

Kinetic energy bounds for particles confined in spherically-symmetric traps with non-standard dimensions

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Abstract. The kinetic energy of non-relativistic single-particle systems with arbitrary D -dimensional central potentials is found to be bounded from below by means of the orbital hyperangular quantum number, the dimensionality and some radial and logarithmic expectation values of the form $\langle r^k \rangle$ and $\langle r^k (\ln r)^m \rangle$. Beyond the intrinsic physico-mathematical interest of this problem, we want to contribute to the current development of the theory of independent particles confined in spherically symmetric traps with non-standard dimensions. The latter has been motivated by the recent experimental achievements of the evaporative cooling of dilute (i.e. almost non-interacting) fermions in magnetic traps.

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1. Introduction

The fundamental relevance and usefulness of spherically-symmetric potentials for the quantum-mechanical description of the natural systems and phenomena is manifest from the early days of quantum physics up until now [1]–[8]. Indeed, the central-field model of the atom [1, 3, 4] is, together with the Pauli exclusion principle and Bohr’s atomic Aufbau principle, the theoretical basis of the periodic system of Mendeleev [6]; see also [9]. Moreover, they have been used as prototypes for numerous other purposes and systems not only in the three-dimensional world but also for non-relativistic [5] and relativistic [2, 7] D -dimensional ($D \geq 2$) physics.

The study of the density-dependent properties of single-particle systems confined in D -dimensional central potentials is of considerable current interest because of quantum dots and wires and recent experiments of dilute bosonic [10, 11] and fermionic [12, 13] systems in magnetic traps of extremely low temperatures. This is provoking a fast development of a density functional theory of independent particles moving in multidimensional central potentials with various analytical forms. Here we shall centre around the kinetic energy.

Since the works of Waller [14], Van Vleck [15] and Pasternack [16] in the thirties until the recent attempts of Dong *et al* [17, 18], many recurrence relations of diverse types have been produced for the calculation of the radial position and momentum expectation values and, at times, matrix elements for some specific central potentials (e.g. harmonic oscillator, Coulomb, Kratzer, . . .) and, less frequently, for arbitrary D -dimensional central potentials. Nevertheless they require for their application knowledge of the analytic form of the potential and, often, their corresponding energy eigenvalues.

Unlike previous approaches, we propose in this paper an inequality-based method which allows us to correlate the non-relativistic single-particle kinetic energy T ($= \langle p^2 \rangle / 2$) with some radial position expectation values for arbitrary D -dimensional central potentials of unknown form. The resulting general inequalities are used to find lower bounds for the kinetic energy of single-particle systems with a D -dimensional central potential of unknown analytic form, by means of various radial position expectation values and the orbital hyperangular quantum number. This procedure leads to the improvement of the corresponding sharp bounds for general

systems existing in the literature, to the generation of novel bounds for these systems, and to the generalization of recent results relative to non-relativistic particles in D -dimensions [19]–[21].

The structure of the paper is as follows. Section 2 gathers the known lower bounds to the kinetic energy of spinless single-particle systems with potential of general form, with emphasis on those which depend on the expectation values $\langle r^{-2} \rangle$, $\langle r^{-1} \rangle$ and $\langle r^2 \rangle$. Then, in section 3, the main results of the paper are described: optimal lower bounds to the kinetic energy of particles moving in central potentials of arbitrary form by means of various expectation values $\langle r^k \rangle$. Later on, in section 4, further bounds in terms of radial logarithmic bounds are obtained; at times, depending on the potential, they improve the previous ones. Finally, the accuracy of some of the novel bounds is numerically studied for the Coulomb and oscillator-like systems.

Atomic units will be used throughout the paper.

2. Kinetic energy lower bounds for general single-particle systems

Here we briefly review the present knowledge of the lower bounds to the non-relativistic kinetic energy T of a spinless particle moving in a D -dimensional potential of unknown analytic form, taking only into account those related results which are relevant for the purposes of the present work.

According to Lieb *et al* [22] the kinetic energy T is known to be bounded from below by means of the frequency moments of the quantum-mechanical probability distribution $\rho(\vec{r})$, i.e. the quantities

$$\omega_t(\rho) \equiv \int d^D r [\rho(\vec{r})]^t, \quad (1)$$

which are also called entropic moments because of their close connection with some information-theoretic quantities such as the Shannon, Renyi and Tsallis [23, 24]. They found [25, 26] that

$$T \geq K_D \omega_{1+(2/D)}(\rho),$$

where the constant

$$K_D \equiv \frac{2\pi D}{D+2} \left[\Gamma\left(\frac{D}{2} + 1\right) \right]^{2/D}. \quad (2)$$

Remark that for $D = 3$ this constant has the value $K_3 = (3/10)(6\pi^2)^{2/3} \simeq 4.5578$. Actually this constant has been numerically argued to be still improved [25] to 4.789. See [27, 28] for the best available constants to date, and [29] for further references.

On the other hand, the entropic moments (1) have been variationally shown [30] to be bounded from below in terms of the two radial expectation values of the form

$$\langle r^k \rangle := \int r^k \rho(\vec{r}) d^D r.$$

It has been variationally found [30] that the frequency moment ω_t , $t > 1$, has the following lower bound

$$\omega_t(\rho) \geq F(\alpha, \beta, t, D) \left[\frac{\langle r^\beta \rangle^{t(\alpha+D)-D}}{\langle r^\alpha \rangle^{t(\beta+D)-D}} \right]^{1/(\alpha-\beta)}, \quad (3)$$

for $\alpha > \beta > -D(t-1)/t$. The constant is given by

$$F(\alpha, \beta, t, D) = \frac{t^t (\alpha - \beta)^{2t-1}}{\left\{ \Omega_D B \left[t(\beta + D) - D/(\alpha - \beta)(t - 1), 2t - 1/t - 1 \right] \right\}^{t-1}} \\ \times \left\{ \frac{[t(\beta + D) - D]^{t(\beta+D)-D}}{[t(\alpha + D) - D]^{t(\alpha+D)-D}} \right\}^{1/(\alpha-\beta)}, \quad (4)$$

where $\Omega_D = 2\pi^{D/2}/\Gamma(D/2)$, and $B(x, y) = \Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the beta function expressed by means of the well-known gamma function $\Gamma(z)$.

Then, from the relations (1)–(4) one can easily obtain the following family of lower bounds to the exact kinetic energy T :

$$T \geq C_D(\alpha, \beta) \left[\frac{\langle r^\beta \rangle^{\alpha(1+2/D)+2}}{\langle r^\alpha \rangle^{\beta(1+2/D)+2}} \right]^{1/(\alpha-\beta)} \quad (5)$$

with $C_D(\alpha, \beta) = K_D F(\alpha, \beta, t = 1 + (2/D), D)$ for $\alpha > \beta > -2D/(D-2)$. Some particular relevant cases are as follows.

1. Bound in terms of $\langle r^2 \rangle$. For $\alpha = 2$ and $\beta = 0$, this relation gives

$$T \geq C_D(2, 0) \frac{1}{\langle r^2 \rangle}, \quad D \geq 1$$

with

$$C_D(2, 0) = \frac{1}{2} \frac{D^2 (D!)^{2/D}}{(D+1)^2}.$$

In particular, for $D = 3$ one has

$$T \geq \frac{9}{16} \frac{3^{2/3}}{2^{1/3}} \frac{1}{\langle r^2 \rangle} \approx 0.92867 \frac{1}{\langle r^2 \rangle}.$$

2. Bound in terms of $\langle r^{-1} \rangle$. For $\alpha = 0$ and $\beta = -1$ one has from (5) that

$$T \geq C_D(0, -1) \langle r^{-1} \rangle^2, \quad D > 2$$

with

$$C_D(0, -1) = \frac{(D!)^{2/D} (D-2)}{2^{1+(2/D)} D}.$$

In particular, for $D = 3$ one has

$$T \geq \frac{1}{2 \times 3^{1/3}} \langle r^{-1} \rangle^2 \approx 0.34668 \langle r^{-1} \rangle^2.$$

The accuracy of these bounds can be increased by improving the value of the constant K_D [27, 28, 31]. In fact, it is known that

$$T \geq \frac{9}{8} \frac{1}{\langle r^2 \rangle}, \quad (6)$$

$$T \geq \frac{1}{2} \langle r^{-1} \rangle^2, \quad (7)$$

and

$$T \geq \frac{\langle r^{-2} \rangle}{8} \left(1 - \frac{\langle r^{-1} \rangle^2}{\langle r^{-2} \rangle} \right)^{-1}, \quad (8)$$

for three-dimensional single-particle systems according to Yue–Janmim [32], Gadre–Pathak [33, 34] and Thirring [35, 36], respectively. Bounds of semiclassical, maximum-entropy-based and/or conjectured types for one- and N -electron systems are also known [32, 34], [36]–[40].

On the other hand, from the Pitt–Beckner inequality [41, 42] one knows that the expectation values ($\langle p^\alpha \rangle$, $\langle r^{-\alpha} \rangle$) are mutually related by

$$\langle p^\alpha \rangle \geq 2^\alpha \left[\frac{\Gamma(D + \alpha/4)}{\Gamma(D - \alpha/4)} \right]^2 \langle r^{-\alpha} \rangle; \quad 0 \leq \alpha < D.$$

The particular case $\alpha = 2$ provides the following lower bound for the kinetic energy.

3. Bound in terms of $\langle r^{-2} \rangle$

$$T \geq \frac{(D-2)^2}{8} \langle r^{-2} \rangle; \quad D > 2,$$

so that for $D = 3$ one has [32, 33]

$$T \geq \frac{1}{8} \langle r^{-2} \rangle.$$

3. Kinetic energy lower bounds for the D -dimensional central force problem

In this section we obtain optimal lower bounds to the kinetic energy of non-relativistic particles confined in a D -dimensional central potential of arbitrary form by means of some radial expectation values $\langle r^k \rangle$, and we illustrate that the resulting bounds with $l = 0$ and $D = 3$ give rise to exact lower bounds for particles subject to general potentials. It happens that the expectation values of lowest orders can be, at times, measured model-independently by low-energy and high-energy experiments.

The non-relativistic motion of a single-particle system in a D -dimensional ($D \geq 2$) central potential $V_D(\vec{r})$ is governed by the Schrödinger equation

$$\left[-\frac{1}{2} \vec{\nabla}_D^2 + V_D(\vec{r}) \right] \Psi_D(\vec{r}) = E_D \Psi_D(\vec{r}), \quad (9)$$

with the Laplacian operator [2, 5, 20, 43] associated with the position vector $\vec{r} = (x_1, \dots, x_D) = (r, \theta_1, \dots, \theta_{D-1}) \equiv (r, \Omega_{D-1})$,

$$\vec{\nabla}_D^2 \equiv \sum_{i=1}^D \frac{\partial^2}{\partial x_i^2} = \frac{\partial^2}{\partial r^2} + \frac{D-1}{r} \frac{\partial}{\partial r} - \frac{\Lambda_{D-1}^2}{r^2},$$

and the squared hyperangular momentum operator Λ_{D-1}^2 known to fulfil the eigenvalue equation

$$\Lambda_{D-1}^2 \mathcal{Y}_{l, \{\mu\}}(\Omega_{D-1}) = l(l + D - 2) \mathcal{Y}_{l, \{\mu\}}(\Omega_{D-1}).$$

The \mathcal{Y} -symbol denotes the hyperspherical harmonics characterized by the $D - 1$ hyperangular quantum numbers $(l \equiv \mu_1, \mu_2, \dots, \mu_{D-1} \equiv m) \equiv (l, \{\mu\})$, which are natural numbers with values $l = 0, 1, 2, \dots$, and $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{D-2} \geq |\mu_{D-1}|$.

The eigensolutions $\{\Psi_D(\vec{r}), E_D\}$ are usually determined by doing the ansatz

$$\Psi_D(\vec{r}) = \frac{u_{\text{El}}(r)}{r^{(D-1)/2}} \mathcal{Y}_{l, \{\mu\}}(\Omega_{D-1}).$$

Then, (9) transforms into the one-dimensional equation in the radial coordinate r ,

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} + V_{\text{eff}}(r) \right] u_{\text{El}}(r) = E_D u_{\text{El}}(r), \quad (10)$$

the so-called reduced radial Schrödinger equation in D -dimensions. The effective potential is

$$\begin{aligned} V_{\text{eff}}(r) &= \frac{l(l + D - 2)}{2r^2} + \frac{(D - 1)(D - 3)}{8r^2} + V_D(r) \\ &= \frac{1}{8r^2} [(D + 2l)^2 - 4(D + 2l) + 3] + V_D(r) \\ &= \frac{L(L + 1)}{2r^2} + V_D(r), \end{aligned} \quad (11)$$

where the notation

$$L = l + \frac{D - 3}{2} \quad (12)$$

was used for the grand orbital quantum number. At this point it is worth making some important observations. Firstly, remark that besides the force coming from the external potential $V_D(r)$ there are two additional forces acting in the system: the centrifugal force associated with non-vanishing hyperangular momentum, and a quantum fictitious force associated to the so-called quantum-centrifugal potential $(D - 1)(D - 3)/(8r^2)$ of purely dimensional origin [44]. This potential vanishes for $D = 1$ and 3, it is negative for $D = 2$ and positive for $D \geq 4$. Then, the quantum fictitious force, which exists irrespective of the hyperangular momentum and has a quadratic dependence on the dimensionality, possesses an attractive character for two dimensions and is repulsive for $D \geq 4$ [19], [44]–[47]. Secondly, the above effective potential depends on D and l through the combination $D + 2l$ [5, 48, 49]. This provokes the phenomenon of interdimensional degeneracy, first noted by Van Vleck [50], which implies, for example, that for an arbitrary potential the energies of the seven-dimensional s states are the same as those of the five-dimensional p states or the three-dimensional d states; see also [5, 48] in this respect.

Thirdly, the Schrödinger equations (10) and (11) for D -dimensions are formally the same as for $D = 3$ but with the orbital quantum number given by (12). This implies the existence of an isomorphism [5, 49] between the dimensionality and the hyperangular quantum number, so that $D \rightarrow D + 2$ is equivalent to $l \rightarrow l + 1$. Finally, note that the physical solutions of the Schrödinger equation (9) require that $u_{\text{El}}(r)$ tends to zero when r goes to zero and to infinity. Moreover, the reduced radial eigenfunctions fulfil

$$\int_0^\infty u_{\text{El}}^2(r) dr = 1$$

because of the normalization to unity of the physical wavefunction $\Psi_D(\vec{r})$.

Let us now consider the following radial inequality for the reduced radial eigenfunction $u_{\text{El}} \equiv u_{\text{El}}(r)$:

$$\int_0^\infty (u'_{\text{El}} - ar^\alpha u_{\text{El}} - \lambda r^\beta u_{\text{El}})^2 dr \geq 0,$$

with $u' = \frac{du}{dr}$ and $\alpha, \beta, a, \lambda \in \mathbb{R}$. Working out the integral, we obtain

$$\lambda^2 \langle r^{2\beta} \rangle - 2\lambda \left[\int_0^\infty r^\beta u_{\text{El}}(r) u'_{\text{El}}(r) dr - a \langle r^{\beta+\alpha} \rangle \right] + 2T - L(L+1) \langle r^{-2} \rangle + a^2 \langle r^{2\alpha} \rangle - 2a \int_0^\infty r^\alpha u_{\text{El}}(r) u'_{\text{El}}(r) dr \geq 0,$$

where T denotes the expectation value of the non-relativistic kinetic energy operator \hat{T} , $T \equiv \langle \hat{T} \rangle$, of the system, and we have used that [21]

$$\int_0^\infty [u'_{\text{El}}(r)]^2 dr = 2T - L(L+1) \langle r^{-2} \rangle, \quad (13)$$

and the following notation for the expectation value of $f(r)$

$$\langle f(r) \rangle = \langle \Psi_D(\vec{r}) | f(r) | \Psi_D(\vec{r}) \rangle = \int_0^\infty f(r) u_{\text{El}}^2(r) dr.$$

Taking into account that

$$\int_0^\infty r^b u_{\text{El}}(r) u'_{\text{El}}(r) dr = -\frac{b}{2} \langle r^{b-1} \rangle, \quad (14)$$

where the known boundary conditions $u_{\text{El}}(r) \sim r^{L+1}$ when $r \sim 0$ are taken into account, so that the real parameter b fulfils $b + 2L + 2 > 0$, one has that

$$2T \geq L(L+1) \langle r^{-2} \rangle - a^2 \langle r^{2\alpha} \rangle - a\alpha \langle r^{\alpha-1} \rangle - \langle r^{2\beta} \rangle \lambda^2 - (\beta \langle r^{\beta-1} \rangle + 2a \langle r^{\beta+\alpha} \rangle) \lambda.$$

The optimization of this lower bound with respect to λ produces

$$2T \geq L(L+1) \langle r^{-2} \rangle - a^2 \langle r^{2\alpha} \rangle - a\alpha \langle r^{\alpha-1} \rangle + \frac{1}{\langle r^{2\beta} \rangle} \left[\frac{\beta}{2} \langle r^{\beta-1} \rangle + a \langle r^{\beta+\alpha} \rangle \right]^2, \quad (15)$$

which occurs for the following λ -value:

$$\lambda_0 = -\frac{1}{2\langle r^{2\beta} \rangle} [\beta\langle r^{\beta-1} \rangle + 2a\langle r^{\beta+\alpha} \rangle].$$

The inequality (15) is valid for $a \in \mathbb{R}$, $\alpha > -L - \frac{3}{2}$ and $\beta > -L - \frac{3}{2}$.

Let us now optimize the lower bound given by the relation (15) with respect to the parameter a . This is attained for the value

$$a = \frac{\beta\langle r^{\beta-1} \rangle\langle r^{\beta+\alpha} \rangle - \alpha\langle r^{2\beta} \rangle\langle r^{\alpha-1} \rangle}{2(\langle r^{2\beta} \rangle\langle r^{2\alpha} \rangle - \langle r^{\beta+\alpha} \rangle^2)},$$

giving rise to the following optimal lower bound to the kinetic energy T in terms of the radial expectation values $\langle r^{-2} \rangle$, $\langle r^{\alpha-1} \rangle$, $\langle r^{2\alpha} \rangle$, $\langle r^{\beta-1} \rangle$, $\langle r^{2\beta} \rangle$ and $\langle r^{\alpha+\beta} \rangle$:

$$2T \geq L(L+1)\langle r^{-2} \rangle + \frac{\alpha^2\langle r^{2\beta} \rangle\langle r^{\alpha-1} \rangle^2 + \beta\langle r^{\beta-1} \rangle[\beta\langle r^{\beta-1} \rangle\langle r^{2\alpha} \rangle - 2\alpha\langle r^{\alpha-1} \rangle\langle r^{\alpha+\beta} \rangle]}{4[\langle r^{2\beta} \rangle\langle r^{2\alpha} \rangle - \langle r^{\alpha+\beta} \rangle^2]}, \quad (16)$$

which are valid for α and β bigger than $-L - \frac{3}{2}$. In the following we describe a few relevant particular cases optimal in λ and a (see section 3.2) or only in λ (see section 3.1).

3.1. Lower bounds optimal in λ but not in a

They are obtained from relation (15). We shall give here only the bounds for three particular values of the parameter a because of its intrinsic interest.

1. The inequality (15) gets simplified when $a^2\langle r^{2\alpha} \rangle + \alpha\langle r^{\alpha-1} \rangle$ vanishes, as occurs for $a = 0$ and $a = -\alpha\langle r^{\alpha-1} \rangle/\langle r^{2\alpha} \rangle$. In both cases one has the lower bounds

$$2T \geq L(L+1)\langle r^{-2} \rangle + \frac{1}{\langle r^{2\beta} \rangle} \left[\frac{\beta}{2}\langle r^{\beta-1} \rangle + a\langle r^{\beta+\alpha} \rangle \right]^2.$$

Some cases are intrinsically interesting for different reasons. Indeed, for $a = 0$ one has that

$$2T \geq L(L+1)\langle r^{-2} \rangle + \frac{\beta^2 \langle r^{\beta-1} \rangle^2}{4 \langle r^{2\beta} \rangle}.$$

This expression extends and improves to central potentials the three-dimensional and D -dimensional bounds of similar type obtained from different means by various authors [26, 32, 33, 40], [51]–[54]. In particular, this relation for $\beta = -1$ gives rise to the best inequality between the expectation values $\langle p^2 \rangle$ and $\langle r^{-2} \rangle$ recently discovered [55]:

$$2T \geq \left(L + \frac{1}{2} \right)^2 \langle r^{-2} \rangle = \left(l + \frac{D-2}{2} \right)^2 \langle r^{-2} \rangle. \quad (17)$$

On the other hand, for $a = -\alpha\langle r^{\alpha-1} \rangle/\langle r^{2\alpha} \rangle$ one obtains

$$2T \geq L(L+1)\langle r^{-2} \rangle + \frac{[\beta\langle r^{\beta-1} \rangle\langle r^{2\alpha} \rangle - 2\alpha\langle r^{\alpha-1} \rangle\langle r^{\beta+\alpha} \rangle]^2}{4\langle r^{2\beta} \rangle\langle r^{2\alpha} \rangle^2}.$$

This expression provides the lower bound

$$2T \geq L(L+1)\langle r^{-2} \rangle + \frac{(\beta+2)^2 \langle r^{\beta-1} \rangle^2}{4 \langle r^{2\beta} \rangle}, \quad D > 2 \quad (18)$$

when $\alpha = -1$, and

$$2T \geq \left(L + \frac{1}{2}\right) \langle r^{-2} \rangle + \frac{1}{\langle r^{-2} \rangle \langle r^2 \rangle^2} + \frac{1}{\langle r^2 \rangle}, \quad D > 2$$

for $\alpha = 1$ and $\beta = -1$, which improves the inequality (17) but is less accurate than the optimal relation (18). Besides, for $\alpha = -1$ and $\beta = 1$ one has

$$2T \geq \frac{9}{4} \frac{1}{\langle r^2 \rangle} + L(L+1)\langle r^{-2} \rangle, \quad (19)$$

which, in particular, considerably improves the three-dimensional Heisenberg-like relation $\langle p^2 \rangle \langle r^2 \rangle \geq D^{2/4}$.

2. Moreover the inequality (15) for $a = L + 1$ leads to the expression

$$2T \geq L(L+1)\langle r^{-2} \rangle - \alpha(L+1)\langle r^{\alpha-1} \rangle - (L+1)^2 \langle r^{2\alpha} \rangle + \frac{1}{\langle r^{2\beta} \rangle} \left[\frac{\beta}{2} \langle r^{\beta-1} \rangle + (L+1)\langle r^{\beta+\alpha} \rangle \right]^2,$$

which for $\alpha = -1$ allows us to obtain the following interesting lower bound in terms of the radial expectation values $\langle r^{\beta-1} \rangle$ and $\langle r^{2\beta} \rangle$:

$$2T \geq \frac{1}{4} (2L + \beta + 2)^2 \frac{\langle r^{\beta-1} \rangle^2}{\langle r^{2\beta} \rangle},$$

for $D > 1 - \beta$, which extends and improves a number of general variational bounds mentioned in section 2. Indeed, for $\beta = -1$ one obtains the lower bound (17) already discussed; and for $\beta = 0, 1$ and 2 one has the lower bounds

$$2T \geq (L+1)^2 \langle r^{-1} \rangle^2 = \left(l + \frac{D-1}{2} \right)^2 \langle r^{-1} \rangle^2, \quad (20)$$

$$2T \geq \left(L + \frac{3}{2} \right)^2 \frac{1}{\langle r^2 \rangle} = \left(l + \frac{D}{2} \right)^2 \frac{1}{\langle r^2 \rangle}, \quad (21)$$

and

$$2T \geq (L+2)^2 \frac{\langle r \rangle^2}{\langle r^{-4} \rangle} = \left(l + \frac{D+1}{2} \right) \frac{\langle r \rangle^2}{\langle r^{-4} \rangle},$$

respectively, which generalize and improve to D -dimensional central potentials similar bounds with different origins obtained by various authors [32, 33, 38, 40, 42, 53] for general three-dimensional single-particle systems. Let us highlight that particular cases of these expressions are the D -dimensional Heisenberg-like relation $\langle p^2 \rangle \langle r^2 \rangle \geq D^2/4$ and the Bialynicki-Birula *et al* relation [19] $\langle p^2 \rangle \geq (D-1)^2 \langle r^{-1} \rangle^2/4$, which correspond to the exact inequalities (6) and (7), respectively, for $D = 3$.

Finally, let us also point out that the reciprocity of the position and momentum spaces allows us to write the conjugate expressions for all the inequalities mentioned above. In particular we have

$$\langle r^2 \rangle \geq \frac{1}{4} (2L + \beta + 2)^2 \frac{\langle p^{\beta-1} \rangle^2}{\langle p^{2\beta} \rangle}$$

for $D > 1 - \beta$, which gives

$$\begin{aligned}\langle r^2 \rangle &\geq (L + 1)^2 \langle p^{-1} \rangle^2, \\ \langle r^2 \rangle &\geq \left(L + \frac{1}{2}\right)^2 \langle p^{-2} \rangle,\end{aligned}$$

for $\beta = 0$ and -1 and $D > 2$, respectively. Again, these expressions extend and improve to D -dimensional central potentials the corresponding three-dimensional relations already known for general systems [32]–[34], [40].

3.2. Lower bounds optimal in λ and a

They are obtained from relation (16).

1. Bound in terms of $\langle r^{-2} \rangle$ and $\langle r^{-1} \rangle$. For $\alpha = -1$ and $\beta = 0$,

$$2T \geq \left(L + \frac{1}{2}\right)^2 \langle r^{-2} \rangle + \frac{1}{4} \frac{\langle r^{-2} \rangle \langle r^{-1} \rangle^2}{\langle r^{-2} \rangle - \langle r^{-1} \rangle^2}, \quad D > 2. \quad (22)$$

2. Bound in terms of $\langle r^{-2} \rangle$ and $\langle r^2 \rangle$. For $\alpha = 1$ and $\beta = -1$,

$$2T \geq \left(L + \frac{1}{2}\right)^2 \langle r^{-2} \rangle + \frac{\langle r^{-2} \rangle}{\langle r^2 \rangle \langle r^{-2} \rangle - 1}, \quad D > 2. \quad (23)$$

3. Bound in terms of $\langle r^{-2} \rangle$, $\langle r \rangle$ and $\langle r^2 \rangle$. For $\alpha = 0$ and $\beta = 1$,

$$2T \geq L(L + 1) \langle r^{-2} \rangle + \frac{1}{4} \frac{1}{\langle r^2 \rangle - \langle r \rangle^2}, \quad D > 3. \quad (24)$$

4. Bound in terms of $\langle r^{-2} \rangle$, $\langle r \rangle$ and $\langle r^4 \rangle$. For $\alpha = 2$ and $\beta = -1$,

$$2T \geq \left(L + \frac{1}{2}\right)^2 \langle r^{-2} \rangle + \frac{9}{4} \frac{\langle r^{-2} \rangle \langle r \rangle^2}{\langle r^{-2} \rangle \langle r^4 \rangle - \langle r \rangle^2}, \quad D > 3. \quad (25)$$

5. Bound in terms of $\langle r^{-2} \rangle$, $\langle r \rangle$, $\langle r^2 \rangle$ and $\langle r^4 \rangle$. For $\alpha = 2$ and $\beta = 0$,

$$2T \geq L(L + 1) \langle r^{-2} \rangle + \frac{\langle r \rangle^2}{\langle r^4 \rangle - \langle r^2 \rangle^2}, \quad D > 3. \quad (26)$$

The bounds (22)–(26) generalize and improve the D -dimensional lower bounds (17) and (19). Moreover, the inequality (22) takes the form

$$T \geq \frac{l(l + 1)}{2} \langle r^{-2} \rangle + \frac{\langle r^{-2} \rangle}{8} \left(1 - \frac{\langle r^{-1} \rangle^2}{\langle r^{-2} \rangle}\right)^{-1}$$

for three-dimensional systems, which reduces to the exact Thirring bound (8) for the ground state ($l = 0$). The inequalities (23)–(26) allow us to find the following lower bounds in a similar manner:

$$T \geq \frac{\langle r^{-2} \rangle}{8} \left(1 + \frac{4}{\langle r^2 \rangle \langle r^{-2} \rangle - 1}\right),$$

$$T \geq \frac{1}{8} \frac{1}{\langle r^2 \rangle - \langle r \rangle^2},$$

$$T \geq \frac{\langle r^{-2} \rangle}{8} \left(1 + \frac{9}{(\langle r^{-2} \rangle \langle r^4 \rangle / \langle r \rangle^2) - 1} \right),$$

and

$$T \geq \frac{1}{2} \frac{\langle r \rangle^2}{\langle r^4 \rangle - \langle r^2 \rangle^2},$$

respectively, for general particles with $l = 0$ moving in the three-dimensional space.

4. Bounds in terms of log-moments

Here we obtain lower bounds to the kinetic energy of single-particle systems moving in a D -dimensional central potential by taking into account not only the radial expectation values $\langle r^\alpha \rangle$ but also the logarithmic expectation values $\langle r^\alpha \ln r \rangle$. This has been motivated by the physical interest of the log-moments in atomic and molecular physics [39], [56]–[58]. These quantities have been analytically determined for one- and D -dimensional hydrogenic systems [57, 59] and numerically for various α -values in all neutral atoms of the periodic table [37, 60] in both position and momentum spaces. The mean logarithmic radius $\langle \ln r \rangle$ is of particular interest because (i) it is experimentally accessible by electron scattering [61] and (ii) it provides tight bounds to the atomic information entropy [58]. Moreover, the log-moments are closely connected with the electron–electron coalescence phenomenon in atoms and molecules [56], and satisfy a number of interesting inequalities and uncertainty relations [60].

We use a methodology similar to that developed in the previous section. We begin with the following inequality fulfilled by the reduced radial wavefunction $u_{\text{El}}(r)$ of the system,

$$\int_0^\infty [u'_{\text{El}} - ar^\alpha \ln ru - \lambda r^\beta u]^2 dr \geq 0,$$

where a , λ , α and β are real parameters.

Working out this integral and taking into account (13) and (14) together with the relation

$$\int_0^\infty r^\alpha \ln r u u' dr = -\frac{\alpha}{2} \langle r^{\alpha-1} \ln r \rangle - \frac{1}{2} \langle r^{\alpha-1} \rangle,$$

one has that

$$2T \geq L(L+1) \langle r^{-2} \rangle - a^2 \langle r^{2\alpha} \ln^2 r \rangle - a\alpha \langle r^{\alpha-1} \ln r \rangle - a \langle r^{\alpha-1} \rangle - \lambda^2 \langle r^{2\beta} \rangle - \beta\lambda \langle r^{\beta-1} \rangle - 2a\lambda \langle r^{\alpha+\beta} \ln r \rangle. \quad (27)$$

From this expression we can obtain a large number of lower bounds, according to the expectation values we want to enter into play. Let us only enumerate a few particular cases.

1. For $\beta = 0$ and optimizing (27) with respect to λ and a , one has

$$2T \geq L(L+1)\langle r^{-2} \rangle + \frac{[\langle r^{\alpha-1} \rangle + \alpha \langle r^{\alpha-1} \ln r \rangle]^2}{4\Delta(r^\alpha \ln r)},$$

where

$$\Delta(r^\alpha \ln r) = \langle r^{2\alpha} \ln^2 r \rangle - \langle r^\alpha \ln r \rangle^2$$

denotes the uncertainty of $r^\alpha \ln r$. In addition, this expression gives

$$2T \geq L(L+1)\langle r^{-2} \rangle + \frac{(1 + \langle \ln r \rangle)^2}{4\Delta(r \ln r)}$$

for $\alpha = 1$, and

$$2T \geq L(L+1)\langle r^{-2} \rangle + \frac{\langle r^{-1} \rangle^2}{4\Delta(\ln r)}$$

for $\alpha = 0$.

2. For $\beta = -1$ and optimizing with respect to λ and a one has the lower bound

$$2T \geq \frac{\langle r^{-2} \rangle}{4} \left[(2L+1)^2 + \frac{(1 + 2\langle \ln r \rangle)^2}{\langle r^{-2} \rangle \langle r^2 \ln^2 r \rangle - \langle \ln r \rangle^2} \right]$$

for $\alpha = 1$, and

$$2T \geq \frac{\langle r^{-2} \rangle}{4} \left[(2L+1)^2 + \frac{\langle r^{-2} \rangle^2}{\langle r^{-2} \rangle \langle r^{-2} \ln^2 r \rangle - \langle r^{-2} \ln r \rangle^2} \right]$$

for $\alpha = -1$.

3. For $\lambda = L+1$, $\beta = -1$ and optimizing with respect to the parameter a , one obtains that

$$2T \geq \frac{1}{4\langle r^{2\alpha} \ln^2 r \rangle} [\langle r^{\alpha-1} \rangle + (2L+2+\alpha)\langle r^{\alpha-1} \ln r \rangle]^2$$

for $\alpha \in \mathbb{R}$. Then we have the following bounds:

$$2T \geq \frac{1}{4\langle r^2 \ln^2 r \rangle} [1 + (2L+3)\langle \ln r \rangle]^2$$

for $\alpha = 1$, and

$$2T \geq \frac{1}{4\langle \ln^2 r \rangle} [\langle r^{-1} \rangle + (2L+2)\langle r^{-1} \ln r \rangle]^2$$

for $\alpha = 0$.

4. For $\lambda = 0$ and optimizing with respect to a , one has

$$2T \geq L(L+1)\langle r^{-2} \rangle + \frac{[\langle r^{\alpha-1} \rangle + \alpha \langle r^{\alpha-1} \ln r \rangle]^2}{4\langle r^{2\alpha} \ln^2 r \rangle}$$

for $\alpha \in \mathbb{R}$. This expression allows us to find

$$2T \geq L(L+1)\langle r^{-2} \rangle + \frac{(1 + \langle \ln r \rangle)^2}{4\langle r^2 \ln^2 r \rangle}$$

for $\alpha = 1$, and

$$2T \geq L(L+1)\langle r^{-2} \rangle + \frac{\langle r^{-1} \rangle^2}{4\langle \ln^2 r \rangle}$$

for $\alpha = 0$.

5. Numerical analysis for oscillator- and hydrogen-like systems

In this section we have performed a comparison between the six lower bounds to the kinetic energy (17), (20)–(23) and (8), in the two most important prototypes of D -dimensional systems: the isotropic harmonic oscillator and the hydrogen atom. To facilitate our discussion, let us introduce the ratios between each of these lower bounds, respectively, and the kinetic energy:

$$\begin{aligned}\Xi_1 &= \frac{1}{2T} \left(L + \frac{1}{2}\right)^2 \langle r^{-2} \rangle \leq 1, \\ \Xi_2 &= \frac{1}{2T} (L + 1)^2 \langle r^{-1} \rangle^2 \leq 1, \\ \Xi_3 &= \frac{1}{2T} \left(L + \frac{3}{2}\right)^2 \langle r^2 \rangle^{-1} \leq 1, \\ \Xi_4 &= \frac{1}{2T} \left[\left(L + \frac{1}{2}\right)^2 \langle r^{-2} \rangle + \frac{1}{4} \frac{\langle r^{-2} \rangle \langle r^{-1} \rangle^2}{\langle r^{-2} \rangle - \langle r^{-1} \rangle^2} \right] \leq 1, \\ \Xi_5 &= \frac{1}{2T} \left[\left(L + \frac{1}{2}\right)^2 \langle r^{-2} \rangle + \frac{\langle r^{-2} \rangle}{\langle r^2 \rangle \langle r^{-2} \rangle - 1} \right] \leq 1, \\ \Xi_6 &= \frac{1}{2T} \frac{\langle r^{-2} \rangle}{4} \left(1 - \frac{\langle r^{-1} \rangle^2}{\langle r^{-2} \rangle}\right)^{-1} \leq 1,\end{aligned}$$

where the last ratio Ξ_6 is only defined for dimensionality $D = 3$. We have numerically studied the dependence of these ratios on the dimensionality and on the principal quantum number of the oscillator and hydrogen-like states.

5.1. Isotropic harmonic oscillator

The potential considered is $V(r) = \frac{1}{2}r^2$. The behaviour of the ratios Ξ_i ($i = 1, \dots, 5$) as a function of the dimension D for the state with quantum numbers $(n, l, m) = (3, 1, 1)$ is shown in figure 1. For the five cases, the ratio monotonically increases, i.e. the bounds improve, as D is augmented. For any given dimensionality, ratios Ξ_4 and Ξ_5 give the highest values, being Ξ_4 a bit higher than Ξ_5 , but both ratios tending to the same value. The third highest ratio is Ξ_1 with a value very close to these of Ξ_4 and Ξ_5 . In the limit $D \rightarrow \infty$, all the ratios approach the unity, i.e. $\Xi_i \rightarrow 1$, independently of the values of the quantum numbers n, l and m .

The ratios Ξ_i ($i = 1, \dots, 6$) are plotted in figure 2 as a function of the principal quantum number n for $D = 3$ and angular quantum numbers $l = m = 1$. For the six cases, Ξ_i has a qualitatively similar but quantitatively different behaviour as a function of n , monotonically decreasing as n is enhanced. The inequalities worsen as the degree of excitation of the level is augmented, and in the $n \rightarrow \infty$ limit, $\Xi_i \rightarrow 0$ for $i = 1, \dots, 6$. For $n = 0$, the inequality is saturated with $\Xi_3 = 1$ and $\Xi_5 = 1$ for these two ratios, and the other two ratios get almost saturated with $\Xi_2 \simeq 0.91$ and $\Xi_4 \simeq 0.97$. However, for the range of values of n considered, the values of Ξ_1 , Ξ_4 and Ξ_5 are reduced by almost two orders of magnitude with $\Xi_i \simeq 1-0.018$ ($i = 1, 4, 5$) for the levels with $n = 0$ and 40 respectively; and the values of these three ratios are higher for larger values of n , with each one asymptotically approaching each other.

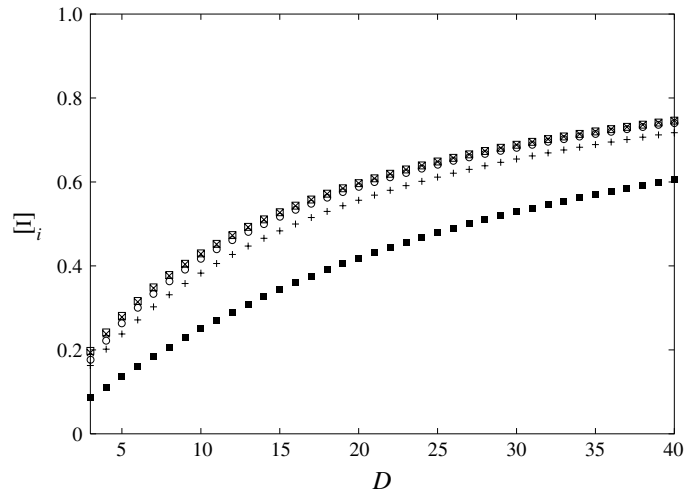


Figure 1. Ratios Ξ_i , $i = 1$ (\circ), 2 ($+$), 3 (\blacksquare), 4 (\square) and 5 (\times), of the lower bounds and the kinetic energy for the harmonic oscillator for the state with quantum numbers $(n, l, m) = (3, 1, 1)$ in terms of the dimension D .

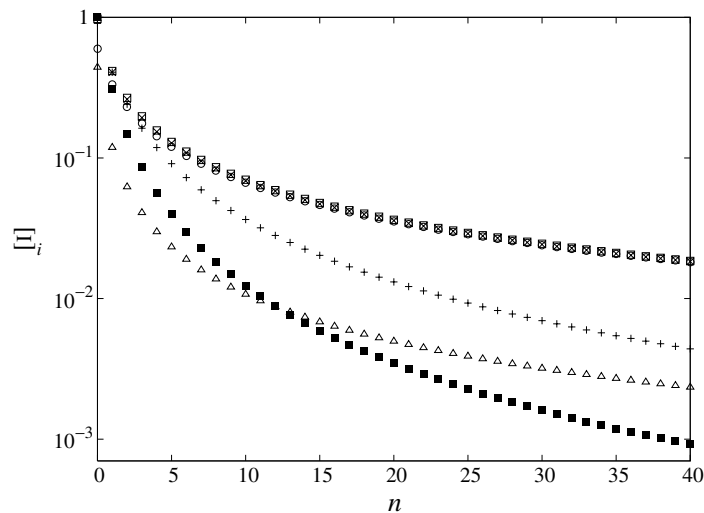


Figure 2. Ratios Ξ_i , $i = 1$ (\circ), 2 ($+$), 3 (\blacksquare), 4 (\square), 5 (\times) and 6 (\triangle), of the lower bounds and the kinetic energy for the harmonic oscillator states with $l = m = 1$ and dimension $D = 3$ in terms of the principal quantum number n .

5.2. Hydrogen atom

Here the potential is $V(r) = -1/r$. Figure 3 shows the behaviour of ratios Ξ_i ($i = 1, \dots, 5$) as a function of the dimension D for the level with quantum numbers $(n, l, m) = (3, 1, 1)$ of the hydrogen atom. These results resemble those given for the harmonic oscillator case in figure 1. All the lower bounds increase as the dimensionality is enhanced. Again the ratios Ξ_4 and Ξ_5 tend to have the same value and are the nearest to the unity, but now Ξ_5 is a bit higher than Ξ_4 .

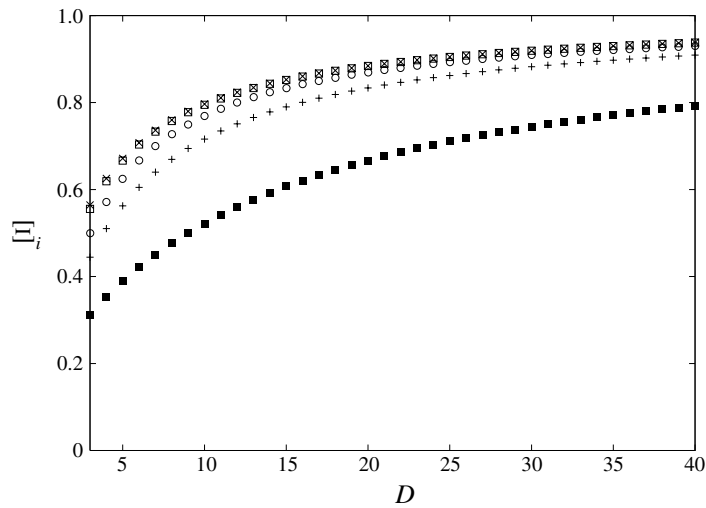


Figure 3. Ratios Ξ_i , $i = 1$ (\circ), 2 ($+$), 3 (\blacksquare), 4 (\square) and 5 (\times), of the lower bounds and the kinetic energy for the hydrogen atom in the state $(n, l, m) = (3, 1, 1)$ in terms of the dimension D .

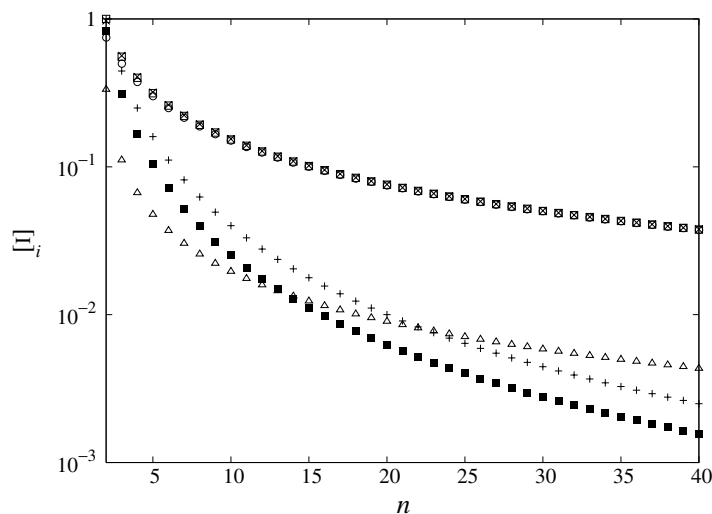


Figure 4. Ratios Ξ_i , $i = 1$ (\circ), 2 ($+$), 3 (\blacksquare), 4 (\square), 5 (\times) and 6 (\triangle), of the lower bounds and the kinetic energy for the hydrogen atom in the state with $l = m = 1$ and dimension $D = 3$ in terms of the principal quantum number n .

With Ξ_1 again with the closest value to these ones. In the five cases, the ratios quickly reaches the asymptotic behaviour for large D values, with $\Xi_i \rightarrow 1$ for $D \rightarrow \infty$, independently of the quantum numbers n , l and m .

As a last example we plot for the hydrogenic levels with angular symmetry $l = m = 1$ the ratios Ξ_i , with $i = 1, \dots, 6$, as a function of the principal quantum number n for a three-dimensional system in figure 4. As for the oscillator case the six bounds worsen as the degree of excitation is enhanced, and they approach zero in the $n \rightarrow \infty$ limit. For $n = 2$, the ratios $\Xi_2 = 1$ and $\Xi_4 = 1$, indicating that the corresponding inequalities (20) and (22) reach saturation.

Actually, this situation occurs for any state with $l = n - 1$. However, again for the range of values of n considered, the values of Ξ_1 , Ξ_4 and Ξ_5 are reduced by almost two orders of magnitude, and have a similar asymptotical behaviour for larger values of n .

6. Conclusions

We have investigated the kinetic energy for single-particle systems subject to a central potential confinement in arbitrary dimensions. Beyond its intrinsic physico-mathematical interest, this theoretical work has been partially motivated by the recent experimental achievements of the evaporative cooling of dilute (i.e. almost non-interacting) fermions [12, 13] in magnetic traps. These experiments have opened the door to exploit the D -dimensional confinement of fermionic gases in atomic traps of spherically symmetric type. This is a most relevant reason for the current development of a density functional theory for independent particles subject to central-potential (e.g. harmonic) confinement in non-standard dimensions [54, 62].

We have obtained sharp lower bounds to the kinetic energy which depend on the orbital hyperangular quantum number, the dimensionality and one or more radial and logarithmic position expectation values. The associated conjugate relations are also fulfilled, so that the magnetic susceptibility of the system (which, a factor apart, is equal to $\langle r^2 \rangle$) is explicitly bounded by means of one or more radial and logarithmic momentum expectation values. They are optimal in the sense mentioned in section 3, so that they extend and improve to central potentials all the corresponding ones for general systems, if they exist, published in the literature. Furthermore, it is also claimed that these bounds with $l = 0$ and $D = 3$ give rise to exact lower bounds for the kinetic energy of particles that are arbitrarily confined, i.e. subject to forces with a non-necessarily central character.

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