Physics Letters A 483 (2023) 129062

Contents lists available at ScienceDirect

Physics Letters A

journal homepage: www.elsevier.com/locate/pla

Quantum recurrence times in nanostructures

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ARTICLE INFO

Article history:
Received 15 June 2023
Received in revised form 27 July 2023
Accepted 3 August 2023
Available online 8 August 2023
Communicated by J.G. Lu

Keywords:
Quantum revivals
Nonparabolic corrections

ABSTRACT

We compute the classical and revival times of electron currents in several bulk nanostructured, semiconductor materials. We have used a nonparabolic Schrödinger equation to model the conduction band of semiconductors. We have calculated the classical and revival periods for quantum dots of Si, Ge and InAs quantum dots. The obtained results are of the order of tenths of nanoseconds to picoseconds, which are within reach of current technologies.

The possibility of creating and manipulating nanobjects has increased dramatically over the last decades. At the same time, quantum physical effects are progressively incorporated into current technologies which, in turn, open up unprecedented possibilities to realize, observe, and control quantum effects. To name but a few examples, current quantum technologies cover quantum communication and cryptography, atomic sensors, matter wave optics, or quantum computers. Many of the aforementioned technologies largely rely on the possibility of creating wave packets and of controlling their subsequent time development. The time evolution of wave packets can be monitored on the attosecond time scale, and even their dynamics can be controlled by changing the phases between their components [1]. Moreover, the technical capacity to excite wave packets to high-energy levels, for instance Rydberg states of atoms or molecules, enables researches to approach the classical limit [2].

A most impressive feature of the time evolution of wave packets is the possibility of occurrence of quantum revivals [3]. Under given conditions to be discussed below, wave packets propagate as classical entities over short periods of time T_{Cl} before they decay into the collapsed phase, only to regain their original form after the so-called revival time, T_{R}, after which the cycle commences again. This phenomenon has a purely quantum origin with no classical analogue. Initially limited to numerical investigations, quantum revivals were soon after observed in many experimental situations, including quantum many-body systems [4], systems exhibiting quantum phase transitions [5], quantum chaos [6], and many-body localization [7]. On the applied side, they have become a feasible, useful tool at the basis of various applications as well. There have been reported quantum-recurrence-dependent methods for wave packet, laser isotope separation [8], factorization into prime numbers [9], and wave packet evolution control through relatively weak laser pulses at fractional revivals which modify the phase between their components [1]. Revivals are observable even in the presence of environmental decoherence, using carbon nanotubes or silicon nanorods with a length of 50 nm [10]. They have also been investigated in other materials of technological interest such as grephene [11] and silicene [12], and used to characterize topological-band insulator transitions [13].

In this paper, we compute the revival times of electron currents in quantum dots of several semiconductor materials, namely, Silicon, Germanium and Indium arsenide. We take advantage of a proposed, modified Schrödinger equation to model the conduction band of semiconductors.

The wave function of electrons in a solid is usually described by the single-band, effective mass equation [14]

$$[\varepsilon(-i\nabla) + V(\mathbf{r})]\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{1}$$

where $\varepsilon(-i\nabla)$ is the operator that results from replacing $\mathbf{k}$ by $-i\nabla$ in the dispersion relation $E_n(\mathbf{k})$ of the perfect crystal and $V(\mathbf{r})$ is an external field. Although Eq. (1) is customarily simplified by expanding ε up to second order in $\mathbf{k}$, simple quadratic approximations such as this are not valid for wave vectors far from the band minimum, whereas further expanding $\varepsilon(\mathbf{k})$ to higher orders leads

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https://doi.org/10.1016/j.physleta.2023.129062

to very complicated expressions. To circumvent this problem, the wave vector can be alternatively expressed in terms of the energy,

$$\frac{\hbar^2 k^2}{2m^*} = \varepsilon + \alpha\varepsilon^2 + \beta\varepsilon^3 \cdots . \tag{2}$$

Truncating the series to two terms provides the approximation

$$\varepsilon(\mathbf{k})[1 + \alpha\varepsilon(\mathbf{k})] = \frac{\hbar^2 k^2}{2m^*} \equiv \gamma(\mathbf{k}), \tag{3}$$

where α is known as the non parabolicity coefficient and the coordinate system has been chosen so that the effective mass tensor is diagonal. Pursing this approach, which is widely used in many materials, López-Villanueva et al. [15,16] have obtained analytical expressions for the energy spectrum of the conducting band of different semiconductors with simple geometries. The gist of their approach is to split the kinetic energy operator along the directions of confinement and propagation, $\gamma = \gamma_c + \gamma_p$. Corresponding to this separation, the energy operator is separated as $\epsilon = \epsilon_c + \epsilon_p$ with [16]

$$\epsilon_c = \frac{1 + 2\alpha\epsilon_p}{2\alpha}\left\{\sqrt{1 + \frac{4\alpha\gamma_c}{(1 + 2\alpha\epsilon_p)^2}} - 1\right\}$$

$$\epsilon_p(1 + \alpha\epsilon_p) = \gamma_p(\mathbf{k}_p). \tag{4}$$

The energy spectrum is all what is needed to compute the revival times. Consider the time evolution of a wave packet for a time-independent Hamiltonian

$$|\psi(t)\rangle = \sum_n c_n |u_n\rangle e^{-iE_n t/\hbar}. \tag{5}$$

Assuming that the initial wave packet is a superposition of eigenstates $|u_n\rangle$ sharply peaked around some n_0, several times scales of evolution can be obtained from the Taylor series of the energy spectrum E_n around E_{n_0},

$$E_n \approx E_{n_0} + E'_{n_0}(n - n_0) + \frac{E''_{n_0}}{2}(n - n_0)^2 + \cdots . \tag{6}$$

Consequently,

$$e^{-iE_n t/\hbar} = \exp\left[- iE_{n_0}\frac{t}{\hbar} - 2\pi i(n - n_0)\frac{t}{T_{\mathrm{Cl}}} - 2\pi i(n - n_0)^2\frac{t}{T_{\mathrm{R}}} + \cdots \right], \tag{7}$$

where $T_{\mathrm{Cl}} \equiv 2\pi\hbar/|E'_{n_0}|$ and $T_{\mathrm{R}} \equiv 4\pi\hbar/|E''_{n_0}|$. Some comments are in order. Revivals are generally only approximate; wave packets do not *exactly* revive after a time T_{R}. But the more tightly peaked is the wave packet around a given quantum number, the more faithful the reproduction of the original wave packet is at T_{R}. Notice that these are sufficient conditions for revivals to exist, but not necessary: In an infinite square well, the separation between energy eigenvalues $E_n = E_1 n^2$ increases with n, and the wave packets do regain exactly their original shape after a time $T_{\mathrm{R}} = 2\pi\hbar/E_1$. [The infinite square well is also special in that T_{R} does not depend on the initial value n_0.] Moreover, in the context of quantum phase transitions revivals have been reported for wave packets centered around energy levels as low as the fundamental state [5]. Finally, we would like to mention that in relativistic quantum mechanics a new periodicity arises, namely the Zitterbewegung or trembling motion. Although nowadays this is considered an artifact of the Dirac equation overcome by quantum field theory, it can show up in electrons in semiconductors whose band structure has a form

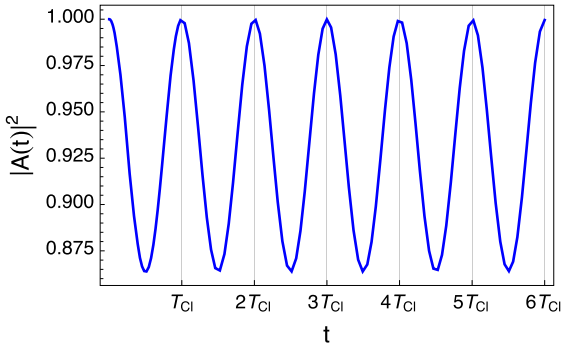

Fig. 1. Time evolution of $|A(t)|^2$ for a particle in a quantum well. The classical time value is $T_{\mathrm{Cl}} = 1.50 \times 10^{-14}$ s.

reminiscent of the Dirac equation [17]. The $\pi\hbar/E_{n_0}$ term then provides the frequency of aforementioned Zitterbewegung oscillations [11].

Next, we apply the nonparabolic approach to various semiconductors and geometries, but first we address the more academic case of a quantum well.

Quantum well. Taking the confinement direction along the z axis and the propagation in the $x - y$ plane, the energy spectrum as derived in [16] is

$$E_n = \frac{1 + 2\alpha E_p}{2\alpha}\left\{\sqrt{1 + \frac{4\alpha}{(1 + 2\alpha E_p)^2}\frac{\hbar^2}{2m_z^*}\left(\frac{\pi n}{L}\right)^2} - 1\right\}, \tag{8}$$

which, upon considering the subband minimum $E_p = 0$, implies

$$T_{\mathrm{Cl}} = \frac{2m_z^* L^2}{\pi\hbar n}\sqrt{1 + 2\alpha\frac{\pi^2\hbar^2}{m_z^* L^2}n^2}, \tag{9}$$

$$T_{\mathrm{R}} = \frac{4m_z^* L^2}{\pi\hbar}\left(1 + 2\alpha\frac{\pi^2\hbar^2}{m_z^* L^2}n^2\right)^{3/2}. \tag{10}$$

Setting $\alpha = 0$ in Eq. (10) recovers the well known parabolic results $T_{\mathrm{Cl}} = 2m_z^* L^2/\pi\hbar n$ and $T_{\mathrm{R}} = 4m_z^* L^2/\pi\hbar$. Note that the nonparabolic correction does depend on the selected central state n, and hence T_{R} is no longer independent from n. Moreover, the nonparabolic correction might not be a small one. In particular, for GaAs $m_z^* = 0.0665$ and $\alpha = 0.697$ [19], which, taking $L = 10$ nm and $n = 10$, leads to $T_{\mathrm{Cl}} = 1.50 \times 10^{-14}$ s and $T_{\mathrm{R}} = 5.03 \times 10^{-12}$ s, to be compared with the parabolic approximation $T_{\mathrm{Cl}} = 3.6 \times 10^{-15}$ s and $T_{\mathrm{R}} = 7.3 \times 10^{-14}$ s. As we will see, this trait carries over to more realistic cases.

For the sake of illustration, Fig. 1 shows the short time development of the squared modulus of the autocorrelation function, $A(t) = \langle\psi(t), \psi(0)\rangle = \sum_n |c_n|^2 e^{iE_n t/\hbar}$.

As can be seen, the wave function initially evolves periodically as denoted by the coming backs of $|A(t)|^2$ to its initial value of unity. This behavior fades away as longer times are considered (not shown) until eventually the almost periodic behavior is resumed at the revival time. This is illustrated in Fig. 2, which shows the time evolution up to $3T_{\mathrm{R}}$. The vertical lines are now located at multiples of $T_{\mathrm{R}} = 5.03 \times 10^{-12}$ s. Finally, note that in this case the first revival occurs at $T_{\mathrm{R}}/2$ [18].

Rectangular quantum wires. Next, we address the case of rectangular cross-section wires. For wires of square-section of size L where the confinement is in the $x - y$ plane and the propagation is along the z-direction, the energy spectrum as derived in [16] is

$$E_{n_x,n_y} = \frac{1 + 2\alpha E_p}{2\alpha} \tag{11}$$

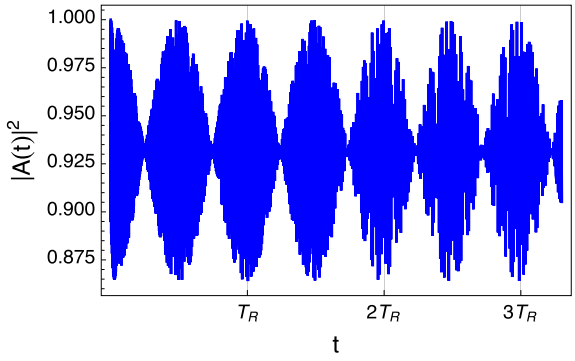

Fig. 2. Time evolution of $|A(t)|^2$ for a particle in a quantum well. The revival time value is $T_R = 5.03 \times 10^{-12}$ s.

$$\times \left\{ \sqrt{1 + \frac{2\alpha\hbar^2}{(1+2\alpha E_p)^2} \left(\frac{\pi}{L}\right)^2 \left(\frac{n_x^2}{m_x^*} + \frac{n_y^2}{m_y^*}\right)} - 1 \right\}.$$

Thus, this case constitutes a simple generalization to a system of two quantum numbers. From the expansion of E_{n_x,n_y}, two different classical periods and three revival times can be defined. Particularizing to n_x and $E_p = 0$ leads to

$$T_{\rm Cl} = \frac{2\pi\hbar}{|E'_{n_x}|} = \frac{2m_x^* L^2}{\pi\hbar n_x} \sqrt{1 + \frac{2\alpha\pi^2\hbar^2}{L^2} \left(\frac{n_x^2}{m_x^*} + \frac{n_y^2}{m_y^*}\right)}, \tag{12}$$

$$T_{\rm R} = \frac{4\pi\hbar}{|E''_{n_x}|} = \frac{4m_x^* L^2}{\pi\hbar} \frac{\left[1 + \frac{2\alpha\pi^2\hbar^2}{L^2}\left(\frac{n_x^2}{m_x^*} + \frac{n_y^2}{m_y^*}\right)\right]^{3/2}}{1 + \frac{2\alpha\pi^2\hbar^2}{L^2}\frac{n_y^2}{m_y^*}},$$

and the mixed term

$$T_{\rm R} = \frac{4\pi\hbar}{|E''_{n_x,n_y}|} = \frac{2m_x^* m_y^* L^4}{\alpha\pi^3\hbar^3 n_x n_y} \left[1 + \frac{2\alpha\pi^2\hbar^2}{L^2}\left(\frac{n_x^2}{m_x^*} + \frac{n_y^2}{m_y^*}\right)\right]^{3/2}. \tag{13}$$

These expressions provide results of the same order of magnitude as the quantum well ones.

Quantum dots. For a spherical quantum dot of radius R, after substituting $\mathbf{k}$ by $-i\nabla$ in Eq. (3), López-Villanueva et al. found solutions of the resulting equation that are the product of radial functions and spherical harmonics (see [16] for details), the ensuing energy spectrum being

$$E_n = \frac{\sqrt{1 + 2\alpha\dfrac{\hbar^2}{m^* R^2} z_{nl}^2} - 1}{2\alpha}, \tag{14}$$

where z_{nl} is the $n^{\rm th}$ zero of the spherical Bessel function $J_{l+1/2}$. Next, we compute the classical and revival times for quantum dots of Si, Ge and InAs. Making use of $z_{nl} \approx [n + (l+1/2)/2 - 1/4]\pi + \mathcal{O}(1/n)$ for $n \gg l$ [20], it is straightforward to obtain

$$T_{\rm Cl} = \frac{2m^* R^2}{\hbar z_{nl}} \sqrt{1 + 2\alpha\frac{\hbar^2}{m^* R^2} z_{nl}^2}, \tag{15}$$

$$T_{\rm R} = \frac{4m^* R^2}{\pi\hbar} \left(1 + 2\alpha\frac{\hbar^2}{m^* R^2} z_{nl}^2\right)^{3/2}. \tag{16}$$

Without loss of generality, we restrict ourselves to zero angular momentum states, $l = 0$, and illustrate in Fig. 3 our results

Material	m^*	α (eV^{-1})	$T_{\rm R}$ (s)	$T_{\rm Cl}$ (s)
Si	0.306	0.520	2.3×10^{-12}	3.2×10^{-14}
Ge	0.136	1.617	1.2×10^{-11}	3.3×10^{-14}
InAs	0.027	4.238	1.1×10^{-10}	2.3×10^{-14}

Fig. 3. Classical and revival times for electron wave packets in a quantum dot of radius $R = 10$ nm made of different materials. $n_0 = 10$ and the effective masses and the non-parabolicity coefficient are taken from [16].

for quantum dots of radius $R = 10$ nm and electron wave packets centered around $n_0 = 10$. The effective masses and the non-parabolicity coefficients are taken from Ref. [16], which contains details on how these parameters were calculated and their values for other materials. The obtained results, of the order of tenths of nanoseconds to picoseconds, are within reach of current technologies.

Notice that the introduction of nonparabolic corrections greatly modifies the energy spectrum and, consequently, the revival times. Setting $\alpha = 0$ in Eq. (16) recovers the parabolic approximation that results in $T_{\rm R}({\rm Si}) = 3.4 \times 10^{-13}$ s, $T_{\rm R}({\rm Ge}) = 1.5 \times 10^{-13}$ s, and $T_{\rm R}({\rm InAs}) = 3 \times 10^{-15}$ s, which are between one and five orders of magnitude smaller than in the nonparabolic case. It ensues from Eq. (10) that the greater the confinement, the stronger the nonparabolic effects. To make this statement more quantitative, we plot in Fig. 4 a comparison between the classical and revival times as computed without (black lines) and with the nonparabolic correction (red lines). The increase of the recurrence times, both classical and quantum, with confinement (smaller radius) is evident and can reach up to 5 or more orders of magnitude for the smallest structures. Interestingly enough, the corrected $T_{\rm R}$ are no longer a monotonic function of the radius. The double-logarithmic scale is just for a better visualization of the data.

In summary, we have calculated the quantum revival times for different nanostructures, namely, quantum wells, rectangular quantum wires, and quantum dots. We have obtained analytically and numerically the revival times for quantum dots of Silicon, Germanium, and Indium Arsenide, showing that the wave-packet, revival times can be largely affected by nonparabolic corrections. Previous theoretical work has focused mainly on the calculation of revival times of single particles in different potentials, ignoring more realistic systems such as semiconductors because of their complex band structure. On the other hand, revival times are difficult to observe directly due to their extremely fast oscillations. We hope this paper helps to overcome both difficulties by showing through explicit calculation that certain nanostructures exhibit considerably higher revival times.

CRediT authorship contribution statement

F. de los Santos: Methodology, Software, Investigation, Writing – original draft. **E. Romera:** Methodology, Software, Investigation, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

Acknowledgements

This work is part of the Project of I+D+i Ref. PID2020-113681GB-I00, financed by MICIN/AEI/10.13039/501100011033 and FEDER "A

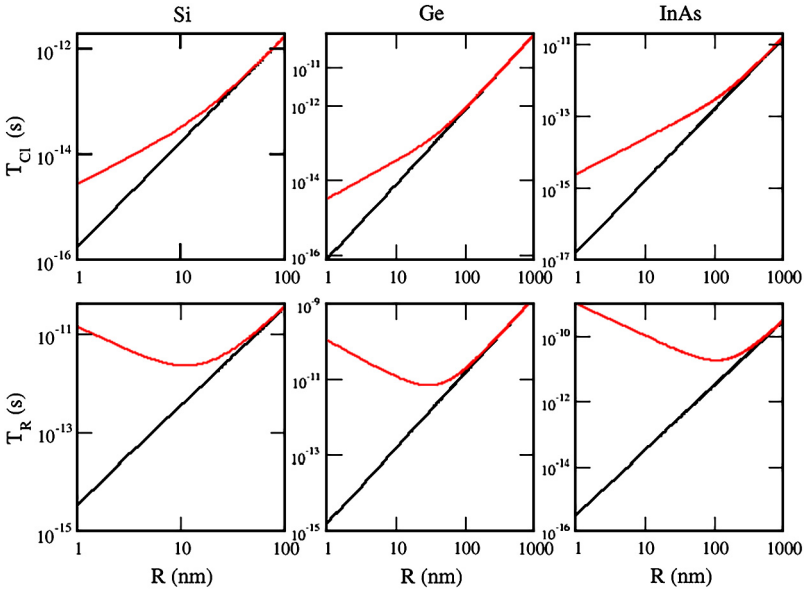

Fig. 4. Classical and revival times as a function of the radius for quantum dots of different materials and $n_0 = 10$. The rest of parameters are as in Fig. 3. Black lines correspond to the parabolic calculus and the red ones to the nonparabolic correction. Notice the double-logarithmic scale.

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