathbb{R}^6)$ up to spatial translations. This argument is based on the sequence of equivalent problems introduced in Theorems 3.3 and 3.4

Proof of Theorem 3.2. For simplicity, along the proof we shall denote all the subsequences with the same name of the original sequence. Let us consider an arbitrary minimizing sequence f_n for the problem (3.9). Then, Theorem 3.3 states that $\rho_n(\cdot) = \int_{\mathbb{R}^3} f_n(\cdot, v)\, dv$ is a minimizing sequence for (3.16). Applying Theorem 3.4 to ρ_n we obtain the existence of a subsequence of f_n and $a_n \in \mathbb{R}^3$ such that $\bar{f}_n(\cdot,\cdot) = f(\cdot - a_n, \cdot)$ and $\bar{\rho}_n(\cdot) = \rho(\cdot - a_n)$ verify that there exists $R > 0$ with

$$\int_{B_R} \bar{\rho}_n(x)\, dx \geq M - \epsilon, \quad n \in \mathbb{N}, \tag{3.48}$$

$$\bar{\rho}_n \rightharpoonup \rho_{M,J} \text{ weakly in } \mathrm{L}^{1+\frac{2}{2\mu+3}}(\mathbb{R}^3), \quad n \to \infty, \tag{3.49}$$

for all $\epsilon > 0$, where $\rho_{M,J}$ is a minimizer of (3.16) such that

$$\int_{B_R} \rho_{M,J} \geq M - \epsilon\,. \tag{3.50}$$

In addition, Theorem 3.4 implies

$$\nabla\phi_{\bar{\rho}_n} \to \nabla\phi_{\rho_{M,J}} \quad \text{strongly in } \mathrm{L}^2(\mathbb{R}^3), \quad n \to \infty\,. \tag{3.51}$$

The sequence $\bar{f}_n$ is also a minimizing sequence for (3.9) because the L^p norms and the total energy functional are invariant under space translations. Then, by using (3.51) we easily deduce that $E_{KIN}(\bar{f}_n)$ is uniformly bounded in n. Now, we are in a position to claim that $\bar{f}_n$ satisfies the hypotheses of the Dunford–Pettis theorem:

i) $\{\bar{f}_n\}_{n\in\mathbf{N}}$ is bounded in $\mathrm{L}^1(\mathbb{R}^6)$.

ii) Let $A \in \mathbb{R}^6$ be a measurable set. Then, there is no concentration in A since
$$\int_A \bar{f}_n \, dxdv \leq \|\bar{f}_n\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} |A|^{\mu+1} \, .$$

iii) As a consequence of (3.48) there is no vanishing:
$$\int_{\{|x|>R_1\}\times\{|v|>R_2\}} \bar{f}_n \, dxdv \leq \int_{|x|>R_1} \bar{\rho}_n \, dx \leq \epsilon_{(R_1)} \, .$$

Hence, we can assume that there exists a function f_M such that
$$\bar{f}_n \rightharpoonup f_{M,J} \text{ weakly in } \mathrm{L}^1(\mathbb{R}^6) \, . \tag{3.52}$$

In order to obtain a relationship between $f_{M,J}$ and $\rho_{M,J}$ we have to check that $\int_{\mathbb{R}^3} f_{M,J}(\cdot, v) \, dv = \rho_{M,J}$. Let us consider $\phi \in \mathrm{L}^\infty(\mathbb{R}^3)$. Then,
$$\begin{aligned} \left| \int_{\mathbb{R}^6} f_{M,J}(x,v)\phi(x) \, dxdv - \int_{\mathbb{R}^3} \rho_{M,J}(x)\phi(x) \, dx \right| \leq & \\ \leq \left| \int_{\mathbb{R}^6} f_{M,J}(x,v)\phi(x) - \int_{\mathbb{R}^6} \bar{f}_n(x,v)\phi(x) \right| & \\ + \left| \int_{\mathbb{R}^3} \bar{\rho}_n(x)\phi(x) - \int_{\mathbb{R}^3} \rho_{M,J}(x)\phi(x) \right| & \\ \leq I_1 + I_2. & \end{aligned} \tag{3.53}$$

Clearly, I_1 tends to 0 according to the weak convergence of $\bar{f}_n$ to $f_{M,J}$. To prove that I_2 is also small, as n goes to ∞, we split it into two parts. Let $\epsilon > 0$ and R be such that (3.48) and (3.50) are verified. Then,
$$I_2 \leq \left| \int_{|x|\leq R} \bar{\rho}_n \phi - \int_{|x|\leq R} \rho_{M,J}\phi \right| + \left| \int_{|x|\geq R} \bar{\rho}_n \phi - \int_{|x|\geq R} \rho_{M,J}\phi \right|$$

Now, an application of (3.49) shows that the first term in the right–hand side of this inequality goes to 0 as $n \to \infty$ while the second one is bounded by $2\epsilon\|\phi\|_{\mathrm{L}^\infty(\mathbb{R}^3)}$. These estimates imply that $\int_{\mathbb{R}^3} f_{M,J}(\cdot, v) \, dv = \rho_{M,J}$ in $\mathrm{L}^1(\mathbb{R}^3)$.

It can be also obtained the existence of a subsequence such that
$$\begin{aligned} &\bar{f}_n \rightharpoonup f_{M,J} \quad \text{weakly in } \mathrm{L}^{1+\frac{1}{\mu}}(\mathbb{R}^6) \, , &&\text{for } \mu \in (0, 7/2) \, , \\ &\bar{f}_n \overset{*}{\rightharpoonup} f_{M,J} \quad \text{weak-* in } \mathrm{L}^\infty(\mathbb{R}^6) \, , &&\text{for } \mu = 0 \, . \end{aligned} \tag{3.54}$$

To deduce (3.54) we use the relative compactness arguments in L^p and the fact that $\bar{f}_n$ is bounded in $\mathrm{L}^{1+1/\mu}$. Then, we can extract subsequences of $\{f_n\}$ converging to some function g. Finally, by using the following inequalities
$$\left| \int_{\mathbb{R}^6} (f_{M,J} - g)\varphi \, dxdv \right| \leq \left| \int_{\mathbb{R}^6} (f_{M,J} - \bar{f}_n)\varphi \, dxdv \right| + \left| \int_{\mathbb{R}^6} (\bar{f}_n - g)\varphi \, dxdv \right|$$

for every continuous function φ with compact support, we conclude that $g = f_{M,J}$ a.e. in $\mathbb{R}^6$.

Once we have proved (3.54), we may claim that $f_{M,J}$ is a minimum of (3.9). To this aim, we distinguish two different cases depending on the value of μ:

1) $\mu \in (0, 7/2)$: Combining (3.50), (3.52) and (3.54) we get

$$\|f_{M,J}\|_{\mathrm{L}^1(\mathbb{R}^6)} = M\,, \quad E_{KIN}(f_{M,J}) \leq E_{KIN}(\bar{f}_n)$$

and

$$\|f_{M,J}\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} \leq \|\bar{f}_n\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)}\,.$$

These estimates together with (3.51) allow to conclude that $f_{M,J}$ is a minimizer for the problem

$$\inf\{E(f)\,;\ f \in \mathrm{L}^1_+(\mathbb{R}^6, M),\ \|f\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} \leq J\}\,.$$

The scaling property stated in Lemma 3.2 *i* allows to enssure that the minimum of this problem coincides with the minimum for (3.9), since any minimizer is in $\mathrm{L}^{1+1/\mu}_+(\mathbb{R}^3, J)$. In particular we have that

$$J = \lim_{n\to\infty} \|\bar{f}\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} = \|f_{M,J}\|_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)}\,.$$

By the uniform convexity of $\mathrm{L}^{1+1/\mu}$ (note that $\mu \in (0, 7/2)$) the above identity and (3.54) imply the strong convergence in $\mathrm{L}^{1+1/\mu}$ of $\bar{f}_n$ to $f_{M,J}$. Consequently, a subsequence of $\bar{f}_n$ exists such that

$$\bar{f}_n(x,v) \to f_{M,J}(x,v) \quad a.e. \text{ in } \mathbb{R}^6\,. \tag{3.55}$$

By standard compactness results we can conclude that (3.52) and (3.55) give the strong convergence in L^1 of a subsequence of $\bar{f}_n$ to $f_{M,J}$. This justifies the notation $f_{M,J}$ and ends this part of the proof.

2) $\mu = 0$: Similarly, (3.50), (3.52) and (3.54) imply

$$\|f_{M,J}\|_{\mathrm{L}^1(\mathbb{R}^6)} = M\,,\ \|f_{M,J}\|_{\mathrm{L}^\infty(\mathbb{R}^6)} \leq 1 \text{ and } E_{KIN}(f_{M,J}) \leq E_{KIN}(\bar{f}_n)\,.$$

These estimates together with (3.51) imply that f_M is a minimizer for (3.7). Thus, by Proposition 3.1 $f_{M,J}$ is defined by (3.14) with associated density function $\rho_{M,J}$. Also, it is well known that $f_{M,J}$ has compact support (see Chapter 2). Since $f_{M,J} \equiv J$ on its support and $\|\bar{f}_n\|_{\mathrm{L}^\infty(\mathbb{R}^6)} \leq J$, we have $f_M - \bar{f}_n \geq 0$ on $Supp(f_{M,J})$ and consequently

$$\begin{aligned}\|f_{M,J} - \bar{f}_n\|_{\mathrm{L}^1(\mathbb{R}^6)} &= \int_{Supp(f_{M,J})} f_{M,J} - \bar{f}_n\,dxdv + \int_{\mathbb{R}^6 - Supp(f_{M,J})} \bar{f}_n\,dxdv \\ &= 2M - 2\int_{Supp(f_{M,J})} \bar{f}_n\,dxdv\,.\end{aligned} \tag{3.56}$$

This estimate clearly goes to 0 as $n \to \infty$ by using (3.52). This concludes the proof of Theorem 3.2. $\square$

Remark. In the case $\mu = 0$ the relative compactness cannot be deduced in $L^\infty(\mathbb{R}^3)$. Let us consider a particular minimizing sequence for the problem (3.7) defined by $f_n(x,v) = f_{M,J}(\frac{n}{n+1}x, \frac{n+1}{n}v)$, $n \in \mathbf{N}$, where f_M is a minimum of (3.7) given by Theorem 3.2. It can be easily proved that $f_n \to f_{M,J}$ in $L^1(\mathbb{R}^6)$ as $n \to \infty$, while

$$\|f_n(x-k,v) - f_{M,J}(x,v)\|_{L^\infty(\mathbb{R}^6)} = 1\,, \quad \forall n \in \mathbf{N},\ \forall k \in \mathbb{R}^3\,.$$

Remark. Combining (3.14), (3.15), Proposition 3.1, Theorem 3.4 and Lemma 3.2 we get that the polytrope ν_μ in $\Gamma^\mu_{M,J}$ is given by

$$\nu_0(x,v) = \begin{cases} J & \text{if } \frac{7}{3}M^{\frac{4}{3}}J^{\frac{2}{3}} - \phi_{\nu_0}(x) \geq \frac{|v|^2}{2} \\ 0 & \text{elsewhere} \end{cases}\,,$$

for $\mu = 0$ and

$$\tilde{\nu}_\mu(x,v) = \left(\frac{3}{2(\mu+1)}\frac{J^{\frac{(\mu+1)(3-2\mu)}{3\mu}}}{M^{\frac{7-2\mu}{3}}(-I^\mu_{1,1})}\right)^\mu \left(\frac{7-2\mu}{3}M^{\frac{4-2\mu}{3}}J^{\frac{2(\mu+1)}{3}}I^\mu_{1,1} - \phi_{\nu_\mu}(x) - \frac{|v|^2}{2}\right)^\mu_+$$

for $\mu \in (0, 7/2)$. This clearly shows the relation between the parameters c and E_0 appearing in the definition of the polytrope with M and J.

Appendix: Polytropes and variational approaches

In this section we will show that the minimizing problem of the energy–Casimir functional under mass constraints:

$$C^\mu_M := \inf\left\{Q_{\mu,0}(f)\,;\ f \in L^1_+(\mathbb{R}^6, M)\right\}\,, \tag{3.57}$$

and the minimization problem of the energy functional under mass–Casimir constraints

$$E^\mu_M := \inf\{E(f)\,;\ f \in \Lambda^\mu_M\}\,, \tag{3.58}$$

can be equivalently reduced to certain problems defined by (3.9), where the parameters M and J are linked. To this aim, we basically use scaling arguments. These simple techniques also help to clarify some other questions:

- Why the technical constraint $\mu \leq 3/2$ in the Casimir minimization problem can be avoided by studying the energy minimization problem with mass–Casimir constraint?
- Why the polytropic solutions depend on two parameters c and $E_0 - \alpha$ (for fixed $\mu \in [0, 7/2]$) while the variational problems proposed in (3.57), (3.58), (3.7) depend only on one parameter?
- Can be the minimum of (3.58) reached by two functions with different orbits?

Our next result allows to read the Casimir minimization problem (3.57) in an equivalent form.

Lemma 3.5. Let $\mu \in (0, 3/2)$ and $M > 0$. Then,

$$C_M^\mu = \left(\frac{\mu}{\mu+1}\right) J_{(\mu,M)}^{1+1/\mu} + I^\mu_{M,J_{(\mu,M)}} , \tag{3.59}$$

where

$$J_{(\mu,M)} = \left(\frac{-3}{2(\mu+1)M^{\frac{7}{3}-\frac{2\mu}{3}} I^\mu_{1,1}}\right)^{\frac{3\mu}{(2\mu-3)(\mu+1)}} .$$

Furthermore, the minimizers of C_M^μ and $I^\mu_{M,J_{(\mu,M)}}$ coincide.

Proof. The proof is based on the following identities

$$\begin{aligned} C_M^\mu &= \inf\left\{\frac{\mu}{\mu+1}\int\int f^{1+1/\mu}\, dxdv + E(f)\, ;\ f \in \Gamma_M^\mu\right\} , \\ &= \inf\left\{\inf\left\{\frac{\mu}{\mu+1} J^{1+1/\mu} + E(f)\, ;\ f \in \Gamma^\mu_{M,J}\right\}\, ;\ J \in \mathbb{R}^+\right\} , \\ &= \inf\left\{\frac{\mu}{\mu+1} J^{1+1/\mu} + \inf\left\{E(f)\, ;\ f \in \Gamma^\mu_{M,J}\right\}\, ;\ J \in \mathbb{R}^+\right\} , \\ &= \inf\left\{\frac{\mu}{\mu+1} J^{1+1/\mu} + I^\mu_{M,J}\, ;\ J \in \mathbb{R}^+\right\} , \\ &= \inf\left\{\frac{\mu}{\mu+1} J^{1+1/\mu} + M^{\frac{7}{3}-\frac{2\mu}{3}} J^{\frac{2(\mu+1)}{3}} I^\mu_{1,1}\, ;\ J \in \mathbb{R}^+\right\} . \end{aligned} \tag{3.60}$$

By standard computations, we can prove that the minimum of (3.60) is reached when $J = J_{(\mu,M)}$ and, as consequence,

$$C_M^\mu = \frac{\mu}{\mu+1} J_{(\mu,M)}^{1+1/\mu} + I^\mu_{M,J_{(\mu,M)}} .$$

Then, we have reduced the problem (3.57) to a particular case of (3.9), so that we can enssure that the minimizers are the same for both problems. □

Remark. In the above sections we have proved that the minimizers for $I^{\mu}_{M,J}$ exist for $0 \leq \mu < 7/2$. However, when we are dealing with the Casimir functional we are only able to find such minimizers for $\mu < 3/2$, because (3.60) shows that C^{μ}_{M} is bounded from below if and only if this condition holds. This explains the original restrictions appearing in the literature [48, 90].

In order to avoid the artificial restriction $\mu < 3/2$, it was proposed in [49, 51] to find the polytropic solutions as minimizers for the energy functional under the mass-Casimir constraint (3.58). In our next result we prove that (3.58) is also related to (3.9).

Lemma 3.6. Let $\mu \in (0, 7/2)$ and $M > 0$. Then

$$E^{\mu}_{M} = I^{\mu}_{a_M, b_M}\,,$$

where $a_M = \frac{2M}{7}$ and $b_M = \left(\frac{2M(\mu+1)}{7}\right)^{\frac{\mu}{\mu+1}}$. Furthermore, the minimizers for both problems coincide.

Proof. Trivially, $E^{\mu}_{M} \leq I_{a_M, b_M}$ since $\Gamma_{a_M, b_M} \subset \Lambda^{\mu}_{M}$. In order to prove the reverse inequality we are going to show that any minimizer for E^{μ}_{M} (whose existence was proved in [49]) is in $\Gamma^{\mu}_{a_M, b_M}$. Let f_M be such a minimizer. The scaled functions $\bar{f}_M(x,v) := a f_M(bx, cv) \in \Lambda^{\mu}_{M}$ lead to

$$c = \frac{a^{\frac{1}{3}}}{M^{\frac{1}{3}} b}\left(a^{\frac{1}{\mu}} \frac{\mu}{\mu+1} \|f_M\|^{1+1/\mu}_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} + \left(\frac{7}{2} - \mu\right) \|f_M\|_{\mathrm{L}^1(\mathbb{R}^6)} \right)^{\frac{1}{3}}\,,$$

where a and b are positive constants. The total energy associated with the scaled function depends on the parameters a and b. Indeed,

$$\begin{aligned} E(\bar{f}_M) = {} & \frac{M^{\frac{5}{3}} b^2}{a^{\frac{2}{3}} \left(a^{\frac{1}{\mu}} \frac{\mu}{\mu+1} \|f_M\|^{1+1/\mu}_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} + \left(\frac{7}{2} - \mu\right) \|f_M\|_{\mathrm{L}^1(\mathbb{R}^6)} \right)^{\frac{5}{3}}} E_{KIN}(f_M) \\ & - \frac{M^2 b}{\left(a^{\frac{1}{\mu}} \frac{\mu}{\mu+1} \|f_M\|^{1+1/\mu}_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} + \left(\frac{7}{2} - \mu\right) \|f_M\|_{\mathrm{L}^1(\mathbb{R}^6)} \right)^{2}} E_{POT}(f_M). \end{aligned}$$

Considering the function $h : \mathbb{R}^+ \times \mathbb{R}^+ \to \mathbb{R}$ defined by $h(a,b) := E(\bar{f}_M)$ and the minimizing character of f_M we have that h admits a relative minimum in $(a,b) = (1,1)$. Then, we find

$$\frac{\partial h}{\partial a}(1,1) = 0\,, \quad \frac{\partial h}{\partial b}(1,1) = 0\,.$$

By computing both equations we obtain

$$\frac{1}{\mu+1}\|f_M\|^{1+1/\mu}_{\mathrm{L}^{1+1/\mu}(\mathbb{R}^6)} = \frac{2M}{7} \quad \text{and} \quad E_{POT}(f_M) = 2E_{KIN}(f_M)\,,$$

which concludes the proof. □

Remark. Notice that (3.58) has a unique minimizer (up to translations). This completes the results established in [51].

Remark. We also observe that Casimir minimization problems as well as energy minimization problems in mass–Casimir restricted spaces allow to study a particular subset of polytropes for which c and $E_0 - \alpha$ are connected.

The above results and the ideas developed in Chapter 2 to treat with the stability of the polytropic solution in the case $\mu = 0$ have motivated the analysis of (3.9). From previous results in Chapter 2 and [48, 49], we can ensure the existence of minimimizers for (3.9). However, we developed in this chapter a constructive argument to solve these type of problems which is based on the equivalence between (3.9) and a problem for the corresponding densities.

Chapter 4

Asymptotic decay estimates for the repulsive Schrödinger-Poisson System

Introduction

The purpose of this chapter is to improve the well–known time decay bounds for the $L^p(\mathbb{R}^3)$-norm, $p > 2$, of solutions to the Schrödinger–Poisson (SP) system in the repulsive case. As we announced in the first chapter the SP system for a wave function $\psi : \mathbb{R}^3 \times (0, \infty) \longrightarrow \mathbb{C}$ can be written as follows

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta_x \psi + V\psi, \qquad \lim_{|x|\to\infty} \psi(x,t) = 0, \tag{4.1}$$

$$\psi(x, t = 0) = \phi(x), \tag{4.2}$$

$$\Delta_x V = -\epsilon\, n, \qquad \lim_{|x|\to\infty} V(x,t) = 0, \tag{4.3}$$

where n is the charge density and $\epsilon = 1$ (repulsive case) or $\epsilon = -1$ (attractive case) depending on the type of interaction considered. (4.3) determines the self–consistent potential V originated by the charge of the particles, which can be equivalently written in integral form as

$$V(x,t) = \frac{\epsilon}{4\pi}\int_{\mathbb{R}^3} \frac{|\psi(x',t)|^2}{|x - x'|} dx'.$$

In the subsequent analysis, the Planck constant and the particle mass, $\hbar$ and m respectively, are normalized to unity for the sake of the simplicity. Throughout this chapter we shall focus on the repulsive case and make some remarks about the attractive case in the last Appendix.

The long time behaviour of solutions to the SP system has been treated in the literature by analyzing the time evolution of $\|\psi(\cdot,t)\|_{L^p(\mathbb{R}^3)}$ and the dispersion, i.e. $\||\cdot|\psi(\cdot,t)\|_{L^2(\mathbb{R}^3)}$, provided that $(1+|x|)\phi \in L^2(\mathbb{R}^3)$.

For both the single–state and the mixed–state case, time decreasing upper bounds have been deduced for the $L^p(\mathbb{R}^3)$ norms of solutions with finite dispersion with $p \in]2,6]$ (See [59, 29]). As consequence, decay upper bounds can be derived for the Coulombian potential. These estimates were deduced from the well–known pseudo–conformal law and the nonnegativeness of the potential energy in [28].

The dispersion equation as well as the fact that the total energy remains always positive in the repulsive case allow to describe the evolution of the dispersion of the solutions, which is shown to be a strictly increasing function of time and behaves like $O(t^2)$ (See [97]). We shall refer to this property as the dispersive character of the solutions.

Let us summarize the results of this chapter. In Section 2 we derive time decreasing lower bounds for the $L^p(\mathbb{R}^3)$-norm of the solutions to the SP system in the repulsive case, with $p \in]2,6]$. Our proof follows from the dispersive character of the solution. Actually, at this point it differs from the more complex arguments (See [83]). Also, our proof provides some consequences for the attractive case which are not deducible from the previous techniques developed in [83], see the Appendix for a wider discussion.

In Section 3 we obtain decreasing upper bounds for the $L^p(\mathbb{R}^3)$-norms that improve the previous results in the literature. These bounds are derived from the pseudo–conformal law and from an equivalent norm induced by the Coulomb potential energy [78]. These estimates are collected in our main result:

Theorem 4.1. Let $\phi \in H^1(\mathbb{R}^3)$ be the initial condition of the SP system such that $(1+|x|)\phi \in L^2(\mathbb{R}^3)$, and let ψ be the associated solution in the repulsive case. Then, there exist positive constants C_1, C_2 depending on $\|\phi(\cdot)\|_{L^2(\mathbb{R}^3)}$, $\||\cdot|\phi(\cdot)\|_{L^2(\mathbb{R}^3)}$, the initial total energy $E[\phi]$ and p, such that

$$\frac{C_1}{|t|^{\frac{3p-6}{2p}}} \leq \|\psi(\cdot,t)\|_{L^p(\mathbb{R}^3)} \leq \frac{C_2}{|t|^{\alpha(p)}}, \quad \forall\, |t| \geq \xi,\ \forall\, p \in [2,6]\,, \tag{4.4}$$

where $\xi > 0$, $\alpha(p) = \begin{cases} 1-\frac{2}{p}, & \text{if } p \in [2,3], \\ \frac{2}{3}-\frac{1}{p} & \text{if } p \in [3,6]\,. \end{cases}$

Remark. The lower bound obtained in this theorem is optimal. In fact in the case of small data, it was shown in [55] that the upper bound of solutions

ψ such that $\phi \in \mathrm{H}^\gamma(\mathbb{R}^3)$ and $\||x|^\gamma\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}$ is bounded with $\gamma > \frac{1}{2}$ is

$$\|\psi(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq \frac{C}{t^{\frac{3}{2}(1-\frac{2}{p})}}\,,$$

for both cases $\epsilon = \pm 1$, where $2 \leq p \leq \infty$ and C depends on $\|\phi\|_{\mathrm{H}^\gamma(\mathbb{R}^3)} + \||x|^\gamma\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}$.

Furthermore, from the pseudo–conformal law it can be deduced a finite bound for $\mathrm{L}^{q,p}$ norms, where (q,p) is an admissible pair. These functional spaces, restricted to a finite time interval, seems to be the natural spaces for the solutions we are dealing with when the existence problem is studied for initial data $\phi \in \mathrm{L}^2(\mathbb{R}^3)$ (See [28, 29]).

Finally in the last Appendix, we make some remarks about the application of these ideas to the attractive case, proving that the decay properties of the repulsive case are not possible. In this case there are stationary solutions (with constant density in time) and also nonstationary solutions with $\mathrm{L}^p(\mathbb{R}^3)$-norm bounded from below by a positive constant. The results of this chapter are collected in [98].

Lower bounds for solutions of the SP system

Lower bounds for solutions of the SP system will be deduced from the dispersion equation, which relates the position and momentum dispersion with the total energy. The total energy $E[\psi]$ associated with a smooth solution $\psi(x,t) \in \mathrm{H}^1(\mathbb{R}^3)$, defined by

$$E[\psi] = \int_{\mathbb{R}^3} \left\{ \frac{1}{2}|\nabla\psi(x,t)|^2 + \frac{1}{8\pi}\int_{\mathbb{R}^3} \frac{|\psi(x,t)|^2|\psi(x',t)|^2}{|x-x'|}\,dx' \right\} dx, \tag{4.5}$$

is one of the time-invariant quantities due to the symmetry properties of the system. The first term on the right hand-side of (4.5) represents the kinetic energy, $E_{KIN}[\psi]$, while the second term is the Coulomb potential energy $E_{POT}[\psi]$. Another important time-preserved quantity is the L^2-norm of the solutions (mass preservation). The dispersion associated with the solutions

$$\langle x^2\rangle(t) = \int_{\mathbb{R}^3} |x|^2\,|\psi(x,t)|^2\,dx\,,$$

is in general a non-bounded operator in the whole space of solutions, nevertheless R. Illner, F. Zweifel and H. Lange showed in [59] that it is well-defined for $H^1(\mathbb{R}^3)$ solutions whose initial condition satisfies $(1+|x|)\phi \in L^2(\mathbb{R}^3)$. By using the dispersion equation

$$\frac{d^2}{dt^2}\langle x^2\rangle = E_{KIN}[\psi] + E[\psi], \tag{4.6}$$

E. Ruiz Arriola and J. Soler [97] proved that the dispersion of a solution to the SP system (in the attractive or repulsive case) with positive finite energy verifies

$$C_1 t^2 \le \langle x^2\rangle(t) \le C_2 t^2, \tag{4.7}$$

where C_1, and C_2 are positive constants.

From (4.7) we deduce the following lower bound for the $L^p(\mathbb{R}^3)$-norms of the solutions.

Proposition 4.1. Let $\phi \in H^1(\mathbb{R}^3)$ the initial condition of the SP system with positive initial energy $E[\phi] > 0$ and finite dispersion $\langle x^2\rangle$. Then, the L^p-norm of the associated solution satisfies

$$\|\psi(\cdot,t)\|_{L^p(\mathbb{R}^3)} \ge \frac{C}{t^{\frac{3p-6}{2p}}}, \qquad \forall t > \xi > 0, \qquad p \in [2,6], \tag{4.8}$$

where C is a positive constant depending on $\|\phi\|_{L^2(\mathbb{R}^3)}$, $E[\phi]$ and p.

Proof. The proof is a straightforward consequence of the following estimates

$$\begin{aligned} \|\psi(\cdot,t)\|^2_{L^2(\mathbb{R}^3)} &= \int_{|x|\le R} |\psi(x,t)|^2 dx + \int_{|x|>R} |\psi(x,t)|^2 dx \\ &\le CR^{\frac{3p-6}{p}} \left(\int_{|x|<R} |\psi(x,t)|^p dx\right)^{\frac{2}{p}} + \frac{1}{R^2}\int_{|x|>R} |x|^2 |\psi(x,t)|^2 dx \\ &\le CR^{\frac{3p-6}{p}} \|\psi(\cdot,t)\|^2_{L^p(\mathbb{R}^3)} + \frac{1}{R^2}\langle x^2\rangle(t). \end{aligned} \tag{4.9}$$

Optimizing in R, we have

$$\|\psi(\cdot,t)\|^2_{L^2(\mathbb{R}^3)} \le C\left(\|\psi(\cdot,t)\|^2_{L^p(\mathbb{R}^3)}\right)^{\frac{2p}{5p-6}} \langle x^2\rangle^{\frac{3p-6}{5p-6}}(t),$$

which allows to conclude as a simple consequence of (4.7) and of the mass preservation property. □

Decay estimates

Time decay estimates were obtained as consequence of the pseudo–conformal law [59, 29]

$$\frac{d}{dt}\left(\|(x+it\nabla)\psi\|^2_{L^2(\mathbb{R}^3)} + t^2\int_{\mathbb{R}^3} Vn dx\right) = t\int_{\mathbb{R}^3} Vn\, dx, \tag{4.10}$$

valid for solutions $\psi(x,t)$ with initial condition ϕ satisfying $(1+|x|)\phi \in L^2(\mathbb{R}^3)$. The pseudo–conformal law was first shown mathematically in [41] for the case of power nonlinearities. To improve these bounds we shall use an estimate relating the kinetic and potential energy with the $\|\psi\|_{L^3(\mathbb{R}^3)}$. Indeed, it was shown by P.L. Lions [78] that there exists a positive constant C_1 such that

$$\int_{\mathbb{R}^3} |u|^3\, dx \le C_1 \left(\int_{\mathbb{R}^3} |\nabla u|^2\, dx\right)^{\frac{1}{2}} \left(\frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|u(x)|^2|u(y)|^2}{|x-y|}\, dx\, dy\right)^{\frac{1}{2}} \tag{4.11}$$

for all $u \in \mathcal{D}(\mathbb{R}^3)$. The argument used in the proof of (4.11) is based on the fact that the norm in the dual space of $\mathcal{D}^{1,2}(\mathbb{R}^3) = \{u \in L^6(\mathbb{R}^3); \nabla u \in L^2(\mathbb{R}^3)\}$, endowed with the norm $\|\nabla u\|_{L^2(\mathbb{R}^3)}$, may be written on its dense subspace $L^{\frac{6}{5}}(\mathbb{R}^3)$ as $E_{POT}[\cdot]$ up to a constant. The Hölder inequality implies that the functional $F_v(w) = \int_{\mathbb{R}^3} v.\bar{w}\, dx$ applies $v \in L^{\frac{6}{5}}(\mathbb{R}^3)$ onto the dual space of $\mathcal{D}^{1,2}(\mathbb{R}^3)$. Since this is a Hilbert space, the Riesz representation theorem states the existence of $u_v \in \mathcal{D}^{1,2}(\mathbb{R}^3)$, such that

$$F_v(w) = \langle u_v, w\rangle_{\mathcal{D}^{1,2}(\mathbb{R}^3)} = \int_{\mathbb{R}^3} \nabla u_v \nabla \bar{w}\, dx\,.$$

Then, it is known that $u_v(x) = \frac{1}{4\pi}\frac{1}{|x|} * v$. As consequence, for any $w \in \mathcal{D}^{1,2}(\mathbb{R}^3)$ we have

$$\begin{aligned}\int_{\mathbb{R}^3} v.\bar{w}\, dx &= \langle u_v w\rangle_{\mathcal{D}^{1,2}(\mathbb{R}^3)} \le \|u_v\|_{\mathcal{D}^{1,2}(\mathbb{R}^3)}\|w\|_{\mathcal{D}^{1,2}(\mathbb{R}^3)} \\ &\le \frac{1}{4\pi}\left(\int_{\mathbb{R}^6} \frac{v(x)v(y)}{|x-y|}\, dxdy\right)^{\frac{1}{2}} \cdot \|\nabla w\|_{L^2(\mathbb{R}^3)}\,.\end{aligned}$$

This clearly concludes (4.11).

Combining the techniques used in previous works [29, 54, 59] with (4.11), we have the following Proposition

Proposition 4.2. Let $\phi \in H^1(\mathbb{R}^3)$ the initial condition of the SP system such that $(1+|x|)\phi \in L^2(\mathbb{R}^3)$, and let ψ be the associated solution in the repulsive case. Then, there exist (various) positive constants C such that

(i) $\forall\, |t| \geq \xi,\ \forall\, p \in [2,3]\,,\ \|\psi(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq \frac{C}{|t|^{(1-\frac{2}{p})}},$
$\forall\, |t| \geq \xi,\ \forall\, p \in [3,6]\,,\ \|\psi(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq \frac{C}{|t|^{(\frac{2}{3}-\frac{1}{p})}},$

(ii) $\forall\, |t| \geq \xi,\ \forall\, p \in [1,\frac{3}{2}]\,,\ \|n(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq \frac{C}{|t|^{2(1-\frac{1}{p})}},$
$\forall\, |t| \geq \xi,\ \forall\, p \in [\frac{3}{2},3]\,,\ \|n(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq \frac{C}{|t|^{(\frac{4}{3}-\frac{1}{p})}},$

(iii) $\forall\, |t| \geq \xi,\ \forall\, p \in]3,6]\,,\ \|V(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq \frac{C}{t^{(1-\frac{3}{p}-\epsilon)}}$ $(\epsilon = 0$ when $p = 6)$,
$\forall\, |t| \geq \xi,\ \forall\, p \in\ [6,\infty[\,,\ \|V(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq \frac{C}{t^{(\frac{2}{3}-\frac{1}{p})}},$

(iv) $\forall\, |t| \geq \xi,\ \forall\, p \in]\frac{3}{2},2]\,,\ \|\nabla V(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq \frac{C}{t^{(2-\frac{3}{p}-\epsilon)}}$ $(\epsilon = 0$ when $p = 2)$,
$\forall\, |t| \geq \xi,\ \forall\, p \in\ [2,\infty[\,,\ \|\nabla V(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq \frac{C}{t^{(1-\frac{1}{p})}},$

where $\xi > 0$ and C depends on $\|\phi(\cdot)\|_{\mathrm{L}^2(\mathbb{R}^3)}$, $\||\cdot|\phi(\cdot)\|_{\mathrm{L}^2(\mathbb{R}^3)}$ and p.

Proof. By integrating the pseudo-conformal law in $[\xi,t]$ we find

$$\begin{aligned}\|(\cdot + it\nabla)\psi(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} &+ t^2\int_{\mathbb{R}^3} V(x,t)n(x,t)\,dx \\ &= C + \int_\xi^t s\int_{\mathbb{R}^3} V(x,s)n(x,s)dx,\end{aligned} \tag{4.12}$$

where

$$C = \|(\cdot + i\xi\nabla)\psi(\cdot,\xi)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} + \xi^2\int_{\mathbb{R}^3} V(x,\xi)n(x,\xi)dx\,.$$

Here, the constant C depends on $\|x\phi\|^2_{\mathrm{L}^2(\mathbb{R}^3)}$ since the integral term in the right-hand side of (4.12) goes to $\|x\phi\|^2_{\mathrm{L}^2(\mathbb{R}^3)}$ as $t \to 0$, and ξ can be chosen small enough. Let $g(t) = t^2\int_{\mathbb{R}^3} V(x,t)n(x,t)\,dx = t^2\int_{\mathbb{R}^3}|\nabla V(x,t)|^2\,dx$. Then, from (4.12) it is clear that

$$g(t) \leq C + \int_\xi^t \frac{g(s)}{s}\,ds. \tag{4.13}$$

Now, the Gronwall inequality yields

$$g(t) = t^2\int_{\mathbb{R}^3}|\nabla V(x,t)|^2\,dx \leq \frac{Ct}{\xi}\,, \tag{4.14}$$

for all $t \geq \xi$. Define $\psi_g(x,t) := exp(-\frac{ix^2}{2t})\psi(x,t)$. An easy computation leads to

$$it\nabla\psi_g(x,t) = exp\left(-\frac{ix^2}{2t}\right)((x+it\nabla)\psi)(x,t), \tag{4.15}$$

for $t > 0$. Then, the pseudo–conformal law can be rewritten as

$$\begin{aligned} t^2\|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} + t^2\int_{\mathbb{R}^3}|\nabla V(x,t)|^2\,dx \\ = C + \int_\xi^t \left(s\int_{\mathbb{R}^3}|\nabla V(x,s)|^2\,dx\right)ds, \end{aligned} \tag{4.16}$$

for all positive times. By applying (4.14) to the integral term in the right-hand side of (4.16) we find

$$\|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} + \int_{\mathbb{R}^3}|\nabla V(x,t)|^2\,dx \le \frac{C}{t\xi} \tag{4.17}$$

for all $t \ge \xi$. Now, the estimates

$$\|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} \le \frac{C}{t\xi} \quad \text{and} \quad \int_{\mathbb{R}^3}|\nabla V(x,t)|^2\,dx \le \frac{C}{t\xi}, \qquad \forall t\ge\xi\,, \tag{4.18}$$

immediately hold. Some additional information can be deduced from (4.11). According to Young's inequality and to the fact that (4.11) can be extended to functions in $\mathrm{H}^1(\mathbb{R}^3)$ by standard density arguments we can write

$$\frac{1}{C_1}\int_{\mathbb{R}^3}|\psi|^3\,dx \le \frac{1}{2}\int_{\mathbb{R}^3}|\nabla\psi|^2\,dx + \frac{1}{4\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|\psi(x)|^2|\psi(y)|^2}{|x-y|}\,dx\,dy, \tag{4.19}$$

where $\psi \in \mathrm{H}^1(\mathbb{R}^3)$ and $C_1 > 0$. Clearly $|\psi(x,t)| = |\psi_g(x,t)|$, so that (4.19) along with (4.17) apply to guarantee that the solution $\psi(x,t)$ of the SP system satisfies

$$\int_{\mathbb{R}^3}|\psi(x,t)|^3\,dx = \int_{\mathbb{R}^3}|\psi_g(x,t)|^3\,dx \le \frac{C}{t}, \qquad \forall t\ge\xi. \tag{4.20}$$

Now, we estimate the L^p-norm of the solutions in terms of p. If $p \in [2,3]$, the Hölder inequality gives

$$\|\psi(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \le \|\psi(\cdot,t)\|^{\beta}_{\mathrm{L}^2(\mathbb{R}^3)}\|\psi(\cdot,t)\|^{(1-\beta)}_{\mathrm{L}^3(\mathbb{R}^3)} \le \frac{C}{t^{(1-\frac{2}{p})}},$$

where $\beta = \left(\frac{6}{p}-2\right)$. On the other hand, if $p\in[3,6]$ we use the Gagliardo–Nirenberg inequality to deduce

$$\begin{aligned} \|\psi(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} = \|\psi_g(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} &\le \gamma(p)\|\nabla\psi_g(\cdot,t)\|^a_{\mathrm{L}^2(\mathbb{R}^3)}\|\psi_g(\cdot,t)\|^{1-a}_{\mathrm{L}^3(\mathbb{R}^3)} \\ &\le \gamma(p)\left(\frac{C}{t^{\frac{1}{2}}}\right)^a\left(\frac{C}{t^{\frac{1}{3}}}\right)^{1-a} \\ &\le \frac{C}{t^{\left(\frac{2}{3}-\frac{1}{p}\right)}}, \end{aligned} \tag{4.21}$$

where $p \in [3,6]$ and $a = \left(2 - \frac{6}{p}\right)$. Here, C only depends on $\|\phi\|_{L^2(\mathbb{R}^3)}$. The proof of (ii) is a consequence of the identity $\|n(\cdot,t)\|_{L^p(\mathbb{R}^3)} = \|\psi(\cdot,t)\|^2_{L^{2p}}$. Then, by the Hardy–Littlewood–Sobolev inequality we get

$$\|\nabla V(t)\|_{L^p(\mathbb{R}^3)} \le \begin{cases} \frac{C}{|t|^{\frac{4}{3}-\frac{2}{p}}} & \forall\, p \in]3/2,3]\,, \\ \frac{C}{|t|^{1-\frac{1}{p}}} & \forall\, p \in [3,\infty[\,. \end{cases}$$

We can improve these estimates thanks to the interpolation inequality and (4.18)

$$\begin{aligned} \|\nabla V(t)\|_{L^p(\mathbb{R}^3)} &\le \|\nabla V(t)\|^{\theta}_{L^2(\mathbb{R}^3)} \|\nabla V(t)\|^{(1-\theta)}_{L^q(\mathbb{R}^3)}\,, \\ &\le \begin{cases} \frac{C}{|t|^{\frac{\theta}{2}+\left(\frac{4}{3}-\frac{2}{q}\right)(1-\theta)}} & \forall\, p \in]3/2,2]\,, \\ \frac{C}{|t|^{1-\frac{1}{p}}} & \forall\, p \in [2,\infty[\,, \end{cases} \end{aligned}$$

which allow to conclude (iv) by setting $q = 3/2$. Finally, (iii) is deduced from (iv) and the Gagliardo–Nirenberg inequality

$$\|V(\cdot,t)\|_{L^p(\mathbb{R}^3)} \le C\|\nabla V(\cdot,t)\|_{L^{\frac{3p}{3+p}}(\mathbb{R}^3)}\,.$$

□

Another interesting consequence of the pseudo–conformal law is the finiteness of $\|\psi\|_{L^{q,p}}$ for all (q,p) admissible pairs, with $p \in (2,6)$.

The spaces $L^{q,p}_T = L^q([0,T], L^p(\mathbb{R}^3))$, where $T > 0$ and (q,p) is an admissible pair, i.e., $2 \le p < 6$ and $q = \frac{4p}{3(p-2)}$, are involved in the existence arguments for $L^2(\mathbb{R}^3)$ initial data [29]. In fact, the existence of mild solutions is proved by using a fixed point argument in $L^{q,p}_T$ spaces. The next result guarantees that the solutions in the repulsive case belong to $L^q([\xi,\infty), L^p(\mathbb{R}^3))$, with $\xi > 0$ and $p \in (2,6]$. From the existence theory and the next Proposition we conclude that the solutions belong to $L^q(\mathbb{R}^+_0, L^p(\mathbb{R}^3))$ with $p \in (2,6)$. This property implies a global-in-time decay estimate for the $L^p(\mathbb{R}^3)$ norm of the solutions.

Define

$$f_\psi(t) = \|(\cdot + it\nabla)\psi(\cdot,t)\|^2_{L^2(\mathbb{R}^3)} + t^2 \int_{\mathbb{R}^3} |\nabla V(\cdot,t)|^2\,dx\,, \quad \forall t \ge 0.$$

In terms of ψ_g, it is clear that

$$f_\psi(t) = t^2\|\nabla\psi_g(\cdot,t)\|^2_{L^2(\mathbb{R}^3)} + t^2 \int_{\mathbb{R}^3} |\nabla V(\cdot,t)|^2\,dx, \qquad \forall t > 0.$$

Since f_ψ only reaches positive values in the repulsive case, we have the following

Proposition 4.3. Let ψ be a solution of the SP system in the repulsive case with initial data $\phi \in \mathrm{H}^1(\mathbb{R}^3)$ such that $\|x\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} < \infty$. Then, the following estimate

$$\int_\xi^\infty \|\psi(\cdot,s)\|^q_{\mathrm{L}^p(\mathbb{R}^3)} ds \le C \tag{4.22}$$

holds for all admissible pair (q,p), with $p \in (2,6]$, where C is a positive constant depending on p, $\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}$, $\|x\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}$ and $\xi > 0$.

Proof. Since $f_\psi > 0$, we have

$$\|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} + \int_{\mathbb{R}^3} V(\cdot,t)n(\cdot,t)\,dx > 0, \qquad \forall t > 0. \tag{4.23}$$

Notice that (4.10) can be also rewritten as

$$\frac{d}{dt}\Big(t\|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} + 2tE_{POT}[\psi](t)\Big) = -\|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)}, \quad \forall t > 0.$$

Now, integrating between $\xi > 0$ and $t > \xi$ we obtain

$$t\|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} + 2tE_{POT}[\psi](t) = \frac{f_\psi(\xi)}{\xi} - \int_\xi^t \|\nabla\psi_g(\cdot,s)\|^2_{\mathrm{L}^2(\mathbb{R}^3)}\,ds, \ \forall t > \xi. \tag{4.24}$$

Then, using (4.23) to estimate the left-hand side of (4.24) we find

$$\int_\xi^t \|\nabla\psi_g(\cdot,s)\|^2_{\mathrm{L}^2(\mathbb{R}^3)}\,ds \le \frac{f_\psi(\xi)}{\xi}, \quad \forall t > \xi. \tag{4.25}$$

Finally, since $\|\psi\|_{\mathrm{L}^p(\mathbb{R}^3)} = \|\psi_g\|_{\mathrm{L}^p(\mathbb{R}^3)}$ the Gagliardo–Nirenberg inequality allows to conclude the proof. □

Remark. Observe that the proof above is still valid for $p = 6$. However, reconstructing the proof of Proposition 4.2 would make (4.22) work only for $p \in (2,6)$.

Appendix: Some remarks on the attractive case

The solutions of the SP system in the attractive case exhibit remarkable qualitative differences when compared to solutions in the repulsive case. The nonpositivity of the potential energy implies now that the energy reaches negative values, so that steady states (constant density solutions) with negative energy exist [70, 97, 78]. The next result shows that analogous time decreasing bounds cannot be generalized to solutions of the attractive SP system. On the other hand, the argument on upper bounds developed in these sections can be adapted to solutions of the SP system in the attractive case with positive total energy. However, this proof involves another time invariant quantity associated with SP solutions: the linear momentum $\langle p\rangle = \frac{1}{i}\int_{\mathbb{R}^3} \overline{\psi}(x,t)\nabla\psi(x,t)\,dx$.

Proposition 4.4. Let $\psi(x,t)$ be a SP solution with initial data $\phi(x)$ such that

$$E[\phi] < \frac{1}{2}\frac{|\langle p\rangle|^2}{\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}}. \tag{4.26}$$

Then, there exist positive constants C and C' depending on $\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}$, $E[\phi]$, $|\langle p\rangle|^2$ and p such that

$$\|\psi(t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \geq C, \quad E_{POT}[\psi] \leq -C'\,, \quad \forall t \geq 0, \quad p \in [\frac{12}{5}, 6]. \tag{4.27}$$

In the case

$$E[\phi] \geq \frac{1}{2}\frac{|\langle p\rangle|^2}{\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}}\,, \tag{4.28}$$

we have

$$\|\psi(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \geq \frac{C''}{t^{\frac{3p-6}{2p}}}, \qquad \forall t > \xi > 0, \qquad p \in [2,6], \tag{4.29}$$

where C'' is a positive constant depending on $\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}$, $E[\phi]$, $|\langle p\rangle|^2$ and p.

Proof. To show the relevance of (4.26) and (4.28) we shall use the Galilean invariance of the system (See [97]). This property ensures that if $\psi(x,t)$ is a solution to the SP system with initial data ϕ_0, then the solution associated with initial data $\phi_N(x,0) = e^{iNx}\phi_0(x)$ is $\psi_N(x,t) = e^{iNx-it\frac{N^2}{2}}\psi(x-tN,t)$, where $N \in \mathbb{R}^3$. The solutions ψ_N have the same $\mathrm{L}^p(\mathbb{R}^3)$ norm and the same potential energy for all N at every time t, while the total energy is

$$E[\phi_N] = \frac{1}{2}N^2\|\phi_N\|_{\mathrm{L}^2(\mathbb{R}^3)} + N\langle p\rangle + E[\phi_0]\,.$$

It is a simple matter to observe that for every ϕ_0 the Galilean invariance gives a parametric family of initial data ϕ_N such that the time evolution of the $\mathrm{L}^p(\mathbb{R}^3)$ norm and of the potential energy are the same. Analyzing a particular member of this family, the Galilean transformation allows to deduce the behaviour of these quantities for the whole family.

By a simple optimization argument one can easily check that (4.26) implies the existence of initial data with negative energy in the family, while if (4.28) holds, then the energy of the initial data is nonnegative.

Under assumption (4.28), we can choose initial data with positive energy belonging to the class of Galilean transforms of ϕ. Since Proposition 4.1 is still valid for solutions of the SP system with positive energy, it can be easily deduced that (4.29) is satisfied.

On the other hand, if ϕ fulfills (4.26), then we can choose a Galilean translation $\phi_{N'}$ whose total energy is negative. Now, thanks to the nonpositivity of the energy we find

$$-\|\nabla V(\psi_{N'}(t))\|^2_{\mathrm{L}^2(\mathbb{R}^3)} < E[\phi_{N'}] < 0\,, \quad \forall t \geq 0\,.$$

The Hardy–Littlewood–Sobolev and Hölder inequalities lead to

$$\|\nabla V(\psi_{N'})\|^2_{\mathrm{L}^2(\mathbb{R}^3)} \leq C\|\psi_{N'}\|^{\frac{2}{3}\frac{5p-12}{p-2}}_{\mathrm{L}^2(\mathbb{R}^3)} \|\psi_{N'}\|^{\frac{4p}{3(p-2)}}_{\mathrm{L}^p(\mathbb{R}^3)},$$

for all $\psi \in \mathrm{L}^2(\mathbb{R}^3) \cap \mathrm{L}^p(\mathbb{R}^3)$, with $p \geq \frac{12}{5}$, where C is a positive constant which only depends on p. The combination of both inequalities yields

$$0 < -E[\phi_{N'}] \leq \|\nabla V(\psi_{N'})\|^2_{\mathrm{L}^2(\mathbb{R}^3)} \leq C\|\psi_{N'}\|^{\frac{2}{3}\frac{5p-12}{p-2}}_{\mathrm{L}^2(\mathbb{R}^3)} \|\psi_{N'}\|^{\frac{4p}{3(p-2)}}_{\mathrm{L}^p(\mathbb{R}^3)}. \tag{4.30}$$

Now, according to the mass preservation and the invariance of the $\mathrm{L}^p(\mathbb{R}^3)$ norm of the solutions under Galilean translations, (4.27) implies (4.30). □

Thus, there do not exist decreasing upper bounds for solutions to the SP system in the attractive case. The argument developed by Ozawa and Hayashi in [83] to derive the upper bounds in the repulsive case strongly uses the estimates on the solutions given in (4.18). Nevertheless, these properties cannot be derived in general for the attractive case since they would imply the existence of decreasing upper bounds.

Chapter 5

Long–time dynamics of the Schrödinger–Poisson–Slater system

Introduction

The aim of this chapter is to analyze the asymptotic behaviour of solutions to the Schrödinger–Poisson–Slater (SPS) system in comparisson with the solutions to the Schrödinger-Poisson (SP) system.

The SPS system is given by:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta_x\psi + V\psi - C_S n^{\frac{1}{3}}\psi, \qquad \lim_{|x|\to\infty}\psi(x,t) = 0, \tag{5.1}$$

$$\psi(x,t=0) = \phi(x), \tag{5.2}$$

$$\Delta_x V = -\epsilon\, n, \qquad \lim_{|x|\to\infty} V(x,t) = 0, \tag{5.3}$$

where n is the charge density associated to the wave function ψ, and $\epsilon = 1$ (repulsive case) or $\epsilon = -1$ (attractive case). Here, C_S hold for the Slater constant. The Planck constant and the particle mass m can be normalized to unity for the sake of simplicity. However, this normalization also modifies the Slater constant, whose value is relevant for the subsequent analysis.

The SPS system describes the evolution of an electron ensemble in a semiconductor crystal. The repulsive effect of the Coulomb potential in the SP system seems to be too strong when we compare the behaviour of the solutions to simulations of superlattice structures (see [89, 111]). These phenomena are also observed in the context of attractive Coulomb potential. Some different approximations have been studied to overcome this problem, obtaining appropriate adaptations of the Poisson potential. The Hartree–Fock (HF) model has been used to analyze a wide variety of phenomena in

Quantum-Chemistry and Solid State Physics (see [8, 75, 78]). The time–dependent HF equation has been analyzed in [38] and [68]. One of the most interesting corrections to the Poisson potential in the SP system is found by deriving nonlinear $|\psi|^\alpha$ terms from the Fock potential via various limits, in particular the low density limit, which gives $\alpha = 2/3$ (see [20]). This kind of $|\psi|^\alpha$ approximations to the Fock term is usually called the X^α-approach. Another motivation for this approximation in Quantum–Chemistry is the enormous quantity of calculations necessary to evaluate the Fock term, usually of order N^4, N being the number of particles. In this direction, the X^α approach to the Fock correction (Dirac, Slater, ...) has been proved relevant in different contexts. These local approximations to nonlocal interaction terms give excellent results when studying stationary states, for example in Quantum Chemistry (see [35] and [26, 72, 76] for some derivations and analysis of these systems). Then, the calculations are reduced from N^4 to N^3, even there might be some place for improvements. However, there is no rigorous foundation of the X^α-model in the time-dependent case. In this direction, following the classical ideas of the thermodynamical limit in Statistical Mechanics (see [36]) some recent advances are being done from the continuum and mean–field limit of the N–quantum–particle system by C. Bardos *et al.*, see [10].

The aim of this work is to analyze the qualitative differences between the Schrödinger–Poisson–Slater ($\alpha = \frac{2}{3}$) evolution system and the Schrödinger–Poisson and Hartree–Fock systems. We are mainly interested in the X^α case studied in semiconductor theory, that is $\alpha = \frac{2}{3}$, which is derived from the Fock term by means of a low density limit, see [20]. This $|\psi|^{2/3}\psi$ correction is also known as the Dirac exchange term. Another interesting approach comes from the limit of heavy atoms, i.e. the high charge of nuclei limit; this leads to the Thomas-Fermi correction ($\alpha = 4/3$) of the kinetic energy, see [72, 73]. In this work we do not approximate the kinetic energy term (which is also called the von Weizsäcker correction). However, the Thomas–Fermi term can be alternatively seen as a correction of the Fock interaction, that always appears as a repulsive potential, see [73]. As we will point out later, these other X^α–approaches, useful in many scientific contexts, can be treated in our mathematical framework.

One important feature of the SPS system is that its associated potential energy can reach negative values depending on the constants of the system (mass, initial energy or Slater constant). This fact implies some relevant properties of the SPS system in the repulsive case: 1) the minimum of the total energy operator is negative for some choices of the physical constants; 2) there are solutions (depending on the initial energy) that do not have dispersive character; 3) there are steady-state solutions, i.e. solutions with constant density; 4) there are solutions, even with positive energy, which preserve the L^p norm and do not decay with the time evolution. These properties show important qualitative differences between the SPS system and the SP and HF systems, see Chapter 4, [29, 38, 59, 68]. On the other hand, the X^α–Slater–model appears as an appropriate correction to the self–consistent Coulomb potential in semiconductor heterostructures modeling, in the sense that it covers different phenomenologies observed in this context. Some of our results hold true under the hypothesis of a relation between the value of the Slater constant, the mass and the energy of the system. However, the Slater constant is a characteristic of the component metals in the semiconductor device as it was pointed out in [53] when interpreting the exchange–correlation potential of Kohn–Sham type. In this way, our study covers the whole range of variation for these constants, and the relation between these constants appears in a natural way and is not a restriction from a physical point of view. As we have commented before, the main differences with respect to the SP system occur in the repulsive case, where non dispersive effects, stationary and periodic solutions appear. However, the attractive case is also of interest in applications related to quantum gravity in the limit of very heavy particles (see for example [84]), thus we analyze both cases. We focus our study in the single–state case.

In [20], the mixed–state case for the SPS system has been dealt with. In particular, the well-posedness and regularity of local–in–time and global solutions was analyzed, with L^2 or H^1 initial data. Also, the basic conservation laws and the minimal energy solutions in the attractive case were derived under a variational framework. A different approach for the single-state case can be seen in [28].

Most of these results are valid for other X^α–approaches. However, motivated by the applications in semiconductor theory, we focus our efforts in the Slater approach to the Fock term. We will comment along the chapter on some extensions of the results to other X^α-terms or some combination of them.

Let us summarize the main results and the techniques used in the chapter in comparison with previous results. Section 2 is devoted to the minimization of the energy functional in the repulsive case. This allows us to deduce the existence of stationary solutions with negative energy as well as optimal bounds for the kinetic energy. To deal with this nonconvex minimization problem we can use different techniques introduced in [72, 74, 77]. This problem was treated in [20] (in the attractive case) by using symmetric decreasing rearrangement inequalities, but this tool seems to be fruitless in the repulsive case. Some minimization problems related to the repulsive case are studied in references [72] and in [26, 78] for small enough values of the mass upon using a perturbative argument. Alternatively, we propose here a scaling argument which provides effective bounds on the mass. In the third section we analize the long time behaviour of SPS solutions. The balance between the Coulombian potential and the Slater correction makes powerless the usual arguments based on the pseudo–conformal law (See Chapter 4). In our analysis we combine this property, or the equivalent dispersion equation, with the Galilean invariance in order to conclude some $L^p(\mathbb{R}^3)$ estimates. Also, from the dispersion equation (which relates the total energy to the momentum and position dispersions) it can be deduced that the solution is expansive in the sense that its second order moment increases with time. Finally, in Section 4 we analyze the asymptotic behaviour of the SPS solutions under attractive Coulomb forces. Actually, we prove the existence of stationary solutions in the case of negative energy. The contents of this chapter are collected in [99].

Minimum of the energy in the repulsive case

The Slater term introduces some qualitative differences in the behaviour of the solutions to the SPS system when compared to solutions to the SP system. While the SP energy in the repulsive case is always positive, this can be negative when the Slater contribution is considered. The total energy operator associated with the solutions to the SPS system has the following form:

$$E[\psi]=\int_{\mathbb{R}^3}\left\{\frac{|\nabla\psi(x,t)|^2}{2}+\int_{\mathbb{R}^3}\frac{\epsilon|\psi(x,t)|^2|\psi(x',t)|^2}{8\pi|x-x'|}dx'-\frac{3C_S}{4}|\psi(x,t)|^{\frac{8}{3}}\right\}dx. \quad (5.4)$$

E is an invariant of motion (i.e., E is preserved along the time evolution) provided that ψ is such that $E[\psi]$ is well–defined (see [20]). We refer to the first term in the right–hand side of (5.4) as the kinetic energy $E_{KIN}(\psi)$, while the sum of the last two terms is the potential energy $E_{POT}(\psi)$. In (5.4), the expression of the Coulombian potential has been identified as

$$\frac{1}{2}\int_{\mathbb{R}^3}V(x)n(x)\,dx=\frac{\epsilon}{2}\int_{\mathbb{R}^3}|\nabla V(x)|^2\,dx.$$

However, in the repulsive case $\epsilon=1$, we can prove that the potential energy is always negative for some choice of the Slater constant in terms of the mass of the system. The following result corroborates this feature.

Lemma 5.1. If the $L^2(\mathbb{R}^3)$ norm of the initial data ϕ associated with the

SPS system verifies

$$\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)} \leq \left(\frac{3C_S}{2C}\right)^{\frac{3}{4}},$$

where C_S is the Slater constant and C is a positive constant determined by

$$\frac{1}{C} = \mathrm{Inf}\left\{\frac{\|\psi(\cdot,t)\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)}}{\|\nabla V(\psi)(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)}};\ \psi \in L^{\frac{8}{3}}(\mathbb{R}^3)\cap L^2(\mathbb{R}^3),\ \|\psi(\cdot,t)\|_{L^2} = 1\right\},$$

then the potential energy of the solutions is negative along the time evolution.

Proof. This result is based on the following inequality, valid for all $\psi \in \mathrm{L}^2(\mathbb{R}^3)\cap L^{\frac{8}{3}}(\mathbb{R}^3)$:

$$\|\nabla V(\psi)(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} \leq C\|\psi(\cdot,t)\|^{\frac{4}{3}}_{\mathrm{L}^2(\mathbb{R}^3)}\|\psi(\cdot,t)\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)}. \tag{5.5}$$

Let us prove (5.5). From the definition of V and the Hölder inequality we have

$$\begin{aligned}\|\nabla V\|^2_{\mathrm{L}^2(\mathbb{R}^3)} &= \int_{\mathbb{R}^3}|\nabla V|^2\,dx = \left|\int_{\mathbb{R}^3} V\Delta V\,dx\right| = \left|\int_{\mathbb{R}^3} Vn\,dx\right| \\ &\leq \|V\|_{L^{12}(\mathbb{R}^3)}\|n\|_{L^{\frac{12}{11}}(\mathbb{R}^3)}.\end{aligned} \tag{5.6}$$

Then, according to the interpolation inequality for L^p spaces we can estimate

$$\|n(\cdot,t)\|_{L^{\frac{12}{11}}(\mathbb{R}^3)} = \|\psi(\cdot,t)\|^2_{L^{\frac{24}{11}}(\mathbb{R}^3)} \leq \|\psi(\cdot,t)\|^{\frac{4}{3}}_{\mathrm{L}^2(\mathbb{R}^3)}\|\psi(\cdot,t)\|^{\frac{2}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)}. \tag{5.7}$$

To obtain an analogous estimate for $\|V\|_{L^{12}}$, we apply the Hardy-Littlewood-Sobolev inequality to find

$$\|V\|_{L^{12}(\mathbb{R}^3)} = C'\left\||\psi|^2 * \frac{1}{|x|}\right\|_{L^{12}(\mathbb{R}^3)} \leq C'\||\psi|^2\|_{L^{\frac{4}{3}}(\mathbb{R}^3)} = C'\|\psi\|^2_{L^{\frac{8}{3}}(\mathbb{R}^3)}. \tag{5.8}$$

Finally, inequality (5.5) holds by substituting (5.7) and (5.8) in (5.6).

Applying (5.5) to solutions ψ of the SPS system and using that the L^2–norm of the initial data is preserved along the time evolution, we conclude the proof by writing

$$E_{POT}(\psi)(t) \leq \left(\frac{C}{2}\|\psi(\cdot,t)\|^{\frac{4}{3}}_{\mathrm{L}^2(\mathbb{R}^3)} - \frac{3}{4}C_S\right)\|\psi(\cdot,t)\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)}.$$

□

Remark. The inequality (5.5) as well as an upper bound for the sharp constant C were found by Lieb and Oxford in [75]. In our context, this bound takes the value $C = \frac{1.092}{2\pi} = 0.1737$.

Furthermore, since the potential energy associated with the initial data can be negative in the repulsive case we can find initial conditions for which the total energy is also negative, as proved in the following

Proposition 5.1. There exist initial data $\phi \in \mathrm{H}^1(\mathbb{R}^3)$ for which the total energy in the repulsive case is negative.

Proof. Let $\psi \in \mathrm{H}^1(\mathbb{R}^3)$ such that the associated potential energy is negative (this may happen by virtue of Lemma 5.1). Then, there is $\sigma > 0$ small enough such that the total energy of $\psi_\sigma(x) = \sigma^{\frac{3}{2}}\psi(\sigma x)$,

$$\begin{aligned} E[\psi_\sigma] &= \int_{\mathbb{R}^3}\left\{\frac{\sigma^2}{2}|\nabla\psi(x)|^2 + \sigma\left(\int_{\mathbb{R}^3}\frac{|\psi(x)|^2|\psi(x')|^2}{8\pi|x-x'|}dx' - \frac{3C_S}{4}|\psi(x)|^{\frac{8}{3}}\right)\right\}dx \\ &= \sigma^2 E_{KIN}(\psi) + \sigma E_{POT}(\psi), \end{aligned} \tag{5.9}$$

is nonpositive. Then, by choosing $\phi = \psi_\sigma$ as initial condition, the energy associated with this problem is nonpositive. □

Remark. The same thing occurs when other X^α terms are considered. The total energy functional also reaches negative values when couplings of the Coulombian potential with power nonlinearities $|\psi|^\alpha\psi$ $\alpha \in (0, 4/3]$ are considered. Combinations of some of these terms could be also possible in their attractive or repulsive versions. However, some other kind of problems appear in the minimization argument, as we will mention in the next subsection.

Proposition 5.1 allows to remark some important differences between the asymptotic behaviour of solutions to our system and those to the SP system. For the repulsive SP system it was proved (see [29],[59]) that the L^p norms of the solutions tend asymptotically in time to zero for $p \in]2, 6]$. However, when we analyze the evolution of solutions to the repulsive SPS system whose initial data has negative energy, we observe that the $L^{\frac{8}{3}}$ norm of the wave function ψ cannot go to zero as $t \to \infty$. This is because the total energy of the system is preserved and the Slater term is the only nonpositive contribution to the total energy.

One of the relevant points in the analysis of this problem is the existence of a global minimum of the energy functional in $\mathrm{H}^1(\mathbb{R}^3)$ under the constraint $\|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M$. This problem has no solution for the repulsive SP system because the infimum of the energy is always 0, which is not a minimum except for the case $M = 0$. In the following section we prove the existence of such a minimum for the SPS problem, for solutions with sufficiently small $\mathrm{L}^2(\mathbb{R}^3)$ norm.

Minimization problem

In this section we study the following minimization problem associated with the total energy of the repulsive SPS system

$$I_M = \inf\left\{E[\psi];\ \psi \in \mathrm{H}^1(\mathbb{R}^3),\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M\right\}, \tag{5.10}$$

where $M > 0$ and $E[\psi]$ is defined by (5.4). The main result of this section claims that this functional reaches a minimum value, which allows us to deduce two interesting consequences. The first one is the existence of stationary profiles, which are periodic-in-time solutions to the SPS system preserving the density. We also note that this kind of solutions does not exist for the repulsive SP system. The second consequence is the derivation of optimal bounds for the kinetic energy of solutions for which the total energy is well-defined.

Let us prove the results that ensure the existence of a minimum of (5.10). Firstly we observe that the energy operator is bounded from below in terms of the problem (5.10). From the Gagliardo–Nirenberg inequality we get

$$\|\psi\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq \gamma \|\nabla\psi\|^a_{\mathrm{L}^2(\mathbb{R}^3)} \|\psi\|^{1-a}_{\mathrm{L}^2(\mathbb{R}^3)},$$

where $p = \frac{8}{3}$ and $a = 3\left(\frac{1}{2} - \frac{1}{p}\right) = \frac{3}{8}$. This can be rewritten equivalently as

$$\frac{\|\psi\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)}}{\gamma^{\frac{8}{3}} \|\psi\|^{\frac{5}{3}}_{\mathrm{L}^2(\mathbb{R}^3)}} \leq \|\nabla\psi\|_{\mathrm{L}^2(\mathbb{R}^3)}, \tag{5.11}$$

which holds for all $\psi(\cdot, t) \in \mathrm{H}^1(\mathbb{R}^3)$. Using (5.11) and the fact that in this case the Coulombian potential term is nonnegative we obtain

$$E[\psi] \geq \left(\frac{\int_{\mathbb{R}^3} |\psi(x)|^{\frac{8}{3}} dx}{\gamma^{\frac{8}{3}} M^{\frac{5}{3}}}\right)^2 - \frac{3}{2} C_S \int_{\mathbb{R}^3} |\psi(x)|^{\frac{8}{3}} dx. \tag{5.12}$$

The right-hand side of (5.12) can be seen as a second order polynomial $ax^2 + bx$ in $\int_{\mathbb{R}^3} |\psi|^{\frac{8}{3}} dx$, where

$$a = \left(\gamma^{\frac{8}{3}} M^{\frac{5}{3}}\right)^{-2} \qquad \text{and} \qquad b = -\frac{3}{2} C_S.$$

Thus, we immediately conclude that the total energy is bounded from below. Furthermore, we can deduce the boundedness in $\mathrm{H}^1(\mathbb{R}^3)$ of any minimizing sequence, which plays an important role in our argument to obtain the minimum of the functional.

The technical difficulties arising in this nonconvex minimization problem come from the invariance of the total energy functional by the non-compact group of translations. The possible loss of compactness due to that invariance has to be detected by the techniques used in the proofs. In this way, two methods are proposed in the previous literature to analize the class of problems (5.10): the concentration–compactness method [77] and the method of the nonzero weak convergence after translations [74]. In fact, we can prove that every minimizing sequence is *in essence* relatively compact provided that a certain sub-additivity property is strict. This condition implies that a minimizing sequence is *concentrated* in a bounded domain. Recently, this lack of compactness has been analyzed in [39] for the Sobolev embedding. Since an important part of the intermediate steps are common to both (concentration–compactness and nonzero weak convergence after translations in Sobolev spaces) techniques, we will comment the application of them.

Concentration–compactnes argument

We can use the following formulation of the concentration–compactness principle adapted to our situation.

Proposition 5.2. For every $M > 0$, the following inequality

$$I_M \leq I_\alpha + I_{M-\alpha}\ , \quad \forall \alpha \in (0, M), \tag{5.13}$$

holds. Furthermore, every minimizing sequence of (5.10) is relatively compact in $\mathrm{H}^1(\mathbb{R}^3)$ (up to a translation) if and only if

$$I_M < I_\alpha + I_{M-\alpha}\ , \quad \forall \alpha \in (0, M). \tag{5.14}$$

Proof. The proof is a consequence of Lemma III.1 and Lemma I.1 in [77]. In order to make the memory self-consistent, we adapt these results to our notation. The general framework for minimization problems proposed by P. L. Lions allows us to establish the condition (5.13). Consider a minimizing sequence $\{u_n\}$ of (5.10). Since this sequence is bounded in $\mathrm{H}^1(\mathbb{R}^3)$ with $||u_n||^2_{\mathrm{L}^2(\mathbb{R}^3)} = M$, then there exists a subsequence $n_k \in \mathbb{N}$ for which either compactness or vanishing or dichotomy occurs (Lemma III.1 [77]). In order to prove compactness let us prove that vanishing and dichotomy cannot occur. The strict sub–additivity condition (5.14) prevents the subsequence from dichotomy. This property is stated as follows: there exists $\alpha \in]0, M[$ such that for every $\varepsilon > 0$, there exist $k_0 \geq 1$ and u_k^1, u_k^2 bounded in $\mathrm{H}^1(\mathbb{R}^3)$ satisfying

$$\begin{cases} \|u_{n_k} - (u_k^1 + u_k^2)\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq \delta_p(\epsilon) \to 0, \ \epsilon \to 0^+, \ 2 \leq p < 6; \\ |\int_{\mathbb{R}^3} |u_k^1|^2 \, dx - \alpha| \leq \varepsilon, \quad |\int_{\mathbb{R}^3} |u_k^2|^2 \, dx - (M - \alpha)| \leq \varepsilon; \\ \mathrm{dist}(\mathrm{Supp}\, u_k^1, \mathrm{Supp}\, u_k^2) \to \infty, k \to \infty; \\ \liminf_k \int_{\mathbb{R}^3} \{|\nabla u_{n_k}|^2 - |\nabla u_k^1|^2 - |\nabla u_k^2|^2\} \, dx \geq 0; \end{cases}$$

for $k \geq k_0$. Indeed, if dichotomy occurs we easily deduce that

$$I_M \geq I_\alpha + I_{M-\alpha},$$

which yields a contradiction. On the other hand, if strict sub–additivity does not occur, then a minimizing sequence can be constructed without convergent subsequences (see [77] for details). Vanishing occurs when

$$\lim_{k \to \infty} \sup_{y \in \mathbb{R}^3} \int_{y + B_R} |u_{n_k}(x)|^2 \, dx = 0, \quad \forall R < \infty, \quad B_R = \{x \in \mathbb{R}^3, \ |x| < R\}.$$

It can be proved that the subsequence does not vanish as follows from the fact that $I_M < 0$ and from the following result (Lemma I.1 [77] with $q = 2$, $p = 2$ and $\alpha = 8/3$):

Lemma 5.2. Let $1 < p \leq \infty$ and $1 \leq q < \infty$ with $q \neq \frac{3p}{3-p}$ if $p < 3$. Assume that u_n is bounded in $\mathrm{L}^q([0, \infty])$, ∇u_n is bounded in $\mathrm{L}^p(\mathbb{R}^3)$ and

$$\sup_{y \in \mathbb{R}^3} \int_{y + B_R} |u_n|^q \, dx \underset{n}{\to} 0 \quad \text{for some } R > 0\,.$$

Then, $u_n \underset{n}{\to} 0$ in $\mathrm{L}^\alpha(\mathbb{R}^3)$ for $\alpha \in [q, \frac{3p}{3-p}]$.

Hence, we have proved that any minimizing sequence satisfies the following compactness criterium: there exists $y_k \in \mathbb{R}^3$ such that $|u_{n_k}(\cdot + y_k)|^2$ is tight

$$\forall \varepsilon > 0, \ \exists R < \infty, \ \int_{y_k + B_R} |u_{n_k}(x)|^2 \geq M - \varepsilon\,.$$

Setting $\tilde{u}_n = u_n(\cdot + y_n)$, we can assume (up to a subsequence) that $\tilde{u}_n \to \tilde{u}$ weakly in $\mathrm{H}^1(\mathbb{R}^3)$ and the compactness property implies

$$\int_{B_R} |\tilde{u}|^2 \, dx \geq M - \varepsilon.$$

Thus, $\widetilde{u}_n$ converges strongly in $L^2(\mathbb{R}^3)$ to $\widetilde{u}$. By using the Gagliardo–Nirenberg inequality, $\widetilde{u}_n$ converges strongly to $\widetilde{u}$ in $L^p(\mathbb{R}^3)$ for $2 \leq p < 6$. This fact allows to assure that $\widetilde{u}$ is a minimum of the problem I_M as consequence of the weak lower semi–continuity of the $H^1(\mathbb{R}^3)$ norm and the convergence $E_{POT}(\widetilde{u}_n) \to E_{POT}(\widetilde{u})$. Thus, *a posteriori* we deduce

$$\int_{\mathbb{R}^3} |\nabla \widetilde{u}_n|^2 \, dx \underset{n}{\to} \int_{\mathbb{R}^3} |\nabla \widetilde{u}|^2 \, dx,$$

showing the compactness in $H^1(\mathbb{R}^3)$. □

To obtain the relative compactness of any minizing sequence (up to translations) has been used the concentration–compactness argument that can be equivalently replaced by the arguments based on nonzero weak convergence after translations [74]. The point which is common to both techniques is that hypothesis (5.14) is required.

Nonzero weak convergence after translations

In this approach, we apply the next two results to any minimizing sequence $\{u_n\}_{n\in\mathbb{N}}$ of (5.10) to guarantee the existence of a nonzero weak convergent subsequence in $H^1(\mathbb{R}^3)$ up to translations (see [74], Theorem 8.10 and exercise 2.22, for more details):

Lemma 5.3 (Exercise 2.22 [74]). Suppose that $1 \leq p < q < r \leq \infty$ and that u is a function in $L^p(\Omega) \cap L^r(\Omega)$ with $\|u\|_{L^p(\Omega)} \leq C_p < \infty$, $\|u\|_{L^r(\Omega)} \leq C_r < \infty$, and $\|u\|_{L^q(\Omega)} \geq C_q > 0$. Then, there are constants $\epsilon > 0$ and $M > 0$, depending only on $p,\ q,\ r,\ C_p,\ C_q,\ C_r$, such that $Meas(\{x\,:\,|u(x)| > \epsilon\}) > M$.

Theorem 5.1 (Theorem 8.10 [74]). Let $1 < p < \infty$ and let $\{u_n\}_{n\in\mathbb{N}}$ be a bounded sequence of functions in $H^1(\mathbb{R}^3)$. Suposse that for some $\epsilon > 0$ the set $E_n := \{x\,:\,|u_n(x)| > \epsilon\}$ satisfies $Meas(E_n) > \delta > 0$ for some δ and all $n \in \mathbb{N}$. Then, there is a sequence of vectors $y_n \in \mathbb{R}^3$ such that the translated sequence $\tilde{u}_n(x) := u(x + y_n)$ has a subsequence that converges weakly in $H^1(\mathbb{R}^3)$ to a nonzero function.

Any function u_n verifies the hypothesis of Lemma 5.3 with $p = 2$, $q = 8/3$, $p = 6$, $C_p = M$ and $C_q = (-4I_M/3C_S)^{\frac{8}{3}}$, C_r being a constant which comes from the boundedness of $\{u_n\}_{n\in\mathbb{N}}$ in $H^1(\mathbb{R}^3)$. Then, the whole sequence satisfies the hypotheses of Theorem 5.1. As consequence, there exist vectors y_n such that a subsequence of u_n verifies

$$\tilde{u}_n := u_n(\cdot + y_j) \to \tilde{u} \text{ weakly in } H^1(\mathbb{R}^3), \quad \|\tilde{u}\|_{H^1(\mathbb{R}^3)} > 0\,. \tag{5.15}$$

In order to deduce that $\tilde{u}$ is a minimizer of (5.10) we have to prove that

$$E_{POT}(\tilde{u}) \leq \liminf E_{POT}(\tilde{u}_n) \,.$$

To this aim, it is enough to observe that no charge *escapes* to infinity, i.e. $\|\tilde{u}\|_{\mathrm{L}^2(\mathbb{R}^3)} = M$, because this would imply the convergence $\tilde{u}_n \to \tilde{u}$ in $\mathrm{L}^2(\mathbb{R}^3)$ and $E_{POT}(\tilde{u}_n) \to E_{POT}(\tilde{u})$. The inequality (5.14) plays a crucial role at this point. If $\|\tilde{u}\|_{\mathrm{L}^2(\mathbb{R}^3)} = \alpha < M$, then it can be proved that $\tilde{u}_n$ is under the dichotomy hypothesis. Indeed, there exists $R > 0$ such that $\int_{B_R} |\tilde{u}|^2\, dx = \alpha - \epsilon/2$, for $\epsilon > 0$. On the other hand, let R_n be such that $\int_{B_{R_n}} |\tilde{u}_n|^2\, dx = \alpha + \epsilon/2$. The sequence $\{R_n\}_{n\in\mathbb{N}} \to \infty$ as $n \to \infty$ (otherwise, this would contradict (5.15)). We define $\tilde{u}_n^1 := \tilde{u}_n \chi_{B_R}$ and $\tilde{u}_n^2 := \tilde{u}_n \chi_{\mathbb{R}^3 - B_{R_n}}$, where $n \in \mathbb{N}$ and χ_Ω denotes the characteristic function of the set Ω. Then, we have that $\{\tilde{u}_n\}$ verifies

$$\begin{cases} \|\tilde{u}_n - (\tilde{u}_n^1 + \tilde{u}_n^2)\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq \delta_p(\epsilon) \to 0, \ \epsilon \to 0^+ , \ 2 \leq p < 6 \,; \\ |\int_{\mathbb{R}^3} |\tilde{u}_n^1|^2\, dx - \alpha| \leq \epsilon, \quad |\int_{\mathbb{R}^3} |\tilde{u}_n^2|^2\, dx - (M - \alpha)| \leq \epsilon; \\ \mathrm{dist}(\mathrm{Supp}\, \tilde{u}_n^1, \mathrm{Supp}\, \tilde{u}_n^2) = R_n - R \to \infty, n \to \infty; \\ \liminf_k \int_{\mathbb{R}^3} \{|\nabla \tilde{u}_n|^2 - |\nabla \tilde{u}_n^1|^2 - |\nabla \tilde{u}_n^2|^2\}\, dx \geq 0; \end{cases}$$

for $n \geq n_0$. The incompatibility between dichotomy and (5.14) allows to conclude that $\|\tilde{u}\|_{\mathrm{L}^2(\mathbb{R}^3)} = M$ as well as the minimizing charater of $\tilde{u}$. This concludes the proof with the technique of nonzero weak convergence after translations in Sobolev spaces.

Before deriving the inequality (5.14) in the SPS context, let us introduce some notations. Let a, b, c be positive constants and consider the operators T_{KIN}, T_{POT}, T, K: $\mathrm{H}^1(\mathbb{R}^3) \longrightarrow \mathbb{R}$ defined by

$$\begin{aligned} T_{KIN}(\psi) &= a \int_{\mathbb{R}^3} |\nabla \psi(x)|^2\, dx \,, \\ T_{POT}(\psi) &= \int_{\mathbb{R}^3} \left\{ b \int_{\mathbb{R}^3} \frac{|\psi(x)|^2 |\psi(x')|^2}{|x - x'|}\, dx' - c\, |\psi(x)|^{\frac{8}{3}} \right\} dx \,, \\ T(\psi) &= T_{KIN}(\psi) + T_{POT}(\psi) \,, \quad K(\psi) = -\frac{1}{4} \frac{(T_{POT}(\psi))^2}{T_{KIN}(\psi)} \,. \end{aligned}$$

Then, we have the following

Lemma 5.4. The minimization problems associated with the operators T and K over the set

$$\mathcal{B}_M = \{\psi \in \mathrm{H}^1(\mathbb{R}^3); \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M, \ T_{POT}(\psi) < 0\}$$

are equivalent in the following sense

$$T_M \equiv \inf\{T[\psi] \,;\psi \in \mathcal{B}_M\} = \inf\{K[\psi] \,;\psi \in \mathcal{B}_M\} \equiv K_M.$$

In addition, if ψ is a function in which T achieves its minimum, then it is also the minimum for the functional K. On the other hand, if ψ is a function in which K achieves its minimum, then the function ψ^σ is a minimum for T, where $\psi^\sigma(x) = \sigma^{\frac{2}{3}}\psi(\sigma x)$ and $\sigma = \frac{-T_{POT}(\psi)}{2\,T_{KIN}(\psi)}$.

Proof. Let $\psi_n \in \mathcal{B}_M,\ n \in \mathbb{N}$, a minimizing sequence for the problem T_M, i.e., $T(\psi_n) \to T_M$, as $n \to \infty$. The scaling $\psi^\sigma(x) = \sigma^{\frac{3}{2}}\psi(\sigma x),\ \sigma > 0$, preserves the properties of $\mathcal{B}_M$. Then, for every $\psi \in \mathcal{B}_M$ we can study the value of the parameter σ for which the total energy reaches the minimum over the uniparametric family of functions $\{\psi^\sigma\ ;\ \sigma \in \mathbb{R}^+\}$. From (5.9) and using that $T_{POT}(\psi) < 0$ we get $\sigma_{min} = \frac{-T_{POT}(\psi)}{2\,T_{KIN}(\psi)}$ and $T(\psi^{\sigma_{min}}) = -\frac{1}{4}\frac{(T_{POT}(\psi))^2}{T_{KIN}(\psi)} = K(\psi)$. This argument can be applied to every $\psi_n,\ n \in \mathbb{N}$, obtaining $\psi_n^{\sigma_{min}}$ such that

$$T(\psi_n) \geq T(\psi_n^{\sigma_{min}}) = K(\psi_n).$$

As consequence, $T_M \geq K_M$.

On the other hand, we now consider a minimizing sequence $\psi_n \in \mathcal{B}_M,\ n \in \mathbb{N}$, such that $K(\psi_n) \to K_M$, as $n \to \infty$. Again from (5.9) it can be seen that the operator K is invariant under the scaling $\psi(x) \to \psi^\sigma(x) \equiv \sigma^{\frac{2}{3}}\psi(\sigma x),\ \sigma \in \mathbb{R}^+$. This property allows us to choose $\sigma_n = -\frac{T_{POT}(\psi_n)}{2\,T_{KIN}(\psi_n)}$. Then,

$$T(\psi_n^{\sigma_n}) = K(\psi_n) = K(\psi_n^{\sigma_n}) \to K_M \quad \text{as } n \to \infty,$$

which implies $K_M \geq T_M$. This concludes the proof. □

As a particular case, we obtain a minimization problem equivalent to (5.10). Denoting $\mathcal{A}_M = \Big\{\psi \in \mathrm{H}^1(\mathbb{R}^3)\ ;\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M,\ E_{POT}[\psi] < 0\Big\}$, we have

$$I_M = \inf\Big\{E[\psi]\ ;\ \ \psi \in \mathrm{H}^1(\mathbb{R}^3),\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M\Big\} = \inf\left\{E[\psi];\ \psi \in \mathcal{A}_M\right\},$$

which shows that our problem is equivalent to

$$\inf\left\{-\frac{1}{4}\frac{(E_{POT}(\psi))^2}{E_{KIN}(\psi)}\ ;\ \psi \in \mathcal{A}_M\right\}. \tag{5.16}$$

Also, note that the set $\mathcal{A}_M$ is nonempty for any value of M, see [78, 26].

Furthermore we have $-E_{POT}(\psi_M) = 2E_{KIN}(\psi_M)$, where ψ_M denotes the minimizer of I_M. Consequently,

$$E(\psi_M) = \frac{1}{2}E_{POT}(\psi_M) = -E_{KIN}(\psi_M). \tag{5.17}$$

Using Lemma 5.4 we can prove the following result, which provides the strict sub–additivity property (5.14).

Proposition 5.3. For all $C_S > 0$ and $M > 0$ such that

$$M < \left(\frac{7\,C_S}{10\,C}\right)^{\frac{3}{4}}, \tag{5.18}$$

the sub–additivity condition (5.14) holds. Here, C_S denotes the Slater constant and C is the sharp constant in (5.5).

Proof. Assume that M satisfies (5.18). Using the scaling

$$\psi(x) \longrightarrow M^4 \psi(M^2 x),$$

the set $\mathcal{A}_M$ can be seen, for each $M \in \mathbb{R}^+$, as a transformation of the set

$$\mathcal{B}'_M := \{\psi \in \mathrm{H}^1(\mathbb{R}^3)\ ;\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = 1,\ E^M_{POT}(\psi) < 0\},$$

where

$$E^M_{POT}(\psi) = \frac{M^6}{8\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|\psi(x)|^2|\psi(y)|^2}{|x-y|}\,dxdy - \frac{3C_S M^{\frac{14}{3}}}{4}\int_{\mathbb{R}^3}|\psi(x)|^{\frac{8}{3}}\,dx\,.$$

In the same way, (5.10) can be rewritten as

$$I_M = \inf\left\{E^M_{KIN}(\psi) + E^M_{POT}(\psi)\ ;\ \psi \in \mathcal{B}'_M\right\},$$

where $E^M_{KIN}(\psi) = \frac{M^6}{2}\int_{\mathbb{R}^3}|\nabla\psi(x)|^2\,dx$. Since $E^M_{POT}(\psi) < 0$ by (5.18) and the proof of Lemma 5.1, we can take $\mathcal{B}'_M = \{\psi \in \mathrm{H}^1(\mathbb{R}^3)\ ;\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = 1\}$. Under this assumption, our minimization problem reads

$$\begin{aligned} I_M = M^{\frac{14}{3}-p}\inf\Bigg\{&\frac{M^{\frac{4}{3}+p}}{2}\int_{\mathbb{R}^3}|\nabla\psi(x)|^2\,dx + \frac{M^{\frac{4}{3}+p}}{8\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{|\psi(x)|^2|\psi(y)|^2}{|x-y|}\,dxdy \\ &-\frac{3C_S M^p}{4}\int_{\mathbb{R}^3}|\psi(x)|^{\frac{8}{3}}\,dx\ ;\ \psi \in \mathrm{H}^1(\mathbb{R}^3),\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = 1\Bigg\}, \end{aligned}$$

where p is a positive parameter to be precised. Then, we can apply Lemma 5.4 to show that this problem is equivalent to

$$\begin{aligned} I_M &= M^{\frac{14}{3}-p}\inf\Bigg\{-\frac{1}{4}\frac{\left(\frac{1}{2}M^{\frac{4}{3}+p}\int_{\mathbb{R}^3}|\nabla V(\psi)|^2\,dxdy - \frac{3C_S}{4}M^p\int_{\mathbb{R}^3}|\psi(x)|^{\frac{8}{3}}\,dx\right)^2}{\frac{M^{\frac{4}{3}+p}}{2}\int_{\mathbb{R}^3}|\nabla\psi(x)|^2\,dx} \\ &\qquad ;\ \psi \in \mathrm{H}^1(\mathbb{R}^3),\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = 1\Bigg\} \\ &= M^{\frac{14}{3}-p}\ \inf\Bigg\{-\frac{\left(M^{\frac{2}{3}+\frac{p}{2}}\int_{\mathbb{R}^3}|\nabla V(\psi)|^2 dxdy - \frac{3C_S}{2}M^{\frac{p}{2}-\frac{2}{3}}\int_{\mathbb{R}^3}|\psi(x)|^{\frac{8}{3}}dx\right)^2}{8\int_{\mathbb{R}^3}|\nabla\psi(x)|^2 dx} \\ &\qquad ;\ \psi \in \mathrm{H}^1(\mathbb{R}^3),\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = 1\Bigg\} \stackrel{def}{=} M^{\frac{14}{3}-p} I^M_1. \end{aligned}$$

Now (5.14) can be written as

$$M^{\frac{14}{3}-p}\, I_1^M < \alpha^{\frac{14}{3}-p}\, I_1^{\alpha} + (M-\alpha)^{\frac{14}{3}-p}\, I_1^{M-\alpha}, \quad \forall \alpha \in (0, M). \tag{5.19}$$

This inequality is based on the bound

$$M^k > \alpha^k + (M-\alpha)^k, \quad \forall \alpha \in (0, M),\ M \in \mathbb{R}^+,\ \forall k > 1\,.$$

We easily deduce

$$M^{\frac{14}{3}-p}\, I_1^M < \alpha^{\frac{14}{3}-p}\, I_1^{M} + (M-\alpha)^{\frac{14}{3}-p}\, I_1^{M}, \quad \forall \alpha \in (0, M),$$

for some $p \in (\frac{4}{3}, \frac{11}{3})$. To get (5.19) it is enough to show that for all $\eta \in (0, M)$, $I_1^M \leq I_1^\eta$ holds. This is true according to the nonincreasing character of the function

$$f_\psi : \quad \eta \longrightarrow -\frac{1}{8}\frac{\left(\eta^{\frac{2}{3}+\frac{p}{2}} \int_{\mathbb{R}^3} |\nabla V(\psi)|^2\, dx - \frac{3C_S}{2}\eta^{\frac{p}{2}-\frac{2}{3}} \int_{\mathbb{R}^3} |\psi|^{\frac{8}{3}}\, dx\right)^2}{\int_{\mathbb{R}^3} |\nabla \psi|^2\, dx}\,,$$

for $\eta \in (0, M)$ and $p \in (\frac{4}{3}, \frac{11}{3})$, independently of ψ. Indeed, given M there exists $p \in (\frac{4}{3}, \frac{11}{3})$ such that

$$\begin{aligned}\frac{df_\psi}{d\eta} = -\frac{1}{4}\frac{1}{\int_{\mathbb{R}^3} |\nabla\psi|^2\, dx}\left(\eta^{\frac{2}{3}+\frac{p}{2}}\int_{\mathbb{R}^3}|\nabla V(\psi)|^2\, dx - \frac{3C_S}{2}\eta^{\frac{p}{2}-\frac{2}{3}}\int_{\mathbb{R}^3}|\psi|^{\frac{8}{3}}\, dx\right) \times \\ \left(\left(\frac{2}{3}+\frac{p}{2}\right)\eta^{\frac{p}{2}-\frac{1}{3}}\int_{\mathbb{R}^3}|\nabla V(\psi)|^2\, dxdy - \left(\frac{p}{2}-\frac{2}{3}\right)\frac{3C_S}{2}\eta^{\frac{p}{2}-\frac{5}{3}}\int_{\mathbb{R}^3}|\psi|^{\frac{8}{3}}\, dx\right)\end{aligned}$$

is nonpositive for every $\psi \in \mathcal{B}_M$, where we have used (5.5). The optimal bound is obtained as p approaches $\frac{11}{3}$. Finally, this allows to establish the inequality $I_1^M \leq I_1^\eta$, which concludes the proof. □

Remark. It is not clear for us if the constant in (5.18) is or not optimal. Some idea about its optimality could open the discussion on the nonexistence of minimizers when (5.14) in Proposition 5.2 is violated.

Remark. Note that the Thomas-Fermi correction usually appears with positive sign (see [73]), which can be seen as a repulsive contribution to the potential. Then, the addition of this kind of correction simplifies the minimizing argument because combining the repulsive Thomas–Fermi with the attractive Slater correction allows to convexify the functional, see [72].

Now, a simple application of Propositions 5.2 and 5.3 yields the existence of a minimum, since every minimizing sequence is bounded in $\mathrm{H}^1(\mathbb{R}^3)$ and relatively compact (up to a translation). Furthermore, by standard arguments (see [70]) the regularity of the minimum can be deduced.

Theorem 5.2. Under the hypothesis of Proposition 5.3, there exists a minimizer $\psi_M \in C^\infty(\mathbb{R}^3)$ of (5.10) which satisfies the following Euler-Lagrange equation associated with the total energy functional $E[\psi]$:

$$-\frac{1}{2}\Delta\psi_M(x) + \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{|\psi_M(x')|^2\psi_M(x)}{|x-x'|}\,dx' - C_S|\psi_M|^{\frac{2}{3}}\psi_M(x) = \beta\psi_M(x) \qquad (5.20)$$

in a distributional sense, for some $\beta < 0$.

The following paragraph is devoted to show some consequences of this result.

Stationary solutions and solutions preserving the L^p norm in the repulsive case with negative energy

From Theorem 5.2 we can deduce the existence of standing waves $\psi(x,t) = e^{-i\beta t}\psi(x)$ as solutions of the SPS system in the repulsive case. Actually, these are time-periodic solutions which preserve the density. For this kind of solutions, the repulsive SPS system is reduced to the time-independent Schrödinger equation

$$\beta\psi = -\frac{1}{2}\Delta\psi + V\psi - C_S n^{\frac{1}{3}}\psi, \qquad \lim_{|x|\to\infty}\psi = 0, \qquad (5.21)$$

coupled to the Poisson equation

$$\Delta V = |\psi|^2, \quad \lim_{|x|\to\infty} V = 0. \qquad (5.22)$$

The system (5.21)-(5.22) can be written as an Euler-Lagrange equation associated with (5.10) (cf. (5.20)). Then, Theorem 5.2 implies the existence of solutions ψ_M. Since these functions minimize the total energy operator, (5.17) holds.

Let us also note that this kind of solutions do not exist for the SP system in the repulsive case, where every solution is dispersive.

Let us now introduce some other solutions which preserve the L^p norm.

Proposition 5.4. There exist solutions of the SPS system with negative potential energy and constant L^p norm along the time evolution.

Proof. The proof is based on the Galilean invariance of the system, see [20]. In fact, this property guarantees that if $\psi(x,t)$ is a solution to the SPS system with initial data ψ_0, then the solution corresponding to initial data $\psi_N(x,0) = e^{iNx}\psi_0(x)$, with $N \in \mathbb{R}^3$, is $\psi_N(x,t) = e^{iNx-itN^2}\psi(x-2tN,t)$. Now, using the minimal energy solution we can construct the solution $e^{-i\beta t}e^{iNx-it\frac{N^2}{2}}\psi_M(x-tN)$, which has initial data $e^{iNx}\psi_M(x)$. This solution preserves the L^p norm, has negative potential energy and its total energy is

$$E(e^{-i\beta t}e^{iNx-it\frac{N^2}{2}}\psi_M(x-tN)) = \frac{1}{2}N^2\|\psi_M\|_{\mathrm{L}^2(\mathbb{R}^3)} + I_M,$$

which obviously exceeds the minimal energy. A similar idea has been used in [65]. □

Optimal kinetic energy bounds

Minimizing the total energy functional implies, by Lemma 5.4, the minimization of the associated functional

$$T(\psi) = -\frac{1}{4}\frac{(E_{POT}(\psi))^2}{E_{KIN}(\psi)}.$$

In the next result we use this fact to deduce optimal bounds for the kinetic energy of a solution, depending on the initial total energy and the minimum of the energy functional.

Proposition 5.5. The kinetic energy associated with a solution of the repulsive SPS system in $\mathrm{H}^1(\mathbb{R}^3)$, E_{KIN}, ranges between the optimal values

$$E_{KIN}^{\pm} = -2I_M\left(1 - \frac{E_0}{2I_M} \pm \sqrt{1-\frac{E_0}{I_M}}\right), \tag{5.23}$$

where E_0 is the initial energy and I_M is the infimum of the total energy over the set $\{\psi \in \mathrm{H}^1(\mathbb{R}^3)\,;\, \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M\}$. Here, M is assumed to satisfy (5.18).

Proof. As before, this is a direct consequence of the equivalence between the energy minimization problem and (5.16). Since ψ_M minimizes (5.10), we have

$$-\frac{1}{4}\frac{(E_{POT}(\psi))^2}{E_{KIN}(\psi)} \geq -\frac{1}{4}\frac{(E_{POT}(\psi_M))^2}{E_{KIN}(\psi_M)} = -\frac{1}{4}\frac{4\,I_M^2}{-I_M} = I_M\,,$$

for all $\psi \in \mathrm{H}^1(\mathbb{R}^3)$ such that $\|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M$. Then, given $\psi(\cdot,t) \in \mathrm{H}^1(\mathbb{R}^3)$ a solution of the SPS system we find

$$E_{POT}(\psi) \geq -2\sqrt{-I_M}\sqrt{E_{KIN}(\psi)}, \quad \forall t \geq 0.$$

This yields a relation between the kinetic and the total energy:

$$E_0(\psi) \geq -2\sqrt{-I_M}\sqrt{E_{KIN}(\psi)} + E_{KIN}(\psi) \quad \forall t \geq 0,$$

or, using that the potential energy is negative,

$$E_{KIN}^2 + (4I_M - 2E_0)E_{KIN} + E_0^2 \leq 0.$$

This concludes the proof. □

Asymptotic behaviour in the repulsive case

In this section we study the time evolution of solutions to the SPS system. The standard arguments used to obtain various bounds on the $L^p(\mathbb{R}^3)$ norms of solutions to nonlinear Schrödinger equations are fruitless in our case. This is due to the fact that the sign of the potential energy depends on the balance between the Coulombian potential and the Slater correction. Then, we have to combine these arguments with some other techniques to find the $L^p(\mathbb{R}^3)$ bounds.

Dispersion equation and Pseudo–Conformal Law

Now we propose an alternative derivation of the well–known Pseudo-Conformal Law (see Chapter 4, [28], [59]) for the SPS system. The argument is based on the equivalence between this law and the dispersion equation obtained by using the quantum formalism.

Define the quantum mechanical expectation of f by

$$\langle f \rangle(t) \stackrel{def}{=} \int_{\mathbb{R}^3} \psi^*(x,t) f(x,t) \psi(x,t)\, dx,$$

where f could be an integrable vector–valued function or an operator acting on $\psi(x,t)$. Two usual examples are the first order moment of the density and the linear momentum

$$\langle x \rangle(t) = \int_{\mathbb{R}^3} \psi^*(x,t)\, x\, \psi(x,t)\, dx\,, \qquad \langle p \rangle(t) = \frac{1}{i} \int_{\mathbb{R}^3} \psi^*(x,t) \nabla \psi(x,t)\, dx. \tag{5.24}$$

We also introduce the usual quantum Poisson's Bracket formalism defined by

$$[A, B] = i(AB - BA).$$

Using the Hamiltonian operator associated with the Schrödinger equation

$$H = \frac{1}{2}p^2 + V_{Tot},$$

where V_{Tot} is defined by

$$V_{Tot}(\psi) = \frac{\epsilon}{4\pi}\int_{\mathbb{R}^3} \frac{|\psi(x')|^2}{|x-x'|}\,dx' - C_S|\psi(x)|^{\frac{2}{3}},$$

the system can be written as

$$i\frac{\partial\psi(x,t)}{\partial t} = H\,\psi.$$

This formalism allows to get an evolution equation for the space dispersion $(\Delta x)^2 \overset{def}{=} \langle x^2\rangle(t) - \langle x\rangle^2(t)$ in terms of the momentum dispersion $(\Delta p)^2 \overset{def}{=} \langle p^2\rangle(t) - \langle p\rangle^2(t)$.

Theorem 5.3. The position and momentum dispersions for a solution $\psi(x,t)$ of the SPS system with initial data in $\Sigma = \{u \in \mathrm{H}^2(\mathbb{R}^3)\,;\, xu \in \mathrm{L}^2(\mathbb{R}^3)\}$ satisfy the following equation

$$\frac{d^2}{dt^2}(\Delta x)^2(t) = 2\left(E(t) - \frac{1}{2}\langle p\rangle^2(t)\right) + (\Delta p)^2(t),$$

or equivalently

$$\frac{d^2}{dt^2}\langle x^2\rangle \;=\; 2\left(\frac{1}{2}\langle p^2\rangle + E(t)\right)\,, \tag{5.25}$$

where $E(t)$ denotes the total energy.

Proof. We compute $\frac{d^2}{d^2t}\langle x^2\rangle(t)$ and $\frac{d^2}{d^2t}\langle x\rangle^2$ by using that for any arbitrary f, the following indentity

$$\frac{d\langle f\rangle}{dt}(t) = \langle[H,f]\rangle(t) + \langle\frac{\partial f}{\partial t}\rangle(t)$$

holds. As consequence, we have

$$\frac{d}{dt}\langle x\rangle = \langle[H,x]\rangle = \langle[p^2,x]\rangle = \langle p\rangle\,,$$

since $V_{Tot}(\psi)$ and the position operator commute. Now, the preservation of the position momentum implies

$$\frac{d^2}{d^2t}\langle x\rangle^2 = 2\left(\frac{d}{dt}\langle x\rangle\right)^2 + 2\langle x\rangle\frac{d^2}{d^2t}\langle x\rangle = 2\langle p\rangle^2\,. \tag{5.26}$$

On the other hand, we have

$$\frac{d}{dt}\langle x^2\rangle = \langle [H,x^2]\rangle = \langle [\frac{1}{2}p^2, x^2]\rangle = \langle (xp+px)\rangle\,, \tag{5.27}$$

where we combined the antisymmetry property of Poisson's Brakets and

$$[AB,C] = A[B,C] + [A,C]B\,.$$

Now, from (5.27) we find

$$\begin{aligned}\frac{d^2}{dt^2}\langle x^2\rangle &= \langle [H,(xp-px)]\rangle = 2\,\langle [H,xp]\rangle \\ &= 2\,\langle p^2 - x\cdot\nabla_x V_{Tot}\rangle = 2\,\langle p^2\rangle - 2\,\langle x\cdot\nabla_x V_{Tot}\rangle\,. \end{aligned}\tag{5.28}$$

The second term in the right–hand side of (5.28) is equal to

$$\langle x\cdot\nabla_x V_{Tot}.\rangle = \int_{\mathbb{R}^3} x\nabla(V)|\psi|^2 dx - C_S\int_{\mathbb{R}^3} x\nabla(|\psi|^{\frac{2}{3}})|\psi|^2 dx\,,$$

where we can split

$$\int_{\mathbb{R}^3} x\,\nabla(|\psi|^{\frac{2}{3}})\,|\psi|^2\,dx = \frac{1}{4}\int_{\mathbb{R}^3} x\,\nabla|\psi|^{\frac{8}{3}}\,dx = -\frac{3}{4}\int_{\mathbb{R}^3}|\psi|^{\frac{8}{3}}\,dx. \tag{5.29}$$

Now, we estimate

$$\int_{\mathbb{R}^3} x\,\nabla(V)|\psi|^2\,dx = -\frac{1}{2}\int_{\mathbb{R}^3} V(x)\,n(x)\,dx \tag{5.30}$$

from

$$\begin{aligned}\int_{\mathbb{R}^3} x\nabla(V)|\psi|^2 dx &= -\frac{\epsilon}{4\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} x\frac{x-y}{|x-y|^3}\,n(x)\,n(y)\,dxdy \\ &= -\frac{\epsilon}{4\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} x\frac{1}{|x-y|}\,n(x)\,n(y)\,dxdy \\ &\quad -\frac{\epsilon}{4\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} y\frac{x-y}{|x-y|^3}\,n(x)\,n(y)\,dxdy \\ &= -\int_{\mathbb{R}^3} V(x)\,n(x)\,dx \\ &\quad +\frac{\epsilon}{4\pi}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} x\frac{x-y}{|x-y|^3}\,n(x)\,n(y)\,dydx \\ &= -\int_{\mathbb{R}^3} V(x)\,n(x)\,dx - \int_{\mathbb{R}^3} x\nabla(V)|\psi|^2\,dx. \end{aligned}$$

Thus, combining (5.28), (5.30) and (5.29) we get

$$\frac{d^2}{d^2t}\langle x^2\rangle = 2\left(\langle p^2\rangle + \frac{1}{2}\langle V\rangle - \frac{3}{4}C_S\langle n^{\frac{2}{3}}\rangle\right) = 2\left(\frac{1}{2}\langle p\rangle + E(t)\right)\,,$$

which concludes the proof. □

Now, we can show the equivalence between the Pseudo–Conformal Law and the dispersion equation (more precisely, equation (5.25). This gives rises to an alternative derivation of the Pseudo–Conformal Law widely studied in the literature ([28], [59]):

$$\frac{d}{dt}\left(\|(x+it\nabla)\psi\|^2_{\mathrm{L}^2(\mathbb{R}^3)} + t^2\int_{\mathbb{R}^3} Vn\,dx - \frac{3}{2}C_S t^2 \int_{\mathbb{R}^3}|\psi|^{\frac{8}{3}}dx\right) = t\int_{\mathbb{R}^3} Vn\,dx - \frac{3}{2}C_S t\int_{\mathbb{R}^3}|\psi|^{\frac{8}{3}}\,dx. \qquad (5.31)$$

To prove this equivalence, we first expand

$$\begin{aligned}\|(x+it\nabla)\psi(t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} &= \int_{\mathbb{R}^3}\{x^2|\psi|^2 + t^2\,|\nabla\psi|^2 + 2t\,\mathrm{Im}\nabla\psi^*\cdot x\psi\}\,dx \\ &= \langle x^2\rangle + t^2\,\langle p^2\rangle + 2t\,\mathrm{Im}\int_{\mathbb{R}^3}\nabla\psi^*\cdot x\psi\,dx \\ &= \langle x^2\rangle + t^2\,\langle p^2\rangle + 2t\, - t\frac{d}{dt}\langle x^2\rangle\,, \qquad (5.32)\end{aligned}$$

where Im denotes the imaginary part and where we have considered (5.27). Therefore, the Pseudo–Conformal Law can be equivalently written as

$$\begin{aligned}&\frac{d}{dt}\left(\langle x^2\rangle - t\,\frac{d}{dt}\langle x^2\rangle + t^2\,\langle p^2\rangle + 2t^2E_{POT}(\psi)\right) = 2t\,E_{POT}(\psi),\\ &\frac{d}{dt}\left(\langle x^2\rangle - t\,\frac{d}{dt}\langle x^2\rangle + 2t^2E(\psi)\right) = 2t\,E_{POT}(\psi),\\ &t\frac{d^2}{dt^2}\langle x^2\rangle = -2t\,E_{POT}(\psi) + 4tE(\psi) = 2t\,E(\psi) + 2t\,E_{KIN}(\psi)\,,\end{aligned}$$

where we have used the time invariance of the energy. Now, it can be easily observed the equivalence between (5.31) and (5.25).

We finally remark that $\langle x^2\rangle$ is in general a nonbounded operator for the SPS solutions. However, we can prove that if $\langle x^2\rangle$ is bounded for the initial condition, then this operator is well–defined for the corresponding solution. The proof is an straightforward adaptation of the proof done in [59] for the SP system.

Asymptotic behaviour

Equation (5.25) allows to deduce (for positive energies) some important consequences about the long time behaviour of the solutions. The first one is that the solutions tend to expand unboundedly when the energy is positive. The second consequence is a decay bound for the potential energy.

Proposition 5.6. Let ϕ the initial data of the SPS system such that $x\phi \in \mathrm{L}^2(\mathbb{R}^3)$ and $E(\phi) > 0$. Then, the system expands unboundedly for large times and the position dispersion $\langle x^2\rangle(t)$ grows like $O(t^2)$.

Proof. To deduce this result we consider again the dispersion equation (5.25), rewritten as

$$\frac{1}{2}\frac{d^2}{dt^2}\langle x^2\rangle = E_{KIN} + E(t) = 2E(t) - E_{POT}. \tag{5.33}$$

Since $\|\phi\|_{L^2} = M$ and $E(\phi) \equiv E$ are time invariant, we can bound the right-hand side of (5.33) by using (5.23) and obtain

$$E + E^-_{KIN} \leq \frac{1}{2}\frac{d^2}{dt^2}\langle x^2\rangle \leq E + E^+_{KIN}.$$

By using the lower bound of the Slater potential, we also find

$$E < \frac{1}{2}\frac{d^2}{dt^2}\langle x^2\rangle \leq 2E + C_{(E,M)}.$$

If E is positive, then the upper and lower bounds are also positive. This allows to deduce the result by integrating twice in time. □

As an immediate consequence we can deduce lower bounds for the L^p norm of the solutions. These lower bounds are either positive constants or coincide with the usual decay rates of the free Schrödinger equation, depending on a relation between the total energy, the mass and the linear momentum (5.24). For simplicity we shall denote $< p > (\psi) = \frac{1}{i}\int_{\mathbb{R}^3}\psi^*(x)\nabla\psi(x)$.

Corollary 5.1. Let ψ be a SPS solution with initial data $\phi \in \Sigma$ such that

$$E[\phi] < \frac{1}{2}\frac{|< p > (\phi)|^2}{\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}}. \tag{5.34}$$

Then, there exist positive constants C, C' and C'' depending on $\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}$, $E[\phi]$, $|< p > (\phi)|^2$ and p such that

$$\|\psi(t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \geq C, \quad E_{POT}[\psi] \leq -C', \quad \forall t \geq 0, \quad p \in [\frac{8}{3}, 6]. \tag{5.35}$$

In the case

$$E[\phi] \geq \frac{1}{2}\frac{|< p > (\phi)|^2}{\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}}, \tag{5.36}$$

the following lower bound

$$\|\psi(\cdot,t)\|_{L^p(\mathbb{R}^3)} \geq \frac{C''}{t^{\frac{3p-6}{2p}}}, \quad \forall t > \xi > 0, \quad p \in [2,6], \tag{5.37}$$

holds.

Proof. To show the relevance of (5.34) and (5.36) we shall use again the Galilean invariance of the system. The solutions ψ_N associated with an initial condition $\phi_N = e^{iNx}\phi_0(x)$ have the same $\mathrm{L}^p(\mathbb{R}^3)$ norm and the same potential energy for every N and time t, while the total energy is

$$E[\phi_N] = \frac{1}{2}N^2\|\phi_N\|_{\mathrm{L}^2(\mathbb{R}^3)} + N < p > (\phi) + E[\phi_0]\,.$$

It is a simple matter to observe that for every ϕ_0 the Galilean invariance gives a parametric family of initial data ϕ_N for which the time evolution of the $\mathrm{L}^p(\mathbb{R}^3)$ norm and of the potential energy are the same. The analysis of a particular member of the family of Galilean transformations allows to deduce the behaviour of the $\mathrm{L}^p(\mathbb{R}^3)$ norm and of the potential energy for the whole family.

By a simple optimization argument one can easily check that (5.34) implies the existence of initial data with negative energy in the family, while the energy of the initial data is nonnegative if (5.36) holds.

Under hypothesis (5.36), the initial data ϕ can be assumed to have positive energy (if not, ϕ can be replaced by $\phi_{N'}$ belonging to the class of Galilean transforms of ϕ with positive energy). We have

$$\begin{aligned}\|\psi(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} &= \int_{|x|\leq R}|\psi(x,t)|^2dx + \int_{|x|\geq R}|\psi(x,t)|^2dx\,,\\ &\leq CR^{\frac{3p-6}{p}}\|\psi(x,t)\|^2_{\mathrm{L}^p(\mathbb{R}^3)} + \frac{1}{R^2}\langle x^2\rangle.\end{aligned}$$

By optimizing over R we obtain

$$\|\psi(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} \leq C\left(\|\psi(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)}\right)^{\frac{4p}{5p-6}}\langle x^2\rangle^{\frac{3p-6}{5p-6}}\,.$$

This concludes (5.37) by using Proposition 5.6 and the positivity of the total energy.

On the other hand, if ϕ fulfills (5.34), then we can choose a Galilean translation $\phi_{N'}$ whose total energy is negative. In this case, we find

$$-\|\psi_{N'}(t)\|^{\frac{8}{3}}_{\mathrm{L}^{\frac{8}{3}}(\mathbb{R}^3)} < E[\phi_{N'}] < 0\,, \quad \forall t \geq 0\,.$$

We conclude (5.37) by using the Hölder inequality, mass preservation and the invariance of the L^p norm of the solutions under Galilean translations. □

The next result provides a rate–of–decay estimate for the potential energy. However, the potential energy may be negative as shown before. For instance, from (5.5) we know that the potential energy is always nonpositive in the repulsive case.

Proposition 5.7. Let $\phi \in \Sigma$ the initial data of the SPS system. Then, the potential energy associated with the solution $\psi(x,t)$ satisfies the inequality

$$E_{POT}(\psi)(t) \leq \frac{C_\xi}{t}, \quad \forall\, t \geq \xi > 0, \tag{5.38}$$

where C_ξ is a positive constant depending on ξ.

Proof. Integrating the pseudo–conformal law from ξ to t we find

$$\begin{aligned}\|(x+it\nabla)\psi(\cdot,t)\|^2_{L^2(\mathbb{R}^3)} &+ t^2\int_{\mathbb{R}^3} |\nabla V(x,t)|^2\,dx - \frac{3}{2}C_S t^2 \int_{\mathbb{R}^3} |\psi(x,t)|^{\frac{8}{3}} dx \\ &= C + \int_\xi^t \left(s\int_{\mathbb{R}^3} V(x,s)n(x,s)dx - \frac{3}{2}C_S s\int_{\mathbb{R}^3} |\psi(x,s)|^{\frac{8}{3}} dx\right) ds,\end{aligned} \tag{5.39}$$

where

$$\begin{aligned}C= \|(x+i\xi\nabla)\psi(\cdot,\xi)\|^2_{L^2(\mathbb{R}^3)} &+ \xi^2\int_{\mathbb{R}^3} |\nabla V(x,\xi)|^2 dx \\ &-\frac{3}{2}\xi^2 C_S\int_{\mathbb{R}^3} |\psi(x,\xi)|^{\frac{8}{3}} dx\end{aligned} \tag{5.40}$$

and $\xi \geq 0$. Notice that this constant can be chosen positive if ξ is small enough because the right-hand side in (5.40) goes to $\|x\phi\|^2_{L^2(\mathbb{R}^3)}$ as $t \to 0$. Let $g(t) = t^2\int_{\mathbb{R}^3} V n dx - \frac{3}{2}C_S t^2 \int_{\mathbb{R}^3} |\psi|^{\frac{8}{3}} dx$. Then, from (5.39) we deduce

$$g(t) \leq C + \int_\xi^t \frac{g(s)}{s}\, ds.$$

Now Gronwall's lemma yields

$$g(t) = t^2\int_{\mathbb{R}^3} V n dx - \frac{3}{2}C_S t^2\int_{\mathbb{R}^3} |\psi|^{\frac{8}{3}} dx \leq \frac{Ct}{\xi} \equiv C_\xi t\,, \quad \forall t \geq \xi,$$

and we are done with the proof. □

Consider the function

$$f_\psi(t)= \|(x+it\nabla)\psi(\cdot,t)\|^2_{L^2(\mathbb{R}^3)} + t^2\int_{\mathbb{R}^3} |\nabla V(x,t)|^2\,dx - \frac{3}{2}C_S t^2\int_{\mathbb{R}^3} |\psi(x,t)|^{\frac{8}{3}} dx.$$

From (5.38) we get

$$f_\psi(t) \le C + \int_\xi^t \frac{C_\xi s}{s} ds \le C_\xi t.$$

The evolution of f_ψ (more precisely, the evolution of its sign) implies qualitative differences in the behaviour of the associated solution. The following result provides a decay estimate for the potential energy in the attractive case or a weak decay property for some $L^{p,q}$–norms of the wave functions.

Corollary 5.2. If there exists $t_0 \in \mathbb{R}^+$ such that $f_\psi(t_0) < 0$, then $f_\psi(t) < 0$ for all $t \ge t_0$. Furthermore,

$$2E_{POT}(\psi) \le \left(\frac{f_\psi(t_0)}{t_0} \right) \frac{1}{t} < 0, \quad \forall t \ge t_0.$$

Otherwise we have

$$\int_\xi^\infty \|\psi(s)\|_{L^p(\mathbb{R}^3)}^{\frac{4p}{3(p-2)}} ds \le C, \quad \forall p \in (2,6],$$

where C is a positive constant depending on p, $\|\phi\|_{L^2}$, $\|x\phi\|_{L^2}$ and ξ.

Proof. The first part of the Corollary is deduced by using similar arguments to those of Proposition 5.7, when taking $\xi = t_0$.

Setting $\psi_g(x,t) := \exp(-\frac{\mathrm{ix}^2}{2\mathrm{t}})\psi(\mathrm{x},\mathrm{t})$ we have

$$it\nabla\psi_g(x,t) = \exp\left(-\frac{\mathrm{ix}^2}{2\mathrm{t}}\right)(\mathrm{x} + \mathrm{it}\nabla)\psi, \tag{5.41}$$

which implies

$$f_\psi(t) = t^2 \|\nabla\psi_g\|^2_{\mathrm{L}^2(\mathbb{R}^3)} + t^2 \int_{\mathbb{R}^3} V(x,t)n(x,t)\,dx - \frac{3}{2} C_S t^2 \int_{\mathbb{R}^3} |\psi(x,t)|^{\frac{8}{3}} dx.$$

In the case $f_\psi > 0$ we have

$$\|\nabla\psi_g\|^2_{\mathrm{L}^2(\mathbb{R}^3)} + \int_{\mathbb{R}^3} V(x,t)n(x,t)\,dx - \frac{3}{2} C_S \int_{\mathbb{R}^3} |\psi(x,t)|^{\frac{8}{3}} dx > 0. \tag{5.42}$$

On the other hand, we can rewrite (5.31) in the following form

$$\frac{d}{dt}\left(t\|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} + 2tE_{POT}(\psi)(t) \right) = -\|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)}.$$

Integrating between $\xi > 0$ and $t > \xi$ yields

$$t\|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} + 2tE_{POT}(\psi)(t) = \frac{f_\psi(\xi)}{\xi} - \int_\xi^t \|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)}. \tag{5.43}$$

Now, the left-hand side of (5.43) can be estimated by using (5.42), which gives

$$\int_\xi^t \|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} \le \frac{f_\psi(\xi)}{\xi}.$$

The proof concludes by noting that the L^p norm of ψ and ψ_g coincide, then we can apply the Gagliardo-Nirenberg inequality to ψ_g. □

Let us now prove some decay properties of the solutions in the case of nonnegative potential energy.

Proposition 5.8. Let $\phi \in \Sigma$ the initial data of the SPS system and let ψ be the corresponding solution. If the potential energy associated with ψ is nonnegative along the time evolution, then there exist constants $C > 0$ which depend on $\|\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}$ and $\|x\phi\|_{\mathrm{L}^2(\mathbb{R}^3)}$ such that

(i) $\forall\, |t| \ge 1,\ \forall\, p \in [2,6]\,,\ \|\psi(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \le \frac{C}{|t|^{\frac{3}{2}(\frac{1}{2}-\frac{1}{p})}}$,

(ii) $\forall\, |t| \ge 1,\ \forall\, p \in [1,3]\,,\ \|n(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \le \frac{C}{|t|^{\frac{3}{2}(1-\frac{1}{p})}}$,

(iii) $\forall\, |t| \ge 1,\ \forall\, p \in]3,\infty[\,,\ \|V(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \le \frac{C}{t^{(\frac{1}{2}-\frac{3}{2p})}}$,

(iv) $\forall\, |t| \ge 1,\ \forall\, p \in]\frac{3}{2},\infty[\,,\ \|\nabla V(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \le \frac{C}{t^{(1-\frac{3}{2p})}}$.

Proof. The proof follows the steps of Proposition 5.7 and the arguments given in [29], [59].

Using (5.41) the pseudo–conformal law can be written as

$$\begin{aligned} t^2\|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} = C + &\int_\xi^t \Big(s\int_{\mathbb{R}^3} |\nabla V(x,s)|^2 dx - \frac{3}{2} C_S s\int_{\mathbb{R}^3} |\psi(s)|^{\frac{8}{3}} dx\Big)\, ds \\ &-t^2 \int_{\mathbb{R}^3} |\nabla V(x,t)|^2 n(x,t) dx + \frac{3}{2} C_S t^2 \int_{\mathbb{R}^3} |\psi(x,t)|^{\frac{8}{3}} dx. \end{aligned}$$

Then, applying (5.38) and taking into account the nonnegativity of the potential energy we find

$$\|\nabla\psi_g(\cdot,t)\|^2_{\mathrm{L}^2(\mathbb{R}^3)} \le \frac{C'}{t\xi},$$

for all $t \ge \xi$, where $C' = C'(C,\xi) > 0$. Now, the Gagliardo–Nirenberg inequality (applied to ψ_g) allows to get (i) for $p \in [2,6]$ and $a = 3\left(\frac{1}{2} - \frac{1}{p}\right)$:

$$\begin{aligned} \|\psi(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} &= \|\psi_g(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} \le \gamma(p)\|\nabla\psi_g(\cdot,t)\|^a_{\mathrm{L}^2(\mathbb{R}^3)}\|\psi_g(\cdot,t)\|^{1-a}_{\mathrm{L}^2(\mathbb{R}^3)} \\ &\le \gamma(p)\|\nabla\psi_g(\cdot,t)\|^a_{\mathrm{L}^2(\mathbb{R}^3)}\|\phi\|^{1-a}_{\mathrm{L}^2(\mathbb{R}^3)} \le \frac{C'}{t^{\frac{3}{2}\left(\frac{1}{2}-\frac{1}{p}\right)}}. \end{aligned}$$

(ii) is a consequence of $\|n(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} = \|\psi(\cdot,t)\|^2_{L^{2p}}$, while (iii) can be deduced from the Hardy–Littlewood-Sobolev inequality and (ii):

$$\begin{aligned}\|V(\cdot,t)\|_{\mathrm{L}^p(\mathbb{R}^3)} &\leq C' \left\|\frac{1}{r} * n(\cdot,t)\right\|_{\mathrm{L}^p(\mathbb{R}^3)} \leq C'\|n(\cdot,t)\|_{L^q(\mathbb{R}^3)} \\ &\leq C' \frac{1}{t^{\frac{3}{2}(1-\frac{1}{q})}} \leq C' \frac{1}{t^{(\frac{1}{2}-\frac{3}{2p})}},\end{aligned}$$

where $\frac{1}{q} = \frac{1}{p} + \frac{2}{3}$ and $q \in]1,3[$. The proof of (iv) is analogous to that of (iii).
□

Minimization of the energy in the attractive case

The aim of this section is to give some results concerning the asymptotic behaviour in time of solutions to the SPS system under the assumption of attractive interactions. In this case the energy functional reads

$$E[\psi]=\int_{\mathbb{R}^3}\left\{\frac{1}{2}|\nabla\psi(x,t)|^2-\int_{\mathbb{R}^3}\frac{|\psi(x,t)|^2|\psi(x',t)|^2}{8\pi|x-x'|}\,dx'-\frac{3}{4}C_S|\psi(x,t)|^{\frac{8}{3}}\right\}dx \quad (5.44)$$

Using the same arguments developed before to bound the energy in the repulsive case and the inequality (5.5), it can be shown that this functional has a lower bound over the set $\{\psi \in \mathrm{H}^1(\mathbb{R}^3)\,;\, \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M\}$. In [20] it was proved the existence of a minimizer ψ_M of the energy functional (5.44) in $\mathrm{H}^1(\mathbb{R}^3)$ under the constraint $\|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M,\ M \in \mathbb{R}^+$. Furthermore, this minimum was found to be spherically symmetric. The proof given above can be also adapted to this case, therefore it might give an alternative way to obtain the existence of a minimum. In this case the restriction on the L^2–norm is not necessary because the potential energy is always negative.

Theorem 5.4. For all $M > 0$ there exists a minimizer $\psi_M \in C^\infty(\mathbb{R}^3)$ of the problem

$$\min\{E[\psi]; \psi \in \mathrm{H}^1(\mathbb{R}^3),\ \|\psi\|_{\mathrm{L}^2(\mathbb{R}^3)} = M\},$$

where $E[\psi]$ denotes the energy functional (5.44). Also, psi_M satisfies the Euler-Lagrange equation

$$-\frac{1}{2}\Delta\psi_M - \frac{1}{4\pi}\int_{\mathbb{R}^3}\frac{|\psi_M(x',t)|^2}{|x-x'|}\,dx'\,\psi_M - C_S|\psi_M|^{\frac{2}{3}}\psi_M = \beta\psi_M$$

in a distributional sense, for some $\beta < 0$.

As an immediate consequence we get the existence of stationary waves of the form $\psi(x,t) = e^{-i\beta t}\psi_M(x)$ and we can construct solutions of the same type than in Proposition 5.4 satisfying (5.17). Also, from the minimization of the total energy operator we can deduce the same bound for the kinetic energy as in (5.23).

The dispersion properties (in the positive energy case) as well as the dispersion and pseudo–conformal laws are also valid in this case. However, since the potential energy is always negative in the attractive case, the decay properties of the solutions are no longer verified.

It is also possible to study the asymptotic behaviour of the solutions at $t = 0$. Actually, this analysis is a straightforward adaptation of the techniques developed in [29] and shall be omitted here.

Chapter 6

Nonlinear stochastic discrete drift-diffusion theory of charge fluctuations and domain relocation times in semiconductor superlattices

Introduction

The current-voltage (I-V) characteristics of highly doped weakly coupled semiconductor superlattices (SL) typically exhibits many sharp branches due to formation of static electric field domains [44]. Two branches are separated by a discontinuity in the current. The electric field profile associated to a given branch consists of two regions of constant electric field (domains) separated by a charge accumulation layer (domain boundary), which is confined to one or several quantum wells. The location of the domain boundary distinguishes I-V branches: as the voltage increases, the domain boundary is located closer to the injecting contact and the high field domain increases at the expense of the low field one [21]. Branches exhibit hysteresis cycles due to coexistence of two or more stable electric field profiles at a given value of the voltage. Many interesting dynamical phenomena are associated to these SL: (i) response of the SL to sudden changes in bias (which may force relocation of electric field domains [64, 102, 80, 3]), and (ii) self-sustained oscillations of the current provided temperature is raised or doping is lowered [63, 101]. Motivated by recent experimental evidence [92, 93], we shall present in this chapter a stochastic theory of domain relocation in highly doped SL.

In relocation experiments [80, 92, 94], a doped SL displaying a multistable I-V characteristic is biased (typically) on the first plateau, say in the middle of a branch. The corresponding field configuration has two domains separated by a domain wall which is an accumulation layer. Then the voltage is suddently increased from V_0 to $V_1 = V_0 + \Delta V$ and the time evolution of the current is recorded. Depending on ΔV, the domain wall has to relocate so that a stable field configuration appropriate to the new voltage is reached [80]. The outcome has been studied numerically using a discrete resonant tunneling model with Ohmic boundary conditions [3]. For any $\Delta V < 0$ as well as for small positive ΔV, the relocation of the domain wall always occurs by a direct movement of the charge monopole forming the domain boundary to its final position. This movement may be either upstream or downstream the electron flow as needed. However, for sufficiently large $\Delta V > 0$, a charge dipole is injected at the emitter contact in addition to the existing monopole, because the latter cannot move upstream beyond one SL period without encountering a stable field configuration [3]. Recent experiments by Rogozia et al.[94] confirm this theoretical picture. Other experiments have shown that the relocation time for up jumps ($\Delta V > 0$) close to the discontinuity in the I-V characteristic is random and have also investigated its probability distribution function [92, 93]. What is causing randomness in the relocation time? In this work we argue in favor of shot noise.

Shot noise occurring during a transport process is due to fluctuations in the occupation number of states caused by (i) thermal random initial fluctuations; (ii) the random nature of quantum-mechanical transmission/reflection (partition noise). The latter is in turn caused by the discrete nature of the electric charge.

The rest of the chapter is organized as follows. In Section 6, we derive a stochastic discrete drift-diffusion model (DDD) from the previously studied deterministic one (see Chapter 1) considering partition only noise (thermal noise is negligible in the low temperature limit). The stochastic DDD model has multiplicative white noise terms obeying Poissonian statistics and it has been solved numerically by means of a second order scheme proposed by Platen [66]. The results of numerically solving the stochastic model are reported in Section 6. Our numerical results agree qualitatively with Rogozia et al experiments [92], thereby enforcing the idea that shot noise is responsible for the observed fluctuations in domain relocation time. Details on the numerical scheme and comparison to rougher schemes and to the results of solving the deterministic model with random initial conditions are contained in the Appendix.

Stochastic Discrete Drift–Diffusion Model

The DDD model given by Poisson equation

$$F_i - F_{i-1} = \frac{e}{\overline{\varepsilon}}(n_i - N_D^w), \quad i \in \{1, \ldots, N\}\,, \tag{6.1}$$

Ampere equation

$$\frac{\overline{\varepsilon}}{e}\frac{dF_i}{dt} + J_{i\to i+1} = J(t), \quad i \in \{0, \ldots, N\} \tag{6.2}$$

and the tunneling current densities defined by (1.16), (1.17) and (1.18), has a conceptual difficulty coming from charge quantization that motivates the introduction of shot noise terms. The electric charge in each SL period, en_iA (A is the SL cross section), should be a multiple of the electron charge e. This implies that the true charge fluctuates about the mean value given by the deterministic DDD model. To analyze charge fluctuations, we may use the Langevin ideas and add an appropriate stochastic term to the deterministic current densities. The SL cross section A is very large (a circular cross section of diameter 120 μm wide as compared to a SL period of $l = 13$ nm) and the barrier transmission coefficient is very small.

Then we may use the classic Poissonian shot noise to model charge fluctuations [19]:

$$J_{i\to i+1} = \frac{n_i v^{(f)}(F_i) - n_{i+1} v^{(b)}(F_i)}{l} + J^{(r)}_{i\to i+1}(t), \tag{6.3}$$

for $i = 1, \cdots N-1$, where $J^{(r)}_{i\to i+1}$ represents the random current which satisfies

$$\langle J^{(r)}_{i\to i+1}\rangle = 0,$$

$$\begin{aligned}&\langle J^{(r)}_{i\to i+1}(t)\ J^{(r)}_{j\to j+1}(t')\rangle = \\ &\delta_{ij}\delta(t-t')\,(Al)^{-1}[n_i v^{(f)}(F_i) + n_{i+1} v^{(b)}(F_i)],\end{aligned} \tag{6.4}$$

and $v^{(b)}$, $v^{(f)}$ are defined as follows

$$v^{(b)}(F) = \frac{D(F)}{l}\,, \quad v^{(f)}(F) = v^{(b)}(F) + v(F), \tag{6.5}$$

The logic behind this form of the random tunneling current is as follows. We consider that uncorrelated electrons are arriving at the ith barrier with a distribution function of time intervals between arrival times that is Poissonian [19]. Then the shot noise spectrum for the current $eJ^{(r)}_{i\to i+1}A$ is given by the average current, $[n_i v^{(f)}(F_i) + n_{i+1} v^{(b)}(F_i)]\, e^2 A/l$, which in turn yields Eq. (6.4). As remarked in Ref. [19], this procedure assumes low transmission through barriers and it yields an upper bound for the shot noise amplitude. In addition, the tunneling current is approximated by a discrete drift-diffusion expression whose transport coefficients (drift velocity, diffusivity, ...) will be quantitatively different from those of the actual sample used in experiments. Given the exponential dependence of several quantities, relatively small differences in the location of extrema of the drift velocity, etc. may produce substantial differences. Thus, the mathematical model provides quantitative differences in the results but it yields the correct qualitative behavior.

The special nature of the emitter and collector layers is considered in the boundary conditions, given by (6.2) with $i = 0$ and $i = N$ and different constitutive relations for the tunneling currents:

$$J_{0\to 1} = j_e^{(f)}(F_0) - \frac{n_1 w^{(b)}(F_0)}{l} + J_{0\to 1}^{(r)}\,, \tag{6.6}$$

$$J_{N\to N+1} = \frac{n_N w^{(f)}(F_N)}{l} + J_{N\to N+1}^{(r)}\,. \tag{6.7}$$

Here we still have $\langle J_{i\to i+1}^{(r)}\rangle = 0$ for $i = 0$ and $i = N$, while the correlations are:

$$\langle J_{0\to 1}^{(r)}(t) J_{0\to 1}^{(r)}(t')\rangle = \frac{j_e^{(f)}(F_0) l + n_1 w^{(b)}(F_0)}{Al}\delta(t-t'), \tag{6.8}$$

$$\langle J_{N\to N+1}^{(r)}(t) J_{N\to N+1}^{(r)}(t')\rangle = \frac{n_N w^{(f)}(F_N)}{Al}\,\delta(t-t'). \tag{6.9}$$

The drift velocity v, the diffusion coefficient D, the emitter current density $ej_e^{(f)}$, the emitter backward velocity $w^{(b)}$ and the collector forward velocity $w^{(f)}$ are functions of the electric field depicted in Figs. 6.1 and 6.2.

In addition to the boundary conditions, the Ampere and Poisson equations should be supplemented as usual with the voltage bias condition,

$$\sum_{i=1}^{N} F_i l = V\,, \tag{6.10}$$

where V denotes voltage. Eqs. (6.1), (6.2), (6.3) to (6.10) form a closed system of stochastic equations for n_i, F_i and J. They constitute the stochastic DDD model. To analyze this model, it is convenient to render all equations dimensionless. Let us denote by (F_M, v_M) the coordinates of the first positive

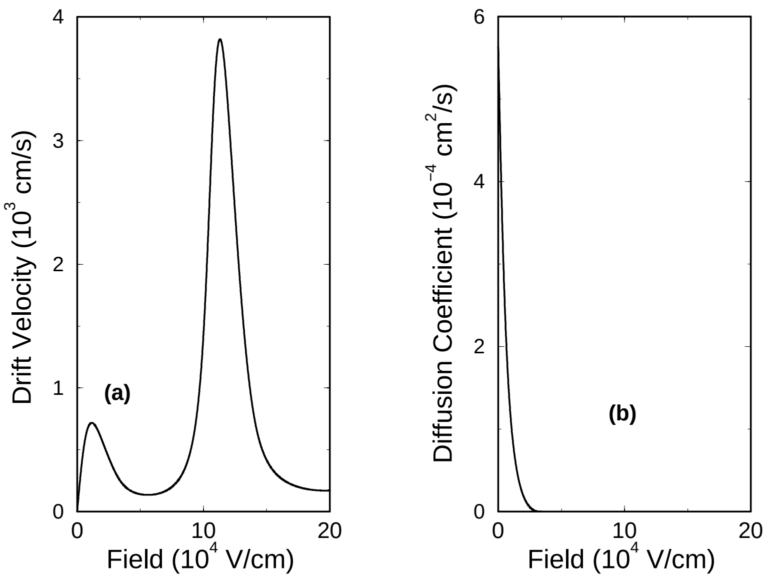

Figure 6.1: Drift velocity and Diffusion coefficient corresponding to the 9/4 GaAs/AlAs SL of Ref. [63].

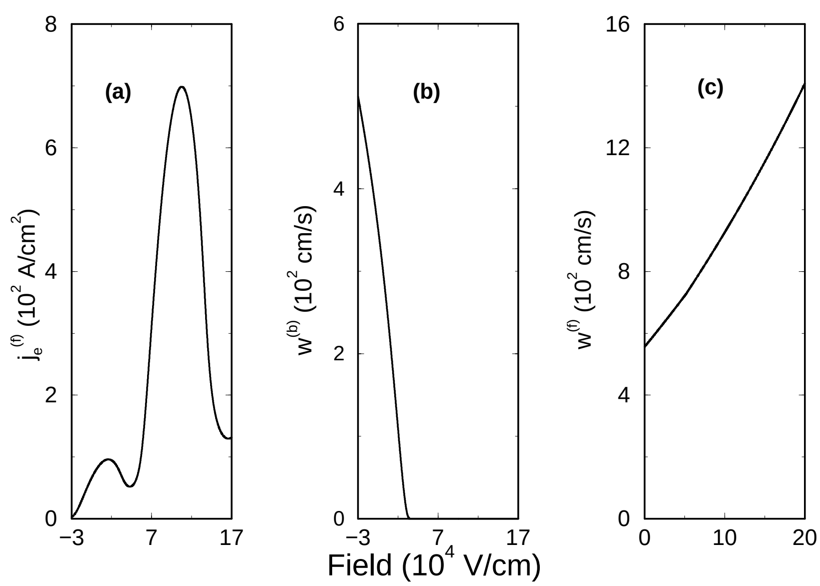

Figure 6.2: Current–field contact characteristics corresponding to the 9/4 GaAs/AlAs SL of Ref. [63].

maximum of the drift velocity $v(F)$. We adopt F_M, N_D^w, v_M, $v_M l$, $eN_D^w v_M/l$ and $\varepsilon F_M l/(eN_D^w v_M)$ as units of F_i, n_i, $v(F)$, $D(F)$, eJ and t, respectively. According to the parameters of the superlattice previously refered we find $F_M = 11.60$ kV/cm, $N_D^w = 1.5\times 10^{11}$ cm $^{-2}$, $v_M = 718$ cm/s, $v_M\, l = 9.33\times 10^{-4}$ cm^2/s and $eN_D^w v_M/l = 13.27$ A/cm^2. For a circular sample with a diameter of 120 μm, the units of current and time are 1.501 mA and 1.021 ns, respectively. Then Eqs. (6.1), (6.2), (6.3) to (6.10) become

$$E_i - E_{i-1} = \nu\,(n_i - 1)\,, \tag{6.11}$$

$$J(t) = \frac{dE_i}{dt} + n_i v_i - D_i(n_{i+1} - n_i) + a\sqrt{n_i(v_i + D_i) + D_i n_{i+1}}\,\xi_i(t)\,, \tag{6.12}$$

$$J(t) = \frac{dE_0}{dt} + J_e(E_0) - W_e(E_0)\,n_1 + a\sqrt{J_e(E_0) + W_e(E_0)\,n_1}\,\xi_0(t)\,, \tag{6.13}$$

$$J(t) = \frac{dE_N}{dt} + W_c(E_N)\,n_N + a\sqrt{W_c(E_N)\,n_N}\,\xi_N(t)\,, \tag{6.14}$$

$$\phi = \frac{1}{N}\sum_{i=1}^{N} E_i. \tag{6.15}$$

Here we have used the same symbols for dimensional and dimensionless quantities except for the electric field and the coefficient functions in the boundary conditions. The parameters $\nu = eN_D^w/(\varepsilon F_M) \approx 1.772$, $\phi = V/(F_M N l)$ and $a = \sqrt{e/(\varepsilon F_M A)} \approx 3.232\times 10^{-4}$ are the dimensionless doping, the average electric field (bias) and the noise amplitude respectively. $\xi_i(t)$ is a zero-mean Gaussian white noise with correlation $\langle \xi_i(t)\xi_j(t')\rangle = \delta_{ij}\delta(t-t')$ ($\xi_i(t) = \xi_i(t_m)/\sqrt{\Delta t}$, where the $\xi_i(t_m)$ are independent identically distributed (i.i.d.) normalized Gaussian random variables for each discrete time t_m and Δt is the dimensionless time step). The rest of the coefficients in Eqs. (6.11) to (6.14) are defined by

$$v_i \equiv v(E_i) = \frac{v(F_M E_i)}{v_M}\,, \qquad D_i \equiv D(E_i) = \frac{D(F_M E_i)}{V_M l}\,,$$
$$J_e(E_0) = \frac{j_e^{(f)}(F_M E_0)l}{N_D^w v_M}\,, \qquad W_e(E_0) = \frac{W^{(b)}(F_M E_0)}{v_M}\,,$$
$$W_c(E_N) = \frac{W^{(f)}(F_M E_N)}{v_M}\,. \tag{6.16}$$

The previous system of equations can be further simplified since the electron densities n_i and the total current density $J(t)$ can be expressed in terms of the electric field and the bias. Differentiating Eq. (6.15) with respect to time, and using Eqs. (6.13) and (6.14), we obtain an expression for the total current density $J(t)$:

$$\begin{aligned}\frac{d\phi}{dt} &= \frac{1}{N}\sum_{i=1}^{N}\frac{dE_i}{dt} = J - \frac{1}{N}\sum_{i=1}^{N-1}[n_i(v_i+D_i) - n_{i+1}D_i] \\ &- \frac{n_N W_c(E_N)}{N} - \frac{a}{N}\sum_{i=1}^{N-1}\sqrt{n_i v_i + (n_i + n_{i+1})D_i}\,\xi_i(t) \\ &- \frac{a}{N}\sqrt{n_N W_c(E_N)}\,\xi_N(t)\,.\end{aligned}$$

Then the total current can be written as

$$J = J_1 + \mathbf{J}_2 \cdot \xi, \tag{6.17}$$

$$J_1 = \frac{d\phi}{dt} + \sum_{i=1}^{N-1}\frac{n_i(v_i+D_i) - n_{i+1}D_i}{N} + \frac{n_N W_c(E_N)}{N} \tag{6.18}$$

$$(\mathbf{J}_2)_0 = 0, \tag{6.19}$$

$$(\mathbf{J}_2)_i = \frac{a\sqrt{n_i v_i + (n_i+n_{i+1})D_i}}{N}, \quad 1 \le i < N, \tag{6.20}$$

$$(\mathbf{J}_2)_N = \frac{a\sqrt{n_N W_c(E_N)}}{N}\,, \tag{6.21}$$

$$\xi = (\xi_0(t), \ldots, \xi_N(t))^T. \tag{6.22}$$

We can now insert these equations in the Ampère equations (6.12) to (6.14) and eliminate n_i by using Eq. (6.11) thereby obtaining a stochastic differential equation of the following form:

$$\frac{d\mathbf{E}}{dt} = \mathbf{H}\left(\mathbf{E}, \frac{d\phi}{dt}\right) + S(\mathbf{E}) \cdot \xi(t), \tag{6.23}$$

for the $(N+1)$-dimensional vector electric field $\mathbf{E} = (E_0, \ldots, E_N)^T$. Here $S(\mathbf{E})$ is a $(N+1)\times(N+1)$ matrix and $\mathbf{H}$ is a $(N+1)$-dimensional vector having obvious forms which we do not write explicitly for the sake of conciseness.

The stochastic differential equation (6.23) has been numerically solved by using two different methods: a first order Heun scheme (modified Euler scheme) and the second order scheme proposed by Platen [66]. The second numerical scheme is rather more costly, but we had to use it to avoid that numerical errors mask the effects due to charge fluctuations. Technical details on numerical schemes and a comparison of their performances are given in Appendix 6. The results of our simulations are reported in the next Section.

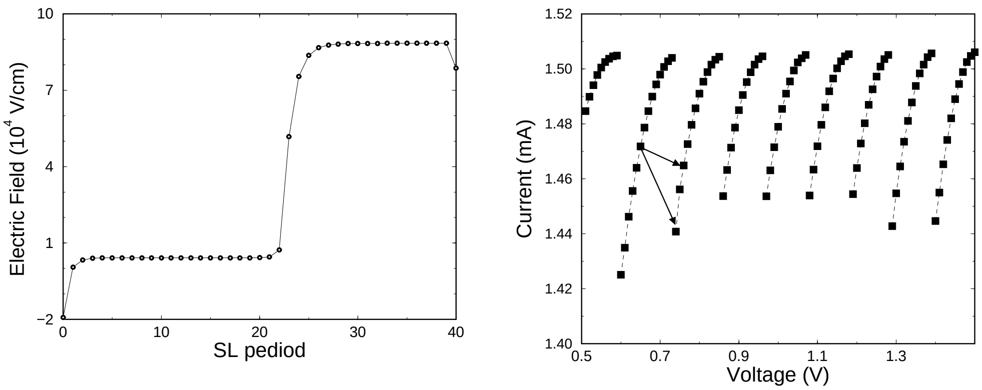

Figure 6.3: (*Left*) Static electric field profile at V=2.1 V. (*Right*) Part of the first plateau of the *I*-*V* characteristics.

Numerical results

We have numerically investigated the sample of Ref. [63] that was used in the relocation experiments [80, 92]. It consists of a $N = 40$-period SL with 9-nm wide GaAs wells and 4-nm wide AlAs barriers, and 2D doping $N_D^w = 1.5 \times 10^{11}$ cm^{-2}, at a temperature $T = 5$ K. We have solved numerically the nondimensional equations in the units and dimensionless parameters introduced in Section 6. Figure 6.3 (*left*) shows a typical static electric field profile (with two coexisting domains) and the first plateau of the time averaged *I*-*V* characteristics (obtained by voltage up sweeping). To ascertain the influence of charge fluctuations in domain relocation, we start by setting a stationary field configuration corresponding to a voltage $V_0 = 0.65$ V on the lower branch of Fig. 6.3 (*Right*). At time $t = 0$, the voltage increases (in one time step) to its final value V_f on the next *I*-*V* branch.

Time traces of the current are depicted in Figures 6.4. Notice that the vertical scale has been augmented sufficiently to see the fluctuations of the current, that are typically about 0.02 in size. To compare our numerical results to experimental ones, we need to characterize the domain relocation times and their distribution function. After a voltage switch, each realization of the random solution of Eq. (6.23) gives rise to jumps in the mean current as depicted in Figures 6.4. We compare the time trace of the current (time averaged over intervals of five time dimensionless units) to the value of the current in static *I*-*V* branches. The first time t_0 that the current time trace differs less than 5×10^{-4} dimensionless units from its final stationary value, we consider that the domain relocation has ended. The distribution of time delays t_0 taken over many realizations is then recorded. For a large voltage

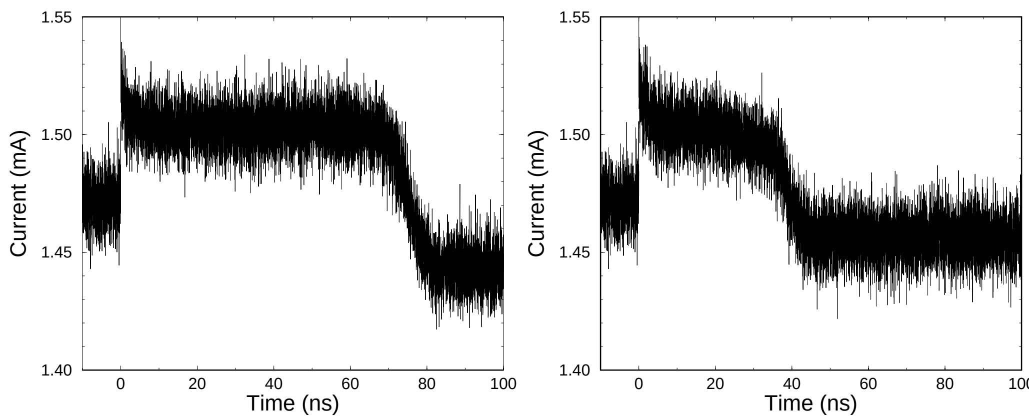

Figure 6.4: Time trace of the current when the voltage is switched from $V_0 = 0.65$ V to $V_f = 0.737$ V (*Left*) and to $V_f = 0.75$ V (*Right*).

switch, the time delay before the current falls from its initial value to its final level is shorter than for a smaller voltage switch; compare Figs. 6.4. The differences between the time delays involved in these two cases (about 40 ns) are smaller than those recorded in experiments [92]. These differences occur because of overestimation of the field F_M and the shot noise amplitude by our theoretical calculations with respect to those of the experimental sample, as we mentioned before.

In Ref.[80] it was claimed that the time delay depends exponentially on the difference between the final value of the stabilized current, I, and the maximum value of the current (or mimimum value in the case of a down switch) at the initial branch, I_m. Then the relocation time (measured in units of 1.021 ns) depends exponentially on the current difference $I - I_m$, i.e.,

$$\exp\left(\frac{b\,|I - I_m|}{I_M} + c\right) . \tag{6.24}$$

We have observed this dependence in our numerical results too. The dimensionless constants b and c are $b = 64.9866$ and $c = 1.6717$. $I_M = 1.501$ mA is the unit of current. In Luo et al's experiments [80], $I_M = 136\mu$A (approximately the height of the first maximum of the current in the inset of Fig. 1), $b = 10.74$ (6 times smaller than the numerically calculated value) and $c = 3.34$ (2 times larger than the numerically calculated value). We thus confirm the exponential dependence of the relocation time on the current difference and observe a good qualitative agreement between numerically and experimentally obtained values. Fig. 6.5(a), shows the mean relocation

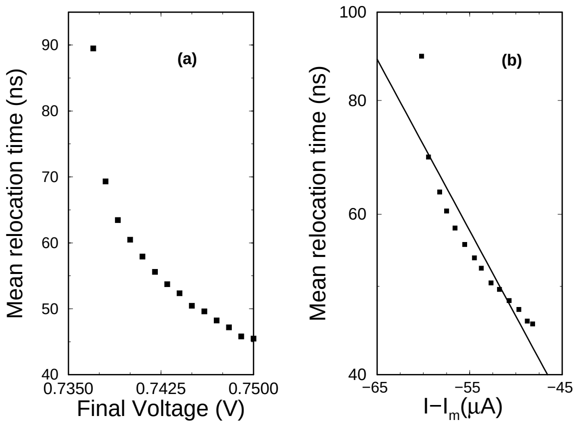

Figure 6.5: (a) Mean relocation time for different final voltages. (b) Logarithm of the mean delay time vs current difference between final current and the maximum or minimum current I_m of the initial branch.

time obtained in our simulations as a function of V_f. As the final voltage approaches that corresponding to I_M, the relocation time increases. Fig. 6.5(b) depicts the mean relocation time as a function of $(I - I_m)$ on a semilogarithmic scale for V_f values between $0.737V$ and $0.735V$. The solid line denotes a linear fit to the data points, that agrees with the exponential law proposed by Luo et al [80]. These figures are qualitatively similar to the corresponding ones depicted from experimental data in Refs.[92] and [80]. Quantitative differences are due to the above mentioned discrepancies in F_M, the tunneling current and the shot noise amplitude. Let us remark a posterior theoretical work [105] deducing exponential dependence for the mean relocation times in a resonant-tunneling structures where the current-voltage characteristics exhibit bistability. In [105] the exponential depends on $|I - I_m|^{\frac{3}{2}}$ instead of a linear dependence. However the region of validity of this fit is only valid localy in a region close to the current jump. This induces to think about different regimes in the exponential approach for this mean relocation times.

Now we focus on the distribution of switching times. Typically, delay distributions are either close to symmetric Gaussians or they are asymmetric, depending on how far V_f is from the limit point of the I-V characteristics. We have fitted our numerical distributions by least squares to either a Gaussian density:

$$W(t,\tau,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(t-\tau)^2}{2\sigma^2}\right), \tag{6.25}$$

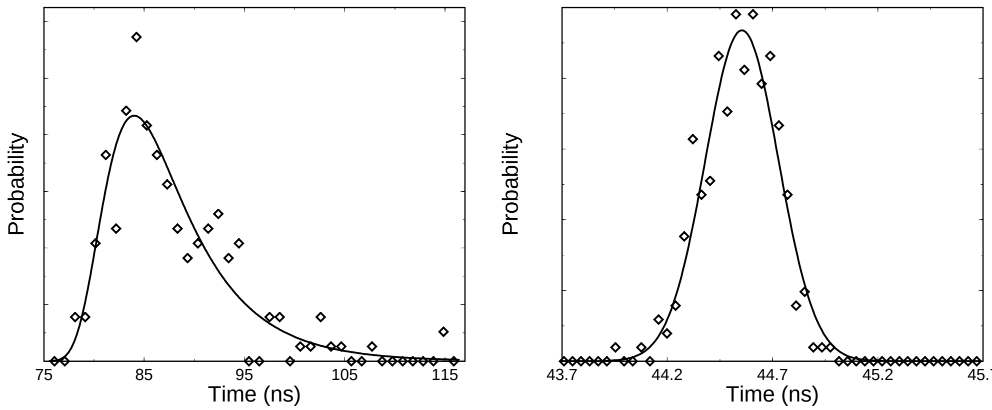

Figure 6.6: Time delay distribution for $V_f = 0.737$ V *(Left)* and $V_f = 0.75$ V *(Right)*. Data from numerical simulations have been fitted to a FPT distribution and to a Gaussian distribution, respectively .

or to a first passage time (FPT) distribution

$$W(t, y, \beta)\, dt = \sqrt{y \frac{2\beta}{\pi}} \exp\left(-\frac{\beta y z^2}{2}\right)\, dz\,, \tag{6.26}$$

where

$$z = \frac{1}{\sqrt{\exp(2\beta t) - 1}}. \tag{6.27}$$

The parameters of these distributions are τ (mean relocation time) and σ (standard deviation) for the Gaussian and y and β for the FPT distribution. The results of our fitting are depicted in Figures 6.6.

These results agree qualitatively with the experimental ones of Rogozia et al's [92]. As in Ref. [92], our Figures 6.6 show that for values of the voltage far away from the current jump the time delay distribution changes from an asymmetric FPT distribution to a very narrow symmetric Gaussian distribution as V_f departs from the voltage corresponding to the current jump. These features have a numerical expression in terms of descriptive statistics like the mean, the standard deviation or the skewness coefficient as shown in the Tables of Appendix 6. The numerically calculated largest and smallest delay times are also presented.

Conclusions

We have studied how the shot noise due to charge quantization affects the relocation time of electric field domains after a suddent switch of the voltage. We find that the mean relocation time depends exponentially on the difference between the value of the current at the final voltage and the value of the current at the end of the branch corresponding to the initial voltage. The distribution function of delay times after a voltage switch changes from Gaussian to a FPT distribution as the final voltage approaches the limit point of the stationary I-V characteristics. These results are in qualitative agreement with experiments.

Appendix: Numerical Scheme

This Appendix is devoted to explain some technical details of the simulations. The Platen second order scheme gives the vector field $\mathbf{E}^{n+1}$ at discrete time $t+\Delta t$ as the following function of $\mathbf{E}^n$ at discrete time t [66]:

$$\begin{aligned}
\mathbf{E}^{n+1} &= \mathbf{E}^n + \frac{1}{2}\left(\mathbf{H}\left(\boldsymbol{\Upsilon}, \frac{d\phi}{dt}\right) + \mathbf{H}\left(\mathbf{E}^n, \frac{d\phi}{dt}\right)\right)\Delta t \\
&+ \frac{1}{4}\sum_{j=1}^{N+1}\Bigg[\left(\mathbf{S}^j(\mathbf{M}_+^j) + \mathbf{S}^j(\mathbf{M}_-^j) + 2\mathbf{S}^j(\mathbf{E}^n)\right)\Delta W^j \\
&+ \sum_{r=1, r\neq j}^{N+1}\left(\mathbf{S}^j(\mathbf{U}_+^r) + \mathbf{S}^j(\mathbf{U}_-^r) - 2\mathbf{S}^j(\mathbf{E}^n)\right)\Delta W^j\Bigg] \\
&+ \frac{1}{4}\sum_{j=1}^{N+1}\Bigg[\left(\mathbf{S}^j(\mathbf{M}_+^j) - \mathbf{S}^j(\mathbf{M}_-^j)\right)\left\{(\Delta W^j)^2 - \Delta t\right\} \\
&+ \sum_{r=1, r\neq j}^{N+1}\left(\mathbf{S}^j(\mathbf{U}_+^r) - \mathbf{S}^j(\mathbf{U}_-^r)\right)\left\{\Delta W^j \Delta W^r + V_{r,j}\right\}\Bigg].
\end{aligned}$$

Here $\mathbf{S}^j(\cdot)$ is the $j-$th column of $S(\cdot)$, $\mathbf{U}_\pm = \mathbf{E}^n \pm \mathbf{S}(\mathbf{E}^n)^j\sqrt{\Delta t}$, and $\mathbf{H}$ and S are evaluated at

$$\begin{aligned}
\boldsymbol{\Upsilon} &= \mathbf{E}^n + \mathbf{H}\left(\mathbf{E}^n, \frac{d\phi}{dt}\right)\Delta t + \sum_{j=1}^{N+1}\mathbf{S}(\mathbf{E}^n)^j \Delta W^j, \\
\mathbf{M}_\pm^j &= \mathbf{E}^n + \mathbf{H}\left(\mathbf{E}^n, \frac{d\phi}{dt}\right)\Delta t \pm \mathbf{S}^j(\mathbf{E}^n)\sqrt{\Delta t}.
\end{aligned}$$

ΔW^j are independent gaussian random variables distributed with zero mean and variance Δt, whereas the V_{j_1,j_2} are independent two point random variables that satisfy

$$P(V_{j_1,j_2} = \pm\Delta t) = \frac{1}{2}\,, \quad V_{j_1,j_1} = -\Delta t\,, V_{j_1,j_2} = -V_{j_2,j_1}\,.$$

We have used a time step of $\Delta t = 10^{-4}$ (in dimensionless units) of the same order as the noise amplitude a. The values of the random variables V and W have been generated through a random number generator improved by using a seed selector depending on the computer clock and an algorithm which allows to avoid the sequential correlation usual in this sort of generators [88]. The Platen scheme is second-order weakly convergent in the following sense. Let $g(\mathbf{E})$ be any sufficiently smooth scalar function (with $2(\beta+1)$ continuous derivatives provided β is the order of the scheme). Let us fix the time instant at t corresponding to discrete time n. Then

$$|\langle g(\mathbf{E}^n)\rangle - \langle g(\mathbf{E})\rangle| \leq C(\Delta t)^2\,,$$

for any $\Delta t \in (0, \delta_0)$, where C and δ_0 are positive constants. The Platen numerical scheme is certainly more complicated and costly than even a stochastic Heun (modified Euler) first order scheme. We have had to use it to minimize the effects of numerical noise coming from floating-point arithmetic (even our high-precision 64-bit arithmetic) and that inherent in interpolating our transport coefficients and contact functions in the boundary conditions. In fact, in the absence of the noise, both the Heun and the Platen schemes become the well-known deterministic Heun (improved Euler) scheme, that is a second-order Runge-Kutta method:

$$\mathbf{E}^{n+1} = \mathbf{E}^n + \frac{\Delta t}{2}\left[\mathbf{H}(\mathbf{E}^n) + \mathbf{H}\Big(\mathbf{E}^n + \mathbf{H}(\mathbf{E}^n)\Delta t\Big)\right]\,.$$

However both schemes differ in their treatment of the noise: the stochastic Heun method is weakly first order whereas the Platen scheme is second order. The result obtained by using the Platen scheme exhibits less dispersion than that reached by the Heun method, as shown in Table 6. An appropriate treatment of the noise term avoids the presence of artificial numerical effects. The effects of the numerical perturbations can be illustrated as follows. Let us use the deterministic Heun scheme with random initial conditions corresponding to disturbances of the stationary field profile at voltage V_0 and suddenly switch to voltage V_f. The domain relocation times have been measured and they give rise to the distributions of Figures 6.7.

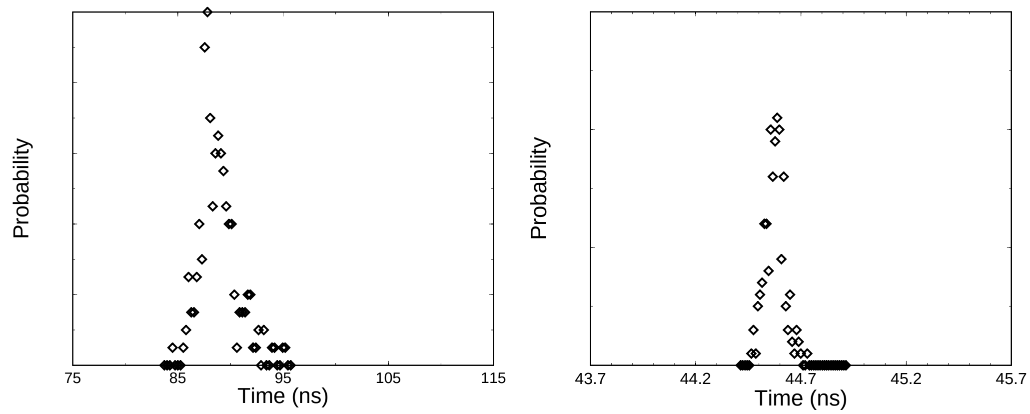

Figure 6.7: Time delay distribution for $V_f = 0.737$ (left) and $V_f = 0.75$ (right) calculated with a deterministic Heun scheme and random initial conditions.

Heun / Platen	$V_f = 0.737$	$V_f = 0.75$	$V_f = 0.737$	$V_f = 0.75$
Lower Limit (ns)	77.692	43.775	77.827	43.942
Upper Limit (ns)	128.048	45.633	115.025	44.960
Mean (ns)	87.863	44.564	87.635	44.541
Standard Dev. (ns)	6.803	0.299	6.339	0.167
Skewness coeff.	1.840	0.131	1.4237	−0.2791

Table 6.1: Descriptive statistics of the relocation time distributions obtained with the Heun and Platen scheme.

We have compared the mean, standard deviation and skewness coefficient, which measures the asymmetry of a distribution, of these distributions to those corresponding to the use of the stochastic Heun and Platen schemes; see Tables 6 and 6.2. Notice that the mean relocation times are similar, while the numerical viscosity contributes to scatter the results. The shot noise does not change the mean values given by the deterministic model, but the dispersion measured by the standard deviation increases due to numerical effects (larger in the Heun scheme). The use of a numerical scheme that reduces these effects is then clearly justified.

	$V_f = 0.737$	$V_f = 0.75$
Mean (ns)	88.916	44.579
Standard Deviation (ns)	1.773	0.045
Skewness coeff.	0.912	0.255

Table 6.2: Descriptive statistics of the relocation time distributions obtained with pertubed initial conditions.

Chapter 7

Low-field limit for a nonlinear discrete drift-diffusion model arising in semiconductor superlattices theory

Introduction

This chapter is concerned with a weakly coupled SL whose electron density inside the device reaches intermediate values. Depending on the charge density (produced by doping or irradiating the SL) and the applied voltage, different qualitative responses of the current can be obtained [22]. At intermediate values of the charge density, stationary responses and self–sustained oscillations are observed depending on the values of the voltage. The solutions corresponding to low voltages are stationary and typically develop low electric fields. We propose to study this regime by identifying some small parameter $h > 0$ by means of physically relevant dimensionless quantities appearing in the Discrete Drift–Diffusion model introduced in Chapter 1. Having set up this discrete problem, we proceed to prove that the solution converges, in an appropriate weak setting, to a continuous Poisson–Drift–Diffusion problem with field–dependent mobilities in the limit. This leads to a parabolic limit equation.

The methodology proposed uses an auxiliar problem to deal with the DDD model. In a first approach, we deduce rigorously the limit for the DDD model replacing the bias condition by an artificial Dirichlet boundary condition at the emitter. At the end, we recover the bias condition by a simple argument. This chapter is structured as follows: In Section 2 we present the DDD model with a Dirichlet boundary condition and study its well–posedness. In Section 3 we derive the dimensionless equations for which the analysis is actually performed and we state our main convergence result for the DDD model. Section 4 is devoted to prove this result. Finally, Section 5 sketches the proof of the continuum limit for the DDD system with the bias condition.

DDD Model with Dirichlet boundary conditions

Let us consider a SL constituted by $2N+1$ consecutive periods, which are well–barrier pairs, labelled by the index $i \in \{-N, \ldots, +N\}$. Then, the barrier in contact with the emitter is considered as the $(-N-1)$–th barrier, while the last barrier of the N–th SL period separates the N–th well from the collector. The DDD model considers that the two–dimensional electron density n_i and the average electric field F_i are goberned by the discrete Poisson equation

$$F_i - F_{i-1} = \frac{e}{\varepsilon}(n_i - N_D^w), \quad i \in \{-N, \ldots, N\}, \tag{7.1}$$

and the continuity equation

$$\frac{dn_i}{dt} = J_{i-1\to i} - J_{i\to i+1}, \quad i \in \{-N, \ldots, N\}, \tag{7.2}$$

being $eJ_{i\to i+1}$ the tunneling current density through the barrier defined by (1.16), (1.17) and (1.18). We remark that one equation is still missing since we have one unknown more than equations. Notice that the set of relations (7.1) involves as an additional unknown the electric field F_{-N-1} at the injecting contact.

There are several ways to close mathematically the system. As we mentioned in Chapters 1 and 6, the most realistic boundary condition is the so–called voltage bias condition:

$$\ell \sum_{i=-N}^{N} F_i = V, \tag{7.3}$$

where V is a given quantity and ℓ is the period length. However, we will replace it in a first approach by a new condition adapted to the analysis of the asymptotic limit. A mathematically convenient recipe is to prescribe the electric field at the emitter:

$$F_{-N-1}(t) = F_{-}(t). \tag{7.4}$$

Here, the right–hand side of (7.4) is a given function $F_- : \mathbb{R}^+ \to \mathbb{R}$. In what follows we essentially deal with the Dirichlet–like boundary condition (7.4) for the electric field. We will come back to the voltage bias condition (7.3) at the end of the chapter.

Relations (7.1), (7.2) and (7.4) form a closed system of equations for n_i and F_i with $i \in \{-N, \dots, N\}$, referred to along this chapter as the Discrete Drift–Diffusion (DDD) model. These equations involve the drift–velocity v, the diffusion coefficient D, the emitter current density $ej^{(e)}$, the emitter backward velocity $W^{(b)}$ and the collector forward velocity $W^{(f)}$, which are given functions of the electric field. All the coefficients v, D, $W^{(b)}$, $W^{(f)}$, $j^{(e)}$ are supposed to be nonnegative and to satisfy some regularity properties (see Chapter 6, where typical profiles of these coefficients are depicted).

We remark that the electric field in the cell $\#i$ can be expressed as a function of the incoming field F_- and the density in the previous cells as follows

$$F_i(t) = F_-(t) + \frac{e}{\varepsilon} \sum_{j=-N}^{i} (n_j(t) - N_D), \quad i \in \{-N, \dots, N\}, \quad \forall t \in [0, T]. \quad (7.5)$$

Consequently, we can rewrite the initial value problem associated to the DDD model in terms of the densities

$$\frac{d\vec{n}}{dt} = g(t, \vec{n}(t)), \qquad \vec{n}(0) = \vec{n}^0, \quad (7.6)$$

where $\vec{n}(t) = (n_{-N}, \dots, n_N)^T \in \mathbb{R}^{2N+1}$, $g : \mathbb{R}^{2N+1} \to \mathbb{R}^{2N+1}$ is a smooth function and $\vec{n}^0 \in \mathbb{R}^{2N+1}$ is the initial condition. Next theorem stablishes the well–posedness of the DDD model.

Theorem 7.1. Let $n_i^0 \geq 0$ for $i \in \{-N, \dots, N\}$ be the initial data for the DDD system. Let F_- be a C^1 function of time. Let also $v, D, W^{(b,f)}, j^{(e)}$ be C^1 nonnegative functions. Then, there exists a unique global solution associated with the initial value problem (7.6). The solution verifies $n_i(t) \geq 0$ for all $i \in \{-N, \dots, N\}$, $t \geq 0$.

Proof. Local existence and uniqueness follows by a direct application of the Cauchy-Lipschitz theorem for ODE, since the function g inherits the regularity properties of the coefficients. The estimates proved in the next section, especially in Lemma 7.1, provides also a uniform bound on the solution which prevents from finite time blow up. Consequently, the solution is globally defined. There only remains to justify the nonnegativeness of the solution. To this end, it is convenient to rewrite (7.2) as a difference between a gain term and a loss term

$$\frac{dn_i}{dt}=\begin{cases} \frac{v(F_{i-1})}{\ell}n_{i-1}+\frac{D(F_i)}{\ell^2}n_{i+1}+\frac{D(F_{i-1})}{\ell^2}n_{i-1}-\left(\frac{v(F_i)}{\ell}+\frac{D(F_i)}{\ell^2}+\frac{D(F_{i-1})}{\ell^2}\right)n_i \\ \qquad \text{for } i\in\{-N+1,\dots,N-1\}, \\ \frac{D(F_{-N})}{\ell^2}n_{-N+1}+j^{(e)}(F_{-N-1})-\left(\frac{v(F_{-N})}{\ell}+\frac{D(F_{-N})}{\ell^2}+\frac{W^{(b)}(F_{-N-1})}{\ell}\right)n_{-N} \\ \qquad \text{for } i=-N, \\ \frac{v(F_{N-1})}{\ell}n_{N-1}+\frac{D(F_{N-1})}{\ell^2}n_{N-1}-\left(\frac{D(F_{N-1})}{\ell^2}+\frac{W^{(f)}(F_N)}{\ell}\right)n_N \\ \qquad \text{for } i=N. \end{cases}$$

Let $t\geq 0$ such that $n_i(t)\geq 0$ for any $i\in\{-N,\dots,N\}$. Suppose $n_j(t)=0$ for some $j\in\{-N,\dots,N\}$. Thus, we notice that its time derivative $\frac{dn_j}{dt}(t)$ is nonnegative and, hence, we deduce the nonnegative character of the solution along the time evolution. □

Dimensionless Equations

The aim of this section is to write the system in dimensionless form. Hence, we will identify some dimensionless physical parameters. Next, we choose suitabily (low–field asymptotics) the ordering of these parameters in terms of a quantity $h>0$ intended to tend to 0. Studying the limit $h\to 0$ we obtain a nonlinear continuous drift–diffusion model. This approach relating discrete to continuous models is reminiscent of hydrodynamic limits in kinetic theory (see [42]). Actually, it has been used for models of phase transition for example in [32].

Let us introduce time and length units, respectively denoted by $\mathcal{T}$, $\mathcal{L}$. They correspond to observation scales. We also need characteristic values for the electron density and for the electric field, respectively denoted by $\mathcal{N}$ and $\mathcal{F}$. For instance, it is quite natural to define $\mathcal{N}$ from the doping profile N_D^w and $\mathcal{F}$ from the emitter field F_-. Then, using the convention that overlined quantities are dimensionless, we set

$$\begin{cases} \mathcal{N}\ \overline{n_i}(\overline{t})=n_i(\mathcal{T}\overline{t}), & \mathcal{N}\ \overline{N_D}=N_D^w, \\ \mathcal{F}\ \overline{F_i}(\overline{t})=F_i(\mathcal{T}\overline{t}), & \mathcal{F}\ \overline{F_-}(\overline{t})=F_-(\mathcal{T}\overline{t}), \\ \dfrac{\mathcal{L}}{\mathcal{T}}\ \overline{v}(\overline{F})=v(\mathcal{F}\overline{F}), & \dfrac{\mathcal{L}}{\mathcal{T}}\ \overline{W^{(b,f)}}(\overline{F})=W^{(b,f)}(\mathcal{F}\overline{F}), \\ \dfrac{\mathcal{L}^2}{\mathcal{T}}\ \overline{D}(\overline{F})=D(\mathcal{F}\overline{F}), & \dfrac{\varepsilon\mathcal{F}}{e}\ \dfrac{1}{\mathcal{T}}\ \overline{j^{(e)}}(\overline{F})=j^{(e)}(\mathcal{F}\overline{F}). \end{cases}$$

Note that the emitter current density has been scaled with respect to the density $\frac{\varepsilon}{e}\mathcal{F}$ instead of with respect to $\mathcal{N}$ (the other choice is also possible;

the proof adapts immediately and the emitter current density disappears as $h \to 0$ in that case). Therefore, we are led to the continuity equations in the following dimensionless form

$$\frac{d\overline{n}_i}{d\overline{t}} = \frac{\mathcal{L}}{\ell}\Big(\overline{v}(\overline{F}_{i-1})\overline{n}_{i-1} - \overline{v}(\overline{F}_i)\overline{n}_i - \frac{\mathcal{L}}{\ell}\overline{D}(\overline{F}_{i-1})(\overline{n}_{i-1} - \overline{n}_i) + \frac{\mathcal{L}}{\ell}\overline{D}(\overline{F}_i)(\overline{n}_i - \overline{n}_{i+1})\Big),$$

for $i \in \{-N+1, \dots, N-1\}$ and

$$\begin{aligned} \frac{d\overline{n}_{-N}}{d\overline{t}} &= \frac{\mathcal{L}}{\ell}\Big(\frac{\ell}{\mathcal{L}}\frac{\overline{\varepsilon}\mathcal{F}}{\epsilon\mathcal{N}}\overline{j}^{(e)}(\overline{F}_{-N-1}) - \overline{n}_{-N}\overline{W}^{(b)}(\overline{F}_{-N-1}) \\ &\quad -\overline{v}(\overline{F}_{-N})\overline{n}_{-N} - \frac{\mathcal{L}}{\ell}\overline{D}(\overline{F}_{-N})(\overline{n}_{-N} - \overline{n}_{-N+1})\Big), \\ \frac{d\overline{n}_N}{d\overline{t}} &= \frac{\mathcal{L}}{\ell}\Big(\overline{v}(\overline{F}_{N-1})\overline{n}_{N-1} + \frac{\mathcal{L}}{\ell}\overline{D}(\overline{F}_{N-1})(\overline{n}_{N-1} - \overline{n}_N) - \overline{n}_{-N}\overline{W}^{(f)}(\overline{F}_N)\Big). \end{aligned}$$

On the other hand, the Poisson equations reads

$$\frac{\overline{\varepsilon}\mathcal{F}}{e\mathcal{N}}\left(\overline{F}_i - \overline{F}_{i-1}\right) = \left(\overline{n}_i - \overline{N}_D\right),$$

for $i \in \{-N, \dots, N\}$.

In these expressions, we indentify two dimensionless parameters

$$\alpha = \frac{e\mathcal{N}}{\overline{\varepsilon}\mathcal{F}}, \quad \beta = \frac{\mathcal{L}}{\ell}.$$

We motivate the limit performed in this chapter by considering a particular example. Fig. 7.1 (left) shows the drift velocity in comparison with the diffusion coefficient for a 9nm/4nm GaAs/AlAs SL at 5^0K (with well dopping $N_D^w = 0.5\ 10^{11}cm^{-2}$ and contact doping $N_D = 2\ 10^{18}cm^{-3}$). Also, Fig. 7.1 (right) shows the electric field distribution of static solutions for a 40 periods 9nm/4nm GaAs/AlAs SL with different voltage values obtained by using the DDD model. There exist two possibilities to dealt with the high field limit. The continuum limit consists of doing $\alpha \to 0$. We can observe that for solutions with high electric fields the conditions $v(F) \approx D(F)/\ell$ or $v(F) >> D(F)/\ell$ are valid. Thus, the appropriate scales in this regime lead to $O(\ell) = O(\mathcal{L})$, which gives rise to the hyperbolic limit studied in previous works. In the opposite regime (low field), the relation

$$v(F) << D(F)/\ell$$

holds. This motivates us to choose typical scales such that

$$O(\bar{v}) = O(\bar{D}/\ell)\,.$$

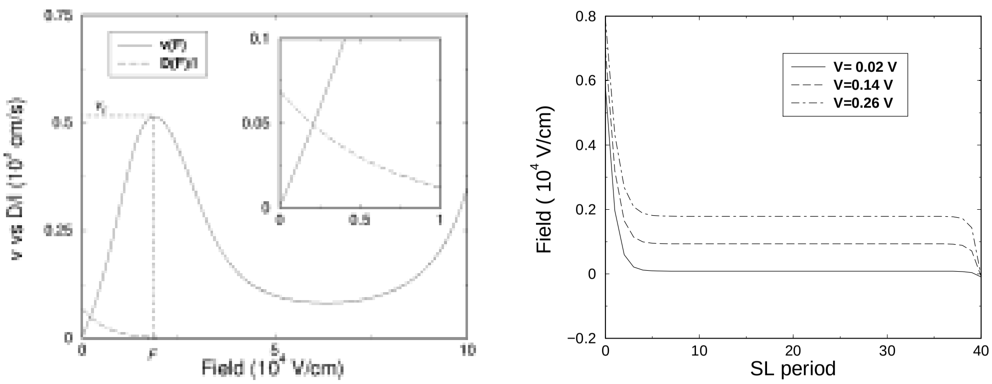

Figure 7.1: (Left) Drift-velocity versus diffusion coefficient for a $9nm/4nm$ GaAs/AlAs SL. (Right) Electric field distribution for stationary solutions 40 periods 9nm/4nm GaAs/AlAs SL for different voltages.

This clearly justifies the choice of the space scale $\ell << \mathcal{L}$.

In this aim, we would like to interpret difference between consecutive cells as differential quotient. This motivates the choice

$$h = \alpha = \beta^{-1},$$

where h is a positive quantity intended to tend to 0. The ordering for β means that the size of the cells is small compared to the observation length scale. The ordering for α can be interpreted as an assumption about the relation between the doping profile N_D^w, which is supposed large compared to the density $\frac{\bar{\varepsilon}}{e} F_-$ associated with the electric field at the injecting contact. Since this implies that the diffusion coefficient is large (order h^{-2}) in comparison with the velocity of the field (order h^{-1}), we call this asymptotic approach low–field limit. Furthermore, we shall assume that the total length of the SL is given and equals to $2X$, so that the number of cells in the SL should be also appropriately rescaled. Namely, the number of cells is defined in terms of the parameter $h > 0$ by

$$N^h = X/h.$$

Let us summarize the low-field problem we are interested in as follows. We drop the overlines and emphasize the dependence of the solution (n, F) with respect to the parameter h by a superscript. Hence, we consider the system

$$\frac{dn_i^h}{dt} = \frac{1}{h}(J_{i-1\to i}^h - J_{i\to i+1}^h), \quad i \in \{-N^h, \dots, N^h\} \tag{7.7}$$

coupled to

$$F_i^h - F_{i-1}^h = h(n_i^h - N_D), \quad i \in \{-N^h, \dots, N^h\}, \tag{7.8}$$

with $F^h_{-N^h-1} = F_-$ given. Remark that, coming back to (7.5), we also have

$$F_i^h(t) = F_-(t) + h \sum_{j=-N^h}^{i} \left(n_j^h(t) - N_D\right), \quad i \in \{-N^h, \ldots, N^h\}. \tag{7.9}$$

Here, we used the following definition for the tunneling currents

$$\begin{cases} J^h_{i\to i+1} = n_i^h v_i^h - \dfrac{1}{h} D(F_i^h)(n^h_{i+1} - n_i^h), \quad i \in \{-N^h, \ldots, N^h - 1\}, \\ J^h_{-N^h-1\to -N^h} = j^{(e)}(F_-) - n^h_{-N^h} W^{(b)}(F_-), \\ J^h_{N^h\to N^h+1} = n_{N^h} W^{(f)}(F^h_{N^h}). \end{cases}$$

The idea is to investigate the limit as $h \to 0$.
To this end, we set $I = (-X, +X) = (-N^h h, N^h h)$ and we associate to the unknowns $(n^h_{-N^h}, \ldots, n^h_{N^h-1}) \in \mathbb{R}^{2N^h}$ and $(F^h_{-N^h}, \ldots, F^h_{N^h-1}) \in \mathbb{R}^{2N^h}$, the stepwise constant functions $n^h(t,x)$ and $F^h(t,x)$ defined almost everywhere on $[0,\infty] \times I$ by saying

$$n^h(t,x) = n_i^h(t), \quad F^h(t,x) = F_i^h(t), \quad ih < x < (i{+}1)h,\ i \in \{-N^h, \ldots, N^h{-}1\}.$$

Note that it is not relevant to define these functions on the negligible set of points $\{ih,\ i \in \{-N^h, \ldots, N^h\}\}$; note also that $F_-, n^h_{N^h}, F^h_{N_h}$ seem to play no role in these definitions. However, they will be used in the definition of traces in the limit $h \to 0$. As a consequence of these definitions, we shall use that sums of n_i^h or F_i^h can be considered as integrals: for example, for any function $\psi : \mathbb{R} \to \mathbb{R}$ we have

$$\int_{-X}^{+X} \psi(n^h)\, dx = h \sum_{i=-N^h}^{N^h-1} \psi(n_i^h)\,,$$

because n_i^h is constant on $ih < x < (i+1)h$. Then, passing to a continuous variable, it is tempting to interpret finite differences as differential quotients. Following this rough idea, we formally guess that the limiting problem corresponding to $h \to 0$ consists of the following nonlinear drift–diffusion equation

$$\begin{cases} \partial_t n + \partial_x J(F,n) = 0, & \text{in } (0,T) \times I, \\ J(F,n) = v(F)n - D(F)\partial_x n & \\ \partial_x F = n - N_D & \text{in } (0,T) \times I, \\ F(-X) = F_- & \text{on } (0,T) \\ J(F,n)(X) = W^{(f)}(F)n(X) & \text{on } (0,T), \\ J(F,n)(-X) = (j^{(e)}(F) - W^{(b)}(F)n)(-X) & \text{on } (0,T), \\ n(t=0,x) = n^0(x) & \text{on } I. \end{cases} \tag{7.10}$$

Thus, the main result of the work is the following.

Theorem 7.2. Let $v, D, W^{(b,f)}, j^{(e)} : \mathbb{R} \to \mathbb{R}$ be continuous and nonnegative functions. Suppose that $D(F) > 0$ and $W^{(b,f)}(F) > 0$ for any $F \in \mathbb{R}$. Let $F_- \in \mathrm{C}^1(\mathbb{R}^+)$. Let $n^{h,0} = (n^{h,0}_{-N^h}, \dots, n^{h,0}_{N^h}) \in \mathbb{R}^{2N^h+1}$ the initial data for the rescaled problem. We suppose that $n_i^{h,0} \geq 0$ satisfy

$$\sup_{h>0} \left(h \sum_{i=-N^h}^{N^h} |n_i^{h,0}|^2 \right) \leq C_0 < \infty. \tag{7.11}$$

Let (n^h, F^h) be the associated solution of (7.7), (7.8). Then, up to a subsequence, we have

$$\begin{cases} n^h \to n & \text{strongly in } \mathrm{L}^2((0,T) \times I) \text{ and in } \mathrm{C}^0([0,T]; \mathrm{L}^2(I) - weak), \\ F^h \to F & \text{uniformly in } [0,T] \times \overline{I}. \end{cases}$$

Furthermore the limits satisfy $n \in \mathrm{L}^2([0,T]; \mathrm{H}^1(I))$, $F \in \mathrm{C}^0([0,T] \times \overline{I})$ and solve the nonlinear problem (7.10) in the sense that

$$\frac{d}{dt} \int_{-X}^{X} n\phi \, dx = \int_{-X}^{X} J(F,n)\phi' \, dx + W^{(f)}(F) n \phi(X) + (j^{(e)}(F) - W^{(b)}(F) n)\phi(-X)$$

holds in $\mathcal{D}'(0,T)$ for any test function $\phi \in \mathrm{C}^\infty(\overline{I})$, coupled to the Poisson equation

$$\partial_x F = n - N_D, \quad F(-X) = F_-$$

considered also in the sense of the distributions.

This kind of nonlinear parabolic equation, coupled to the Poisson equation, have been investigated by Liang [69]. Actually, in [69] the diffusion coefficient is constant and the boundary conditions are slightly different. In the convergence proof, we only need to assume the continuity of the coefficients; however, using locally Lipschitz properties of them, we can prove the uniqueness of solution for (7.10), see Appendix 7. Consequently, assuming the convergence of the initial data, in Theorem 7.2 the entire sequence converges.

A priori Estimates

This section is devoted to the derivation of the crucial estimates on the solutions (n^h, F^h) that will lead us to rigorously perform the limit $h \to 0$. We assume that the initial data $n_i^{h,0} \geq 0$ satisfies (7.11). This implies that the $\mathrm{L}^1[-X, X]$ norm is bounded as follows

$$h \sum_{i=-N^h}^{N^h} n_i^{h,0} \leq \left(h \sum_{i=-N^h}^{N^h} |n_i^{h,0}|^2 \right)^{1/2} \sqrt{(2N^h+1)h}$$

is bounded independently of $h \in (0,1)$. We recall that

$$\begin{cases} D, W^{(b,f)}, j^{(e)}, v \in \mathrm{C}^0(\mathbb{R}), \\ v(F) \geq 0,\ j^{(e)} \geq 0, \\ W^{(b,f)}(F) > 0,\ D(F) > 0. \end{cases} \tag{7.12}$$

We split our argument into several steps. We shall use the convention that C_T stands for a constant possibly depending on T, and on the data $F_-, j^{(e)}, W^{(b,f)}$, or on the estimates (7.11), but which does not depend on h. Also, we denote as usual by $\mathcal{M}(I)$ the set of Radon measures on the open interval I. Elements of $\mathcal{M}(I)$ identify with distributions Φ on I satisfying $|\langle \Phi, \varphi \rangle| \leq C\|\varphi\|_{L^\infty(I)}$ $\forall \varphi \in C_c^\infty(I)$ for some $C > 0$ being independent of the support of the test function (see e.g. [95]). As usual we denote by $\mathrm{BV}(I)$ the set of bounded variation functions, i.e. functions which are in $\mathrm{L}^1(I)$ and such that their distributional derivative belongs to $\mathcal{M}(I)$.

Lemma 7.1 (L^1 ESTIMATE OF THE DENSITY.). The sequence n^h is bounded in $\mathrm{L}^\infty(0,T;\mathrm{L}^1(I))$.

Proof. Summing up the equations in (7.7) we obtain

$$\begin{aligned} h\, \frac{d}{dt} \sum_{i=-N^h}^{N^h} n_i^h &= \sum_{i=-N^h}^{N^h} (J_{i-1\to i}^h - J_{i\to i+1}^h) = J^h_{-N^h-1\to -N^h} - J^h_{N^h\to N^h+1} \\ &= j^{(e)}(F_-) - n^h_{-N^h} W^{(b)}(F_-) - n^h_{N^h} W^{(f)}(F^h_{N^h}). \end{aligned}$$

Therefore, integrating with respect to time and using $n_i^h \geq 0$ and $W^{(b,f)} \geq 0$, we find

$$\begin{aligned} &h \sum_{i=-N^h}^{N^h} n_i^h(t) + \int_0^t n^h_{-N^h} W^{(b)}(F_-(s))\, ds + \int_0^t n^h_{N^h} W^{(f)}(F^h_{N^h})(s)\, ds \\ &= h \sum_{i=-N^h}^{N^h} n_i^{h,0} + \int_0^t j^{(e)}(F_-(s))\, ds \leq C_0 + \|j^{(e)}(F_-)\|_{L^1(0,T)} \leq C_T\,, \end{aligned} \tag{7.13}$$

which concludes the proof. □

Lemma 7.2 (ESTIMATING THE ELECTRIC FIELD.). The sequence F^h is bounded in $\mathrm{L}^\infty((0,T)\times I)$ and in $\mathrm{L}^\infty(0,T;BV(I))$, while $F^h_{N_h}$ is bounded in $\mathrm{L}^\infty(0,T)$.

Proof. We combine the estimate in Lemma 7.1 with the identity (7.9) to yield

$$\begin{aligned}
|F_i^h(t)| &= \left|F_-(t) + h\sum_{j=-N^h}^{i}(n_j^h(t) - N_D)\right| \\
&\leq |F_-(t)| + h\sum_{j=-N^h}^{i} n_j^h(t) + h(i + N^h + 1)N_D \\
&\leq |F_-(t)| + h\sum_{j=-N^h}^{N^h} n_j^h(t) + (2X + h)N_D \leq C_T\,,
\end{aligned}$$

which proves that F^h is bounded in $L^\infty((0,T)\times I)$ and implies the estimate on $F^h_{N^h}$.

Next, let $\phi \in \mathrm{C}_0^\infty(I)$ a test function. We have

$$\begin{aligned}
\langle \partial_x F^h, \phi\rangle &= -\int_{-X}^{X} F^h(t,x)\phi'(x)\,dx = -\sum_{i=-N^h}^{N^h-1} F_i^h \int_{ih}^{(i+1)h} \phi'(x)\,dx \\
&= \sum_{i=-N^h}^{N^h-1} F_i^h(\phi(ih) - \phi((i+1)h)) \\
&= \sum_{i=-N^h}^{N^h} \Big((F_i^h - F_{i-1}^h)\ \phi(ih)\Big) + F^h_{-N^h-1}\phi(-N^h h) - F^h_{N^h}\phi(N^h h) \\
&= h\sum_{i=-N^h}^{N^h} \Big((n_i^h - N_D)\ \phi(ih)\Big) + F_-\phi(-X) - F^h_{N^h}\phi(X),
\end{aligned}$$

where we have used (7.8). Hence, by using the above bounds we deduce that the following estimate

$$|\langle \partial_x F^h, \phi\rangle| \;\leq\; \|\phi\|_{\mathrm{L}^\infty(I)} \left(h\sum_{i=-N^h}^{N^h} n_i^h + (2X+h)N_D\right) \leq \|\phi\|_{\mathrm{L}^\infty(I)}\ C_T\,,$$

holds. This proves that $\partial_x F^h$ is bounded in $\mathrm{L}^\infty(0,T;\mathcal{M}(I))$. □

Remark 1. Since the functions $W^{(b,f)}$ and D are continuous and positive in $\mathbb{R}$, the uniform bound on F_i^h guarantees that

$$\begin{cases}
\displaystyle\inf_{h>0, i\in\{-N^h,\dots,N^h\}, 0\leq t\leq T} D(F_i^h(t)) \geq \delta > 0, \\
\displaystyle\inf_{h>0, 0\leq t\leq T} W^{(f)}(F^h_{N^h}(t)) \geq \delta > 0, \\
\displaystyle\inf_{0\leq t\leq T} W^{(b)}(F_-(t)) \geq \delta > 0,
\end{cases}$$

for some $\delta > 0$. Coming back to (7.13), we deduce that the boundary terms $n_{\pm N^h}$ are bounded in $\mathrm{L}^1(0,T)$. Similarly, there exists $0 < M < \infty$ such that

$$\begin{cases} \sup\limits_{h>0, i\in\{-N^h,\dots,N^h\}, 0\le t\le T} |D(F_i^h)| \le M, \\ \sup\limits_{h>0, i\in\{-N^h,\dots,N^h\}, 0\le t\le T} |v(F_i^h)| \le M, \\ \sup\limits_{h>0, 0\le t\le T} |W^{(f)}(F_{N_h}^h)| \le M, \\ \sup\limits_{h>0, 0\le t\le T} |W^{(b)}(F_-^h)| \le M, \\ \sup\limits_{0\le t\le T} |j^{(e)}(F_-)| \le M. \end{cases}$$

Lemma 7.3 (L^2 ESTIMATE OF THE DENSITY.). The sequence n^h is bounded in $\mathrm{L}^\infty(0,T;\mathrm{L}^2(I))$. The "boundary terms" $n^h_{\pm N^h}$ are bounded in $\mathrm{L}^2(0,T)$. Moreover, we have

$$\int_0^T \sum_{i=-N^h}^{N^h-1} \frac{|n_{i+1}^h - n_i^h|^2}{h}\, ds \le C_T\,.$$

Proof. Multiplying (7.7) by n_i^h and summing over i, we obtain

$$\begin{aligned} \frac{h}{2}\frac{d}{dt}\sum_{i=-N^h}^{N^h} |n_i^h|^2 &= \sum_{i=-N^h}^{N^h} (J^h_{i-1\to i} - J^h_{i\to i+1}) n_i^h \\ &= \sum_{i=-N^h}^{N^h-1} J^h_{i\to i+1}(n^h_{i+1} - n^h_i) + J^h_{-N^h-1\to -N^h} n^h_{-N^h} - J^h_{N^h\to N^h+1} n^h_{N^h} \\ &= \sum_{i=-N^h}^{N^h-1} \left(n_i^h v(F_i^h) - \frac{1}{h} D(F_i^h)(n^h_{i+1} - n^h_i)\right)(n^h_{i+1} - n^h_i) \\ &\qquad + j^{(e)}(F_-) n^h_{-N^h} - |n^h_{-N^h}|^2 W^{(b)}(F_-) - |n_{N^h}|^2 W^{(f)}(F^h_{N^h}). \end{aligned}$$

By using Remark 1, we deduce the inequality

$$\begin{aligned} &\frac{h}{2}\sum_{i=-N^h}^{N^h} |n_i^h(t)|^2 + \delta \int_0^t \left(\sum_{i=-N^h}^{N^h-1} \frac{|n^h_{i+1} - n^h_i|^2}{h} + |n^h_{-N^h}|^2 + |n_{N^h}|^2 \right) ds \\ &\le \frac{h}{2}\sum_{i=-N^h}^{N^h} |n_i^h(0)|^2 + M \int_0^t \left(\sum_{i=-N^h}^{N^h-1} n_i^h |n^h_{i+1} - n^h_i| + n^h_{-N^h} \right) ds\,. \end{aligned}$$

Now, by using the Young inequality we estimate

$$\int_0^t \sum_{i=-N^h}^{N^h-1} n_i^h |n^h_{i+1} - n^h_i|\, ds \le \frac{2Mh}{\delta}\int_0^t \sum_{i=-N^h}^{N^h} |n_i^h|^2\, ds + \frac{\delta}{2M}\int_0^t \sum_{i=-N^h}^{N^h-1} \frac{|n^h_{i+1} - n^h_i|^2}{h}\, ds.$$

It follows that

$$\frac{h}{2}\sum_{i=-N^h}^{N^h}|n_i^h(t)|^2+\frac{\delta}{2}\int_0^t\sum_{i=-N^h}^{N^h-1}\frac{|n_{i+1}^h-n_i^h|^2}{h}\,ds+\delta\int_0^t(|n_{-N^h}^h|^2+|n_{N^h}|^2)\,ds$$
$$\leq\frac{h}{2}\sum_{i=-N^h}^{N^h}|n_i^h(0)|^2+\frac{2M^2}{\delta}\int_0^t\Big(h\sum_{i=-N^h}^{N^h}|n_i^h|^2\Big)\,ds+M\int_0^t n_{-N^h}^h\,ds.$$

We conclude the proof by applying the Gronwall inequality and by taking into account that $n_{-N^h}^h$ is bounded in $\mathrm{L}^1(0,T)$ (see Remark 1). □

In order to study the limit in boundary terms we consider the next statement.

Lemma 7.4 (H^1 ESTIMATE OF THE ELECTRIC FIELD AT THE BOUNDARY.). The sequence $F_{N^h}^h$ is bounded in $\mathrm{H}^1(0,T)$.

Proof. We have proved that $F_{N^h}^h$ is bounded in $\mathrm{L}^\infty(0,T)$. There remains to bound its time derivative in $\mathrm{L}^2(0,T)$. This is a consequence of (7.9) together with the estimates in Lemma 7.2 and 7.3. Indeed, we get (see the argument given in Lemma 7.1)

$$\begin{aligned}\left|\frac{d}{dt}F_{N^h}^h(t)\right| &= \left|\frac{d}{dt}F_- + \frac{d}{dt}\Big(h\sum_{i=-N^h}^{N^h}(n_i^h-N_D)\Big)\right| \\ &= \left|\frac{d}{dt}F_- + j^{(e)}(F_-) - n_{-N^h}^h W^{(b)}(F_-) - n_{N^h}^h W^{(f)}(F_{N^h}^h)\right| \\ &= \left\|\frac{d}{dt}F_-\right\|_{\mathrm{L}^\infty(0,T)} + M(1+n_{-N^h}^h+n_{N^h}^h).\end{aligned}$$

By Lemma 7.3 the right hand side is bounded in $\mathrm{L}^2(0,T)$, which ends the proof. □

Lemma 7.5 (BV ESTIMATE OF THE DENSITY.). The sequence n^h is bounded in $\mathrm{L}^2(0,T;\mathrm{B}V(I))$.

Proof. Once the L^2 estimate on n^h is known, we derive some bounds for

$\partial_x n^h$. Consider $\phi \in \mathrm{C}_0^\infty(I)$. We have

$$\begin{aligned}
|\langle \partial_x n^h, \phi\rangle| &= \left| -\int_{-X}^{X} n^h \phi' \, dx \right| = \left| -\sum_{i=-N^h}^{N^h-1} n_i^h \int_{ih}^{(i+1)h} \phi' \, dx \right| \\
&= \left| -\sum_{i=-N^h}^{N^h-1} n_i^h \, (\phi((i+1)h) - \phi(ih)) \right| \\
&= \left| \sum_{i=-N^h+1}^{N^h} (n_i^h - n_{i-1}^h) \, \phi(ih) + n_{-N^h}^h \phi(-N^h h) - n^h N^h \phi(N^h h) \right| \\
&\le \left(h \sum_{i=-N^h+1}^{N^h} |\phi(ih)|^2 \right)^{1/2} \left(\frac{1}{h} \sum_{i=-N^h+1}^{N^h} |n_i^h - n_{i-1}^h|^2 \right)^{1/2} \\
&\le \|\phi\|_{\mathrm{L}^\infty(I)} \, (2X)^{1/2} \left(\sum_{i=-N^h}^{N^h-1} \frac{|n_{i+1}^h - n_i^h|^2}{h} \right)^{1/2} . \qquad (7.14)
\end{aligned}$$

Lemma 7.3 implies that the $\mathrm{L}^2(0,T)$ norm of the right–hand side of (7.14) is bounded uniformly with respect to h. Hence, we conclude that $\partial_x n^h$ is in $\mathrm{L}^2(0,T;\mathcal{M}(I))$. □

Lemma 7.6 (Estimating the time derivative.). The sequences $\partial_t n^h$ and $\partial_t F^h$ are bounded in $\mathrm{L}^2(0,T;\mathcal{M}(I)) + \mathrm{L}^2(0,T;\mathrm{W}^{-1,1}(I))$ and in $\mathrm{L}^2(0,T;\mathcal{M}(I))$, respectively.

Proof. Let $\phi \in \mathrm{C}_0^\infty(I)$ and denote

$$\Gamma_i^h = \int_{ih}^{(i+1)h} \phi(x) \, dx \, ,$$

for $i \in \{-N^h, \ldots, N^h - 1\}$. Since the support of ϕ is included in I, we can extend Γ_i^h by 0 for $i \ge N^h$. We shall use the following basic estimates

$$\begin{cases} |\Gamma_i^h| \le h \, \|\phi\|_{\mathrm{L}^\infty(I)}, \\ |\Gamma_{i+1}^h - \Gamma_i^h| \le h^2 \, C \|\phi'\|_{\mathrm{L}^\infty(I)}. \end{cases}$$

Now we estimate the time derivative of the electric field by using the Ampère equations (1.15). We have

$$\begin{aligned}
\langle \partial_t F^h, \phi\rangle &= \sum_{i=-N^h}^{N^h-1} \frac{d}{dt} F_i^h \int_{ih}^{(i+1)h} \phi(x) \, dx \\
&= J^h \sum_{i=-N^h}^{N^h-1} \Gamma_i^h - \sum_{i=-N^h}^{N^h-1} J_{i\to i+1}^h \Gamma_i^h = I_1 + I_2,
\end{aligned} \qquad (7.15)$$

where $J^h(t)$ stands for the total current density, which is defined by the $(-N^h-1)$th Ampère equation

$$J^h(t) = \frac{d}{dt}F_- + J^h_{-N^h-1\to -N^h} = \frac{d}{dt}F_- + j^{(e)}(F_-) - W^{(b)}(F_-)n^h_{-N^h}.$$

By Lemma 7.3, this quantity is bounded in $\mathrm{L}^2(0,T)$. Therefore, the first term of the right–hand side of (7.15) is bounded by

$$|I_1| \leq \|\varphi\|_{\mathrm{L}^\infty(I)}\ 2hN^h\ |J^h| = \|\varphi\|_{\mathrm{L}^\infty(I)}\ 2X\ |J^h|,$$

which belongs to a bounded set in $\mathrm{L}^2(0,T)$. Next, I_2 is estimated as follows

$$\begin{aligned}
|I_2| &\leq \Big|\sum_{i=-N^h}^{N^h-1} n_i^h v(F_i^h)\ \Gamma_i^h\Big| + \Big|\sum_{i=-N^h}^{N^h-1}\frac{1}{h}D(F_i^h)(n_i^h - n_{i+1}^h)\ \Gamma_i^h\Big| \\
&\leq M\ \|\phi\|_{\mathrm{L}^\infty(I)}\ h\left(\sum_{i=-N^h}^{N^h-1} n_i^h + \sum_{i=-N^h}^{N^h-1}\frac{|n_i^h - n_{i+1}^h|}{h}\right) \\
&\leq M\ \|\phi\|_{\mathrm{L}^\infty(I)}\left(h\sum_{i=-N^h}^{N^h-1} n_i^h + \sqrt{2hN^h\sum_{i=-N^h}^{N^h-1}\frac{|n_i^h - n_{i+1}^h|^2}{h}}\right).
\end{aligned}$$

We conclude that $\partial_t F^h$ is bounded in $\mathrm{L}^2(0,T;\mathcal{M}^1(I))$.

Similarly, we deal with the time derivative of n^h. We have

$$\begin{aligned}
&|\langle\partial_t n^h, \varphi\rangle| = \Big|\sum_{i=-N^h}^{N^h-1}\frac{dn_i^h}{dt}\int_{ih}^{(i+1)h}\phi(x)\,dx\Big| = \Big|\frac{1}{h}\sum_{i=-N^h}^{N^h-1}(J^h_{i-1\to i} - J^h_{i\to i+1})\ \Gamma_i^h\Big| \\
&= \frac{1}{h}\Big|\sum_{i=-N^h}^{N^h-1} J^h_{i\to i+1}\ (\Gamma^h_{i+1} - \Gamma^h_i) + J^h_{-N^h-1\to -N^h}\Gamma^h_{-N^h} - J^h_{N^h-1\to N^h}\Gamma^h_{N^h}\Big| \\
&\leq \frac{1}{h}\Big|\sum_{i=-N^h}^{N^h-1} v(F_i^h)n_i^h\ (\Gamma^h_{i+1} - \Gamma^h_i)\Big| \\
&\quad + \frac{1}{h^2}\Big|\sum_{i=-N^h}^{N^h-1} D(F_i^h)(n_i^h - n_{i+1}^h)(\Gamma^h_{i+1} - \Gamma^h_i)\Big| \\
&\quad + \frac{1}{h}|j^{(e)}(F_-) - n^h_{-N^h}W^{(b)}(F_-)|\ |\Gamma^h_{-N^h}| \\
&\leq C\ h^2\ \|\phi'\|_{\mathrm{L}^\infty(I)}\left(\frac{M}{h}\sum_{i=-N^h}^{N^h-1} n_i^h + \frac{M}{h^2}\sum_{i=-N^h}^{N^h-1}|n_i^h - n_{i+1}^h|\right) \\
&\quad + h\ \|\phi\|_{\mathrm{L}^\infty(I)}\ \frac{M}{h}(1 + n^h_{-N^h}) \\
&\leq C\ \|\phi'\|_{\mathrm{L}^\infty(I)}\left(h\sum_{i=-N^h}^{N^h-1} n_i^h + \sqrt{2hN^h\sum_{i=-N^h}^{N^h-1}\frac{|n_i^h - n_{i+1}^h|^2}{h}}\right) \\
&\quad + \|\phi\|_{\mathrm{L}^\infty(I)}\ M(1 + n^h_{-N^h}),
\end{aligned}$$

which proves the estimate on $\partial_t n^h$. □

Continuous Model

Let us combine the estimates discussed in the previous section with the following classical compactness result (see e.g. [7], [103]):

Proposition 7.1. Consider Banach spaces B, X and Y. We suppose that $X \subset B \subset Y$, the first embedding being compact. Let $\mathcal{C}$ be a bounded set in $\mathrm{L}^p(0,T;X)$, $1 \le p \le \infty$. Assume that $\partial_t \mathcal{C} = \{\partial_t f,\ f \in \mathcal{C}\}$ is a bounded set in $\mathrm{L}^r(0,T;Y)$. Then, $\mathcal{C}$ is relatively compact in $\mathrm{L}^p(0,T;B)$ if $1 \le p < \infty$ and $r \ge 1$, or in $\mathrm{C}^0([0,T];B)$ if $p = \infty$ and $r > 1$.

Hence, from the previous estimates we have, possibly at the cost of extracting subsequences, that

$$\begin{cases} n^h \to n & \text{strongly in } \mathrm{L}^2((0,T)\times I) \text{ and in } \mathrm{C}^0([0,T];L^2(I)-weak), \\ \partial_x n^h \rightharpoonup \partial_x n & \text{weakly}-* \text{ in } \mathrm{L}^2(0,T;\mathcal{M}(I)), \\ F^h \to F & \text{strongly in } \mathrm{C}^0([0,T];L^p(I)) \text{ for any } 1 \le p < \infty, \end{cases} \tag{7.16}$$

as h goes to 0. Notice in particular that the convergence of traces in time makes sense and

$$n^h(t,x)_{|t=0} = n^{h,0}(x) \rightharpoonup n^0(x) = n(t,x)_{|t=0}\,,\ \text{weakly in } \mathrm{L}^2(I)$$

holds, with $n^{h,0}(x) = n_i^h$ for $ih < x < (i+1)h$, $i \in \{-N^h, \dots, N^h - 1\}$. In other words, we recover the initial condition in the limit $h \to 0$. Finally, we can also assure from Lemmas 7.3 and 7.4 the following properties

$$\begin{cases} n^h_{\pm N^h} \rightharpoonup n_\pm\,, & \text{weakly in } \mathrm{L}^2(0,T), \\ F^h_{N^h} \to F_+\,, & \text{uniformly in } \mathrm{C}^0([0,T]). \end{cases} \tag{7.17}$$

We first get the continuous Poisson equation.

Proposition 7.2. The electric field limit F and the density limit n satisfy the continuous Poisson equation

$$\partial_x F = n - N_D, \quad F_{|x=-X} = F_-$$

in a weak sense.

Remark 2. The Poisson relation with $n \in \mathrm{L}^2((0,T)\times I)$, implies, by Sobolev's imbedding, that F is in $\mathrm{L}^2(0,T;\mathrm{C}^0(\overline{I}))$ so that the traces of F are well-defined.

Proof. Let $\phi \in C^\infty(\overline{I})$ and $\phi_i^h = \phi(ih)$, for $i \in \{-N^h,\ldots,N^h\}$. We denote by ϕ^h the associated stepwise constant function. For the sake of simplicity it will be convenient to introduce also the stepwise constant function $\nabla^h(\phi)(x) = \frac{\phi_{i+1}^h - \phi_i^h}{h}$, for $x \in (ih,(i+1)h)$. Multiplying (7.8) by ϕ_i^h, we get

$$\begin{aligned} h \sum_{i=-N^h}^{N^h} \frac{F_i^h - F_{i-1}^h}{h}\,\phi_i^h &= h \sum_{i=-N^h}^{N^h} (n_i^h - N_D)\,\phi_i^h \\ &= \int_{-X}^{X} (n^h - N_D)\,\phi^h\,dx + h\,(n_{N^h}^h - N_D)\,\phi(X) \\ &= h \sum_{i=-N^h}^{N^h-1} F_i^h\,\frac{\phi_i^h - \phi_{i+1}^h}{h} + F_{N^h}^h \phi(X) - F_- \phi(-X) \\ &= -\int_{-X}^{X} F^h\,\nabla^h(\phi)\,dx + F_{N^h}^h \phi(X) - F_- \phi(-X). \end{aligned}$$

Since $\nabla^h(\phi)$ converges uniformly to $\phi'(x)$ on $\overline{I}$, we have

$$\int_{-X}^{X} (n^h - N_D)\,\phi^h\,dx \to -\int_{-X}^{X} F\,\phi'(x)\,dx + F_+\phi(X) - F_-\phi(-X)$$

as $h \to 0$.

We conclude that $\partial_x F = n - N_D \in \mathrm{L}^2((0,T)\times I)$ and, by the Sobolev embedding, F lies in $\mathrm{L}^2(0,T;\mathrm{C}^0(\overline{I}))$ and the traces of F are well-defined and are given by $F(t,\pm X) = F_\pm(t)$. □

Let us now show that the limit n is more regular that n^h is. In fact, we will prove that $n \in \mathrm{L}^2(0,T;\mathrm{H}^1(I))$, which guarantees that $n \in \mathrm{L}^2(0,T;\mathrm{C}^0(\overline{I}))$ due to the Sobolev embedding, so that the traces of the limit n with respect to the space variable are also well-defined.

Proposition 7.3. The density limit n of n^h belongs to $\mathrm{L}^2(0,T;\mathrm{H}^1(I))$.

Proof. Let $\phi \in \mathrm{C}_c^\infty(I)$. We have seen in the proof of Lemma 7.5 that the following estimate

$$\|\langle \partial_x n^h, \phi\rangle\|_{\mathrm{L}^2(0,T)} \le C_T \left(h \sum_{i=-N^h+1}^{N^h} |\phi(ih)|^2 \right)^{1/2} = C_T\,\|\phi^h\|_{\mathrm{L}^2(I)}$$

holds. We also check readily that ϕ^h tends to ϕ in $\mathrm{L}^2(I)$. Hence, letting $h \to 0$ leads to

$$\|\langle \partial_x n, \phi\rangle\|_{\mathrm{L}^2(0,T)} \le C_T\,\|\phi\|_{\mathrm{L}^2(I)}.$$

By a density argument the estimate can be extended for any function $\phi \in \mathrm{L}^2(I)$. We conclude that $\partial_x n \in L^2((0,T)\times I)$. $\square$

Convergence properties stronger than (7.16) will be necessary due to the nonlinear term. The idea is that the estimate in Lemma 7.3 is close to a $\mathrm{L}^2(0,T;\mathrm{H}^1(I))$ estimate on n^h. To this end we introduce the following $\mathbb{P}_1$ approximation: for $x \in (ih,(i+1)h)$, $i \in \{-N^h,\dots,N^h-1\}$, we set

$$\begin{cases} m^h(t,x) = \dfrac{n_{i+1}^h - n_i^h}{h}\,(x-ih) + n_i^h, \\ G^h(t,x) = \dfrac{F_{i+1}^h - F_i^h}{h}\,(x-ih) + F_i^h. \end{cases} \tag{7.18}$$

Then, the sequences (m^h, G^h) are close to the original quantities (n^h, F^h) and enjoy better compactness properties:

Lemma 7.7. The following estimates are verified

$$\begin{cases} \|n^h - m^h\|_{\mathrm{L}^2((0,T)\times I)} \le C_T\ h, \\ \|F^h - G^h\|_{\mathrm{L}^\infty((0,T)\times I)} \le C_T\ \sqrt{h}. \end{cases}$$

Furthermore, $\left(m^h\right)_{h>0}$ is relatively compact in $\mathrm{L}^2(0,T;\mathrm{C}^0(\overline{I}))$ and $\left(G^h\right)_{h>0}$ is relatively compact in $\mathrm{C}^0([0,T]\times\overline{I})$.

Proof. By taking into account the definition of the P_1 approximations, we have

$$m^h(t,x) - n^h(t,x) = \frac{n_{i+1}^h - n_i^h}{h}\,(x-ih)$$

in the interval $(ih,(i+1)h)$, $i \in \{-N^h,\dots,N^h-1\}$. Hence, by using Lemma 7.3 we get

$$\begin{aligned} \|m^h - n^h\|^2_{\mathrm{L}^2((0,T)\times I)} &= \int_0^T \sum_{i=-N^h}^{N^h-1} \left|\frac{n_{i+1}^h - n_i^h}{h}\right|^2 \int_{ih}^{(i+1)h} (x-ih)^2\,dx\,ds \\ &= \frac{h^2}{3}\int_0^T \sum_{i=-N^h}^{N^h-1} \frac{|n_{i+1}^h - n_i^h|^2}{h}\,ds \le C_T\ h^2\,. \end{aligned}$$

On the other hand, (7.8) yields

$$\begin{aligned} |G^h(t,x) - F^h(t,x)| &= \left|\frac{F_{i+1}^h - F_i^h}{h}\,(x-ih)\right| \\ &= |n_{i+1}^h - N_D|\,(x-ih) \le |n_{i+1}^h - N_D|\ h, \end{aligned}$$

for $x \in (ih,(i+1)h)$, $i \in \{-N^h,\dots,N^h-1\}$. Therefore, Lemma 7.3 allows to control this quantity as follows

$$\begin{aligned}
|G^h(t,x)-F^h(t,x)| &\leq \sqrt{h}\,\sqrt{h}\,(n^h_{i+1}+N_D)\\
&\leq \sqrt{h}\left(\left(h|n^h_{i+1}|^2\right)^{1/2}+\sqrt{h}N_D\right)\\
&\leq \sqrt{h}\left(\left(h\sum_{j=-N^h}^{N^h}|n^h_j|^2\right)^{1/2}+\sqrt{h}N_D\right)\leq C_T\,\sqrt{h}.
\end{aligned}$$

This proves the first part of the result.

Note that m^h and G^h are bounded in $\mathrm{L}^2(0,T;\mathrm{H}^1(I))$ and $\mathrm{L}^\infty(0,T;\mathrm{H}^1(I))$, respectively. Indeed, we have $\partial_x m^h = (n^h_{i+1}-n^h_i)/h$ on $(ih,(i+1)h)$ and the bound for $\partial_x m^h$ in L^2 follows directly from Lemma 7.3. For the approximate electric field we have $\partial_x G^h = (F^h_{i+1}-F^h_i)/h = n^h_{i+1}-N_D$, so that

$$\begin{aligned}
\|\partial_x G^h\|^2_{\mathrm{L}^2(I)} &= \sum_{i=-N^h}^{N^h}|n^h_{i+1}-N_D|^2\int_{ih}^{(i+1)h}dx \leq 2\sum_{i=-N^h}^{N^h}\left(|n^h_{i+1}|^2+N_D^2\right)h\\
&\leq 2\left(h\sum_{i=-N^h}^{N^h}|n^h_{i+1}|^2+(2X+h)N_D^2\right)\leq C_T.
\end{aligned}$$

Hence, to justify the compactness properties there remains to obtain some estimates on the time derivatives. We check that (see Appendix 7)

$$\begin{aligned}
&\partial_t(G^h-F^h) \quad \text{is bounded in } \mathrm{L}^2(0,T;\mathcal{M}(I)),\\
&\partial_t(m^h-n^h) \quad \text{is bounded in } \mathrm{L}^2(0,T;\mathcal{M}(I))+\mathrm{L}^2(0,T;\mathrm{W}^{-1,1}(I)).
\end{aligned} \tag{7.19}$$

Then, combining this information with Lemma 7.6 we deduce the asserted compactness by application of Proposition 7.1. □

As a consequence of the compactness property, and identifying limits, we can assure that

$$\begin{cases}
G^h \to F\,, & \text{uniformly on } [0,T]\times\overline{I},\\
m^h \to n\,, & \text{strongly in } \mathrm{L}^2(0,T;C^0(\overline{I})),\\
\partial_x m^h \rightharpoonup \partial_x n\,, & \text{weakly in } \mathrm{L}^2((0,T)\times I).
\end{cases} \tag{7.20}$$

Since G^h is $\sqrt{h}$–close to F^h in the L^∞–norm, we can improve the convergence in (7.16). Actually, we have

$$F^h \to F\,,\ \text{uniformly on } [0,T]\times\overline{I}. \tag{7.21}$$

Notice also in (7.20) that the traces are well-defined and the following convergences

$$\begin{cases} m^h(\pm X) = n^h_{\pm N^h} \to n(\pm X) = n_\pm\,, & \text{strongly in } \mathrm{L}^2(0,T),\\ G^h(\pm X) = F^h_{\pm N^h} \to F(\pm X) = F_\pm\,, & \text{strongly in } \mathrm{L}^2(0,T),\end{cases}$$

hold. In particular, the traces of n at $\pm X$ can be identified with the limits $n_\pm$ respectively, which were defined in (7.17).

In order to pass to the limit in the equation, we write a discrete weak formulation. Let $\phi \in \mathrm{C}^\infty(\overline{I})$. We denote $\phi^h_i = \phi(ih)$ and ϕ^h stands for the associated piecewise constant approximation. Then, we get

$$\begin{aligned} h\sum_{i=-N^h}^{N^h} \frac{d}{dt} n^h_i\ \phi^h_i &= \sum_{i=-N^h}^{N^h} (J^h_{i-1\to i} - J^h_{i\to i+1})\ \phi^h_i \\ &= \sum_{i=-N^h}^{N^h-1} J^h_{i\to i+1}\ (\phi^h_{i+1} - \phi^h_i) - J^h_{N^h\to N^h+1}\phi^h_{N^h} + J^h_{-N^h-1\to -N^h}\phi^h_{-N^h} \\ &= \sum_{i=-N^h}^{N^h-1} v(F^h_i) n^h_i\ (\phi^h_{i+1} - \phi^h_i) - \sum_{i=-N^h}^{N^h-1} D(F^h_i)\frac{1}{h}\ (n^h_{i+1} - n^h_i)\ (\phi^h_{i+1} - \phi^h_i) \\ &\quad -W^{(f)}(F^h_{N^h}) n^h_{N^h}\phi^h_{N^h} + (j^{(e)}(F_-) - W^{(b)}(F_-) n^h_{-N^h})\phi^h_{-N^h}. \end{aligned} \tag{7.22}$$

Let us rewrite the discrete sums as integrals as follows

$$\begin{aligned} &\frac{d}{dt}\int_{-X}^{X} n^h\ \phi^h\, dx + h\frac{d}{dt} n^h_{N^h}\ \phi(X) \\ &\quad = \int_{-X}^{X} v(F^h) n^h\ \nabla^h\phi\, dx - \int_{-X}^{X} D(F^h)\partial_x m^h\ \nabla^h \phi\, dx \\ &\qquad -W^{(f)}(F^h_{N^h}) n^h_{N^h}\phi(X) + (j^{(e)}(F_-) - W^{(b)}(F_-) n^h_{-N^h})\phi(-X), \end{aligned} \tag{7.23}$$

following the notation $\nabla^h\phi(x) = (\phi^h_{i+1} - \phi^h_i)/h$, for $x \in (ih, (i+1)h)$. We can now pass to the limit $h \to 0$.

We check that $\phi^h \to \phi$ and $\nabla^h\phi \to \phi'$ uniformly on $\overline{I}$. Let us pass to the limit in each term of (7.23). Taking into account that $n^h \to n$ in $\mathrm{C}^0([0,T]; \mathrm{L}^2(I) - \mathit{weak})$, we have $\int_{-X}^X n^h\phi^h\,dx \to \int_{-X}^X n\phi\,dx$ in $\mathrm{C}^0([0,T])$. Since $n^h_{N^h}$ is bounded in $\mathrm{L}^2(0,T)$, the second term in the left–hand side of (7.23) vanishes as $h \to 0$ in $\mathcal{D}'(0,T)$. Next, by using (7.21), $v(F^h)\nabla^h\phi \to v(F)\phi'$ and $D(F^h)\nabla^h\phi \to D(F)\phi'$ uniformly on $[0,T]\times\overline{I}$. To do that we combine the strong convergence $n^h \to n$ and the weak convergence $\partial_x m^h \to \partial_x n$ in $\mathrm{L}^2((0,T)\times I)$ so that the integrals in the right–hand side of (7.23) tend to

$$\int_X^X v(F) n\ \phi', dx - \int_X^X D(F)\partial_x n\ \phi'\, dx$$

as $h \to 0$ in $\mathcal{D}'(0,T)$. Finally, for the boundary terms we combine the convergence properties in (7.17) to find as limit as $h \to 0$ the expression

$$-W^{(f)}(F)n\phi(X) + \left(j^{(e)}(F) - W^{(b)}(F)n\right)\phi(-X)\,.$$

Therefore, letting $h \to 0$ in (7.23) we have

$$\frac{d}{dt}\int_X^X n\ \phi, dx = \int_X^X v(F)n\ \phi', dx - \int_X^X D(F)\partial_x n\phi'\, dx$$
$$+W^{(f)}(F)n\phi(X) + \left(j^{(e)}(F) - W^{(b)}(F)n\right)\phi(-X)$$

in $\mathcal{D}'(0,T)$. This ends the proof of Theorem 7.2.

The bias constraint

In this Section we reconsider the bias condition (7.3) as an alternative to the prescription of the emitter electric field (7.4). The arguments are exactly those of the previous section and we only point out the main differences in the proof. In rescaled form the condition is

$$h\sum_{i=-N^h}^{N^h} F_i^h = V, \tag{7.24}$$

which is added to the system (7.7), (7.8). This scaling means that the ratio $\frac{\mathcal{LF}}{\mathcal{V}}$ has order 1, $\mathcal{V}$ being a characteristic value for the total voltage. Of course, the L^1 estimate in Lemma 7.1 still holds, provided that $j^{(e)}$ is a bounded function. Then, the keypoint in the previous analysis is to establish a uniform estimate (with respect to h) on the electric field $F^h_{-N^h-1}$.

Lemma 7.8. The quantity $F^h_{-N^h-1}$ is bounded in $L^\infty((0,T))$.

Proof. Let us sum the relations (7.9). We get

$$\begin{aligned}
h\sum_{i=-N^h}^{N^h} F_i^h &= V = h\sum_{i=-N^h}^{N^h}\left(F^h_{-N^h-1} + h\sum_{j=-N^h}^{i}(n_j^h - N_D)\right)\\
&= (2N^h+1)h\ F^h_{-N^h-1} + h^2\sum_{j=-N^h}^{N^h}\left((n_j^h - N_D)\sum_{i=j}^{N^h} 1\right)\\
&= (2N^h+1)h\ F^h_{-N^h-1} + h^2\sum_{j=-N^h}^{N^h}(n_j^h - N_D)(N^h - j + 1).
\end{aligned}$$

Consequently, the electric field at the emitter is given by

$$F^h_{-N^h-1} = \frac{V}{(2N^h+1)h} - \frac{h}{2N^h+1} \sum_{j=-N^h}^{N^h} (n^h_j - N_D)(N^h - j + 1). \qquad (7.25)$$

It follows that

$$\begin{aligned} |F^h_{-N^h-1}| &\leq \frac{|V|}{(2N^h+1)h} + \frac{h^2}{(2N^h+1)h} \sum_{j=-N^h}^{N^h} |n^h_j - N_D| \; |N^h - j + 1| \\ &\leq \frac{|V|}{2X} + \frac{h}{(2N^h+1)h} \Big(h \sum_{j=-N^h}^{N^h} n^h_j + (2N^h+1) h N_D \Big) (2N^h+1) \\ &\leq \frac{|V|}{2X} + h \sum_{j=-N^h}^{N^h} n^h_j + (2X + h) N_D. \end{aligned}$$

This leads to the estimate of $F^h_{-N^h-1}$ in $\mathrm{L}^\infty((0,T))$. □

Once we have this estimate, we can justify the bounds in Lemma 7.2 and Lemma 7.3. We also need some control on the time derivative of $F^h_{-N^h-1}$.

Lemma 7.9. The quantity $F^h_{-N^h-1}$ is bounded in $\mathrm{H}^1((0,T))$.

Proof. Differentiating (7.25), we find

$$\begin{aligned} \frac{d}{dt} F^h_{-N^h-1} &= \frac{h}{2N^h+1} \sum_{i=-N^h}^{N^h} \Big(\sum_{j=-N^h}^{i} \frac{d}{dt} n^h_j \Big) \\ &= \frac{1}{2N^h+1} \sum_{i=-N^h}^{N^h} \Big(\sum_{j=-N^h}^{i} (J^h_{j-1\to j} - J^h_{j\to j+1}) \Big) \\ &= \frac{1}{2N^h+1} \sum_{i=-N^h}^{N^h} (J^h_{-N^h-1\to -N^h} - J^h_{i\to i+1}) \\ &= J^h_{-N^h-1\to -N^h} - \frac{1}{2N^h+1} \; J_{N^h \to N^h+1} \\ &\quad + \frac{1}{2N^h+1} \sum_{i=-N^h}^{N^h-1} \Big(v(F^h_i) n^h_i - D(F^h_i) \frac{n^h_{i+1} - n^h_i}{h} \Big). \end{aligned}$$

Using the bounds of Lemma 7.8 and Lemma 7.2, we can bound $v(F^h_i)$, $D(F^h_i)$, $j^{(e)}(F^h_{-N^h-1})$, $W^{(b)}(F^h_{-N^h-1})$ and $W^{(f)}(F^h_{N^h})$ by some constant $0 < M < \infty$.

Hence, we deduce that

$$\begin{aligned}\left|\frac{d}{dt}F^h_{-N^h-1}\right| &\le M(1+n^h_{-N^h}+n^h_{N^h})\\ &\quad+\frac{M}{(2N^h+1)h}\left(h\sum_{i=-N^h}^{N^h} n_i^h+\sum_{i=-N^h}^{N^h}|n^h_{i+1}-n^h_i|\right)\\ &\le M(1+n^h_{-N^h}+n^h_{N^h})+\frac{M}{2X}\,h\sum_{i=-N^h}^{N^h} n_i^h\\ &\quad+\frac{M}{\sqrt{2X}}\left(\sum_{i=-N^h}^{N^h}\frac{|n^h_{i+1}-n^h_i|^2}{h}\right)^{1/2}.\end{aligned}$$

We conclude by applying the estimates of Lemma 7.3. □

By using these estimates, we can reproduce *mutatis mutandis* the arguments of the previous section. We conclude with the following result.

Theorem 7.3. Assume that $j^{(e)}$ is a bounded function. Then, the conclusions of Theorem 1 are still valid by replacing the condition (7.4) by (7.24). Accordingly, in the limit problem the electric field satisfies the Poisson equation $\partial_x F = n - N_D$ coupled to the constraint $\int_{-X}^{X} F\,dx = V$.

Appendix A: Proof of (7.19)

We write $m^h = \nu^h + n^h$, $G^h = \Phi^h + F^h$. Recall that ν^h, Φ^h are defined on $(0,T)\times(ih,(i+1)h)$, $i\in\{-N^h,\dots,N^h-1\}$, by

$$\nu^h(t,x)=\frac{1}{h}\,(n^h_{i+1}-n^h_i),\qquad \Phi^h(t,x)=\frac{1}{h}\,(F^h_{i+1}-F^h_i)=n^h_{i+1}-N_D\,,$$

where we have used (7.8) in the second relation. As in the proof of Lemma 7.6, we consider a test function $\phi\in C_0^\infty(I)$ and set $\Gamma_i^h=\int_{ih}^{(i+1)h}(x-ih)\phi(x)\,dx$, which verifies $|\Gamma_i^h|\le\|\phi\|_{L^\infty(I)}h^2/2$. We have

$$\begin{aligned}\langle\partial_t\Phi^h,\phi\rangle &= \sum_{i=-N^h}^{N^h-1}\frac{dn^h_{i+1}}{dt}\int_{ih}(i+1)h(x-ih)\phi(x)\,dx\\ &= \sum_{i=-N^h}^{N^h-1}\frac{1}{h}\,(J^h_{i\to i+1}-J^h_{i+1\to i+2})\,\Gamma_i^h\\ &= \sum_{i=-N^h}^{N^h-1}J^h_{i\to i+1}\,\frac{1}{h}\,(\Gamma_i^h-\Gamma_{i-1}^h)-\frac{1}{h}J^h_{N^h\to N^h+1}\Gamma^h_{N^h-1}\,.\end{aligned}$$

We can bound this expression as follows

$$\begin{aligned}
|\langle \partial_t \Phi^h, \phi\rangle| &\le \|\phi\|_{\mathrm{L}^\infty(I)} h \left(\sum_{i=-N^h}^{N^h-1} |v(F_i^h) n_i^h + \frac{1}{h} D(F_i^h)(n_{i+1}^h - n_i^h)| \right) \\
&\quad + \|\phi\|_{\mathrm{L}^\infty(I)} h \ |W^{(f)}(F_{N^h}^h) n_{N^h}^h| \\
&\le \|\phi\|_{\mathrm{L}^\infty(I)} \ M \left(h \sum_{i=-N^h}^{N^h-1} n_i^h + \Big(\sum_{i=-N^h}^{N^h-1} \frac{|n_{i+1}^h - n_i^h|^2}{h} \Big)^{1/2} \sqrt{2X} + n_{N^h}^h \right).
\end{aligned}$$

Thus, from Lemma 7.3 we deduce that $\partial_t \Phi^h$ is bounded in $\mathrm{L}^2(0,T;\mathcal{M}(I))$.

We proceed with ν^h in a similar way. Indeed, we can write

$$\begin{aligned}
\langle \partial_t \nu^h, \phi\rangle &= \frac{1}{h} \sum_{i=-N^h}^{N^h-1} \Big(\frac{dn_{i+1}^h}{dt} - \frac{dn_i^h}{dt} \Big) \int_{ih} (i+1)h(x-ih)\phi(x)\, dx \\
&= \frac{1}{h^2} \sum_{i=-N^h}^{N^h-1} (-J_{i+1\to i+2}^h + 2J_{i\to i+1}^h - J_{i-1\to i}^h) \ \Gamma_i^h \\
&= \frac{1}{h^2} \sum_{i=-N^h}^{N^h-1} J_{i\to i+1}^h \ (-\Gamma_{i+1}^h + 2\Gamma_i^h - \Gamma_{i-1}^h) \\
&\quad - \frac{1}{h^2} J_{N^h\to N^h+1}^h \Gamma_{N^h-1}^h - \frac{1}{h^2} J_{-N^h-1\to -N^h}^h \Gamma_{-N^h}^h .
\end{aligned} \tag{7.26}$$

The boundary terms in (7.26) are bounded by

$$M(1 + n_{-N^h}^h + n_{N^h}^h)\|\phi\|_{\mathrm{L}^\infty(I)},$$

which belongs to a bounded set of $\mathrm{L}^2(0,T)$. Next, we have the bound

$$\frac{1}{h^2} | -\Gamma_{i+1}^h + 2\Gamma_i^h - \Gamma_{i-1}^h| \le C\|\phi'\|_{\mathrm{L}^\infty(I)} \ h.$$

Therefore, the sum in the right–hand side of (7.26) can be estimated by

$$\begin{aligned}
C\|\phi'\|_{\mathrm{L}^\infty(I)} \ h \sum_{i=-N^h}^{N^h-1} |J_{i\to i+1}^h| \ &\le \ CM\|\phi'\|_{\mathrm{L}^\infty(I)} \left(h \sum_{i=-N^h}^{N^h-1} n_i^h \right. \\
&\quad \left. + \Big(\sum_{i=-N^h}^{N^h-1} \frac{|n_{i+1}^h - n_i^h|^2}{h} \Big)^{1/2} \sqrt{2X} \right),
\end{aligned}$$

as we did in the previous proof for Φ^h. We conclude that $\partial_t \nu^h$ is bounded in $\mathrm{L}^2(0,T;\mathcal{M}(I)) + \mathrm{L}^2(0,T;\mathrm{W}^{-1,1}(I))$. This ends the proof of (7.19).

Appendix B: Uniqueness for the limiting problem

In this section, we show the uniqueness of the solution of (7.10). Let us consider two solutions (n_1, F_1) and (n_2, F_2) of (7.10) with $n_i \in \mathrm{C}^0([0,T]; \mathrm{L}^2(I)) \cap \mathrm{L}^2(0,T; \mathrm{H}^1(I))$. For the difference, we have

$$\partial_t(n_1 - n_2) + \partial_x J(F_1, n_1 - n_2) + \partial_x \Big((v(F_1) - v(F_2))n_2 - (D(F_1) - D(F_2))\partial_x n_2 \Big) = 0,$$

where $J(F,n) = v(F)n - D(F)\partial_x n$. The boundary conditions read

$$\begin{cases} J(F_1, n_1 - n_2)(X) = W^{(f)}(F_1)(n_1 - n_2) + (W^{(f)}(F_1) - W^{(f)}(F_2))n_2, \\ J(F_1, n_1 - n_2)(X) = j^{(e)}(F_1) - j^{(e)}(F_2) - W^{(b)}(F_1)(n_1 - n_2) \\ \qquad\qquad\qquad\qquad\qquad -(W^{(b)}(F_1) - W^{(b)}(F_2))n_2. \end{cases}$$

Thus, we are only left with the task of evaluating

$$\begin{aligned} \frac{d}{dt}\int_{-X}^{X} \frac{|n_1 - n_2|^2}{2}\,dx &+ \int_{-X}^{X} D(F_1)|\partial_x(n_1 - n_2)|^2\,dx \\ = \int_{-X}^{X} & v(F_1)(n_1 - n_2)\partial_x(n_1 - n_2)\,dx \\ & + \int_{-X}^{X} (v(F_1) - v(F_2))n_2\partial_x(n_1 - n_2)\,dx \\ & - \int_{-X}^{X} (D(F_1) - D(F_2))\partial_x n_2 \partial_x(n_1 - n_2)\,dx \\ & + J(F_1, n_1 - n_2)(n_1 - n_2)(-X) - J(F_1, n_1 - n_2)(n_1 - n_2)(X). \end{aligned} \tag{7.27}$$

Denote by A, B, C, D and E the five terms in the right hand side of (7.27). Recall that F_i belongs to L^∞, so that the coefficients are lying in a bounded set. Also denote by Λ a Lipschitz constant for the functions $v, D, j^{(e)}$ and $W^{(b,f)}$ in the range of values of F_1 and F_2. Let $\nu > 0$ be a parameter to be precised later on. By using the Cauchy-Schwarz and Young inequalities, we can estimate

$$|A| \leq C_\nu \int_{-X}^{X} |n_1 - n_2|^2\,dx + \nu \int_{-X}^{X} |\partial_x(n_1 - n_2)|^2\,dx.$$

Next, we have

$$\begin{aligned} |B| &\leq \Lambda \|F_1 - F_2\|_{\mathrm{L}^\infty(I)} \int_{-X}^{X} |n_2|\ |\partial_x(n_1 - n_2)|\,dx \\ &\leq C_\nu \Lambda^2 \int_{-X}^{X} |n_2|^2\,dx\ \|F_1 - F_2\|^2_{\mathrm{L}^\infty(I)} + \nu \int_{-X}^{X} |\partial_x(n_1 - n_2)|^2\,dx. \end{aligned}$$

The Poisson equations yield to

$$(F_1 - F_2)(t,x) = F_{-,1} - F_{-,2} + \int_{-X}^{x} (n_1 - n_2)(t,y)\, dy,$$

which provides the bound

$$\|F_1 - F_2\|^2_{L^\infty(I)} \le 2|F_{-,1} - F_{-,2}|^2 + 4X \int_{-X}^{X} |n_1 - n_2|^2\, dx.$$

Hence, we get (changing the value of C_ν...)

$$|B| \le C_\nu \int_{-X}^{X} |n_2|^2 dx \left(|F_{-,1} - F_{-,2}|^2 + \int_{-X}^{X} |n_1 - n_2|^2\, dx \right) + \nu \int_{-X}^{X} |\partial_x (n_1 - n_2)|^2 dx.$$

A similar reasoning for C leads to

$$|C| \le C_\nu \int_{-X}^{X} |\partial_x n_2|^2 dx \left(|F_{-,1} - F_{-,2}|^2 + \int_{-X}^{X} |n_1 - n_2|^2 dx \right) + \nu \int_{-X}^{X} |\partial_x (n_1 - n_2)|^2 dx.$$

For the boundary terms, we get rid of the terms $-W^{(b,f)}(F_1)|n_1 - n_2|^2$ which are nonnegative and get

$$D + E \le \Lambda\Big((1 + n_2)\ |F_1 - F_2|\ |n_1 - n_2|(-X) + n_2\ |F_1 - F_2|\ |n_1 - n_2|(+X) \Big).$$

Then, we use the Sobolev embedding to control the traces of $n_1 - n_2$ with the H^1 norm. Finally, we obtain

$$\begin{aligned} D + E \le{}& C_\nu (1 + |n_2(-X)|^2 + |n_2(X)|^2) \left(|F_{-,1} - F_{-,2}|^2 + \int_{-X}^{X} |n_1 - n_2|^2 \right) \\ &+ \nu \Big(\int_{-X}^{X} |n_1 - n_2|^2\, dx + \int_{-X}^{X} |\partial_x (n_1 - n_2)|^2\, dx \Big). \end{aligned}$$

Having disposed of these preliminaries, recall that $D(F_1)$ is bounded from below by some $\delta > 0$. Then, we put all the pieces together and choose $\nu = \nu(\delta)$ appropriately so that we finally find

$$\begin{aligned} &\frac{d}{dt} \int_{-X}^{X} |n_1 - n_2|^2\, dx + \frac{\delta}{2} \int_{-X}^{X} |\partial_x (n_1 - n_2)|^2\, dx \\ &\qquad \le f(t) \int_{-X}^{X} |n_1 - n_2|^2\, dx + g(t) |F_{-,1} - F_{-,2}|^2, \end{aligned}$$

where the nonnegative functions $f, g \in L^1(0,T)$ depend on Λ, δ and $\int_{-X}^{X} (n_2^2 + |\partial_x n_2|^2)\, dx$. The Gronwall Lemma provides the inequality

$$\begin{aligned} &\int_{-X}^{X} |n_1 - n_2|^2(t,x)\, dx \\ &\qquad \le e^{\int_0^t f(s)\, ds} \Big(\int_{-X}^{X} |n_1 - n_2|^2(0,x)\, dx + \int_0^t g(s) |F_{-,1} - F_{-,2}|^2(s)\, ds \Big). \end{aligned}$$

This proves the continuity of the solution with respect to the data and, consequently, the uniqueness of the solution. We skip the adaptation of the proof to the bias condition.

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