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2-d finite barrier rectangular quantum dots II: Dirac description

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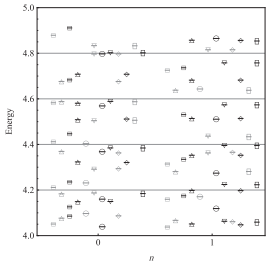
HIGHLIGHTS

- Inseparable piecewise potential is used as the relativistic confinement potential of the quantum dot.
- Theoretical approach is based on elimination of the inexactness of the wave vector components employing the transfer matrices, and the reflection and the rotation symmetries of the dot.
- The transcendental energy relations of the dot are obtained as 2fold degenerate and quantized by half of the rotation angles, similar to non-relativistic case.
- Considerable energy differences between these descriptions are observed due to spin effect.

GRAPHICAL ABSTRACT

Comparison of the finite-barrier rectangular quantum dot energy solutions for Schrödinger and Dirac descriptions, where gray geometric objects are for energy solutions of inside wave vector component κ_x defined quantized transcendental energy relations of Schrödinger and Dirac descriptions, while black ones for those of the inside wave vector component κ_y defined relations, for $n=0,1$ values. Schrödinger description results of inseparable finite barrier rectangular quantum dots are expanded to relativistic Dirac description.



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ABSTRACT

The Schrödinger description of 2-d finite barrier rectangular quantum dots [1] is expanded to Dirac description through transfer matrices and reflection and rotation symmetries of the dot system. Inexactness of wave vector components of spinors is then reduced to two relations which lead to two different bispinors and four quantized transcendental energy relations corresponding to even–even, odd–odd and even–odd, odd–even factorizing functions of each bispinor. In order to show the spin effect on the dot energy levels, the solutions of the transcendental relations of the Schrödinger and Dirac descriptions are plotted.

1. Introduction

Quantum dots that have the ability to confine tunable number of carriers in all spatial dimensions [2,3], have been intriguing theoretical and experimental research area due to their possible implementations in future electronic devices [4]. In addition to the charge at which all electronic properties rely on, since the carriers have also spin aspect, it turns out that individual spins of the carriers can also be controlled and measured in quantum dots [5–7]. This fact has originated the investigations of single spin dynamics in solid-state physics context such as spintronics [8,9] in analogy to single electronics, and quantum bits [10,6,11,12].

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The spin of an electron trapped in a quantum dot interacts with its environment which consists of charge and spin degrees of freedom. The attractive potential and the spin–orbit and hyperfine interactions are these degrees of freedom due to charge and spin respectively [13,14,6].

Spin is a fully relativistic aspect of electrons and should be properly treated by the Dirac equation [15,16]. To our knowledge, Dirac equation has never been used to model even a single-electron state of quantum dots, except in the investigations represented by [17–19] in which graphene quantum dots have been studied. After the discovery of wonder material graphene, a honeycomb lattice of carbon atoms [20–22], the massless Dirac equation has been employed to explain electronic properties of graphene [23]. It is now a necessity to employ the Dirac equation in order to analyze honeycomb lattice carbon materials such as graphene [24], carbon nanotubes [25], and fullerenes [26,27].

Since the shape of the potential is crucial to analyze the dot system, chosen shape of the potential must have a solution in the Dirac description for dot system. However Dirac equation has quite limited number of exact solutions for 2-d and 3-d potentials [28,15], since an electrostatic potential is quadratically coupled with the energy. For instance the Dirac oscillator potential is essentially a scalar potential instead of an electrostatic one [29,30]. These facts make the finite high piecewise potential

$$V(x,y)=\begin{cases}-V_0 & \text{inside of the dot}\\ 0 & \text{outside of the dot}\end{cases} \tag{1}$$

a perfect candidate for Dirac description of an electron confined in a rectangular shape quantum dot.

An algebraic approach to finite barrier rectangular quantum dot system has been accomplished [1] in which outside wave vector components have been obtained by means of inside wave vector components employing the transfer matrices on the boundaries of the dot. Then inexact definitions of inside wave vector components have been reduced to two different relations by means of inside wave vector imposing parity and rotation symmetries of the dot on the wavefunction. It has turned out that the two definitions of inside wave vector components lead two different wavefunctions and two quantized transcendental energy relations corresponding to even–even and odd–odd factorizing functions of each wavefunction.

In this work we intend to expand the Schrödinger description [1] to relativistic domain finding quantized energy relations of a single-electron confined in an inseparable piecewise potential (1) within a non-noise circumstances using the well-known transfer matrix method. First which conditions are necessary to define a Dirac Hamiltonian in a solid-state continuum are explained. Then from the continuity condition of the Dirac equation in the semiconductor continuum, the transfer matrices of the spinor are written, then relations between inside and outside wave vector components are found by means of the continuity condition which is the relativistic counterpart of the BenDaniel–Duke conditions. In order to obtain the constraints of inside wave vector components, parity and rotation symmetries of the dot are imposed on the spinor. Consequently, energy relations of bound states which correspond to both spin-up and spin-down states of the dot occur in a quantized transcendental form.

2. Dirac description of the quantum dots

When the Fermi energy level is set to zero while the energy differences $E_C - E_F$ and $E_F - E_V$ correspond to the rest mass energies of the particle and antiparticle respectively, an analogy can be drawn between conduction and valance bands of a semiconductor and rest mass energies of the field-free vacuum. The energy differences of electron and hole carriers are defined by

$$E_C - E_F = m_e^* v^2 \qquad \text{and} \qquad E_F - E_V = m_h^* v^2, \tag{2}$$

where v being speed of light, and m_e^* and m_h^* are effective masses of electron and hole carriers in the semiconductor, respectively. Therefore the transition of an electron from the occupied states of valance band to the unoccupied states of conduction band which gives rise an electron–hole pair [31, chapter 5] can be considered as the solid-state counterpart of the particle–antiparticle creation of vacuum. With this analogy the time-independent Dirac Hamiltonian of the electron–hole carrier pair can be written as

$$H = v\alpha.\, p_{e,h} + \beta m_{e,h}^* v^2 + V(x,y,x), \tag{3}$$

where α and β are usual Dirac matrices, and $p_{e,h}$ represents momentums of electron and hole respectively.

Despite the fact that there is a similarity between the transition and the particle–antiparticle creation, the discrete charge conjugation symmetry by which particle and its antiparticle are interchanged [32, section 3.6] is not fundamental, since the effective masses of the carrier pair depend on the their energy bands in a solid. The electron–hole symmetry, the solid-state counterpart of charge conjugation symmetry, only occurs permanently when the effective masses of the carrier pair are equal or zero. Since the broken electron–hole symmetry is the general case in which the Dirac Hamiltonian of a semiconductor cannot be a proper description of the system, only a semiconductor quantum dot system that posses equal effective masses can be considered in the Dirac description.

Since a quantum dot structure consists of two different semiconductor materials, the speed of light and the effective mass quantities of the Dirac Hamiltonian (3) should be considered as piecewise functions:

$$v=\begin{cases}v_{in} & \text{inside of the dot}\\ v_{out} & \text{outside of the dot}\end{cases} \tag{4}$$

$$m^*=\begin{cases}m_{in}^* & \text{inside of the dot}\\ m_{out}^* & \text{outside of the dot}\end{cases} \tag{5}$$

It is important to note that, inside of the dot has to be electron–hole symmetric since the Dirac Hamiltonian (3) must be Lorentz-invariant. When inside and outside materials of the structure have different electron–hole symmetries, the charge carriers have the same amount of potential value in opposite signs. Therefore when one has solved the Dirac equation of one carrier, the energy values of other carrier appear exactly with opposite sign. On the other hand if outside of the dot is made of a material which does not possess the symmetry, then the confinement potentials of the carriers differ from each other and hence their energies.

3. Rectangular quantum dot with inseparable potential

In order to employ the approach given by [1] in the relativistic domain, we choose a 2-d rectangular semiconductor quantum dot structure whose time-independent Dirac equation of confined negative charge carrier reads

$$[-i\hbar v(\sigma_x\partial_x \pm \sigma_y\partial_y) + \sigma_z m^* v^2 + V(x,y)]\chi_{\pm}(x,y) = E\chi_{\pm}(x,y), \tag{6}$$