Treating Some Solid State Problems with the Dirac Equation

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Abstract

The ambiguity involved in the definition of effective-mass Hamiltonians for nonrelativistic models is resolved using the Dirac equation. The multistep approximation is extended for relativistic cases allowing the treatment of arbitrary potential and effective-mass profiles without ordering problems. On the other hand, if the Schrödinger equation is supposed to be used, our relativistic approach demonstrate that both results are coincidents if the Ben-Daniel and Duke prescription for the kinetic-energy operator is implemented. Applications for semiconductor heterostructures are discussed.

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The effective-mass theory has been successfully used in semiconductor heterostructures [1]. An interesting aspect arises when we treat materials whose properties change from region to region. In particular, when the effective mass depends on position, the Schrödinger equation for an arbitrary potential profile is usually solved numerically by different methods. However, one of the problems of the effective-mass theory for semiconductors heterostructures, is to decide how to write out the Hamiltonian operator. This problem arise from canonical quantization of the classical Hamiltonian. For position-dependent carrier effective mass, we have an ordering problem with the kinetic energy operator (KEO). Some authors proposed different forms for the kinetic energy operator, all having the generic form proposed by von Roos [2]

$$\hat{T} = \frac{1}{4} \left( m^\alpha(x) \hat{p} m^\beta \hat{p} m^\gamma(x) + m^\gamma(x) \hat{p} m^\beta \hat{p} m^\alpha(x) \right), \quad (1)$$

where $\alpha + \beta + \gamma = -1$, but the problem was not resolved because there is not a first principle to fix only one operator.

This ambiguity indicates that the Schrödinger equation is not rigorously suitable in the effective-mass approximation with position-dependent effective mass. It is reasonable to try

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other equation that represents the same physics of the Schrödinger equation in the low energy limit.

The object of this Letter is to demonstrate that, in fact, the Dirac equation (at adequate limits) can successfully be used to describe quantum-mechanical systems where position-dependent effective mass is present. We recall that, in Dirac equation, the kinetic energy operator and the mass term appear separately, so there is no ordering problems in this context.

Obviously the considerations of this work only concern the mathematical issues related with the equations of motion. Indeed, a physically sensible application of the Dirac equation to semiconductor heterostructures would have to take in to account a relativistic extension of the Wannier-Slater theorem [3].

In this work we use a numerical method (multistep potential approximation [4]) which has been applied to solve Schrödinger equation for an arbitrary potential profile. Here we extend this algorithm to the relativistic case, in such a way that the ambiguity problem is overcome. In particular, we consider the Dirac equation with a one dimensional arbitrary potential well and find the energy levels for a particle. Also we apply the method for a particular type of heterostructure and compare the results to those obtained in the context of the Schrödinger equation with the form (1) for the KEO and several choices for the parameters $\alpha, \beta$ and $\gamma$. For a KEO in the Schrödinger equation of the form suggested by BenDaniel and Duke ($\beta = -1, \gamma = 0$) [3], we conclude that both equations lead to the same solutions in the energy range concerned.

Let us now introduce the numerical method that allows us to obtain the energy levels for a Dirac equation with space-dependent effective mass.

We will consider a particle with mass $m(z)$ that is submitted to an arbitrary one dimensional potential well $V(z)$. The time-independent Dirac equation is written as (in units with $\hbar = c = 1$) [8]

$$\left(\alpha \hat{p} + \beta m(z)\right) \Psi = (E - V(z)) \Psi,$$

where, $\hat{p} = -i \frac{d}{dz}$ is the momentum operator, $E$ is the electron energy, $\alpha$ and $\beta$ are $4 \times 4$ matrices given by

$$\alpha = \begin{pmatrix} 0 & \sigma^3 \\ \sigma^3 & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix},$$

$I$ is the $2 \times 2$ identity matrix and $\sigma^3$ is a $2 \times 2$ Pauli matrix defined as

$$\sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$  

Consider now an arbitrary well as sketched in fig.1. We split up the interval $[a, b]$ into $N$ infinitesimal intervals of length $\Delta z = (b - a)/N$. For the $i$-th interval, we approximate the potential and the mass by

$$V(z) = V(z_i) = V_i \quad and \quad m(z) = m(z_i) = m_i, \quad for \quad z_i \leq z < z_{i+1}.$$  

The wave function of the electron in Dirac’s equation with no spin flip in the $i$–th interval is
\[ \psi_i(z) = A_i e^{i p_i z} \begin{pmatrix} 1 \\ 0 \\ p_i \\ E - v_i + m_i \end{pmatrix} + B_i e^{-i p_i z} \begin{pmatrix} 1 \\ 0 \\ -p_i \\ E - v_i + m_i \end{pmatrix}, \tag{6} \]

where \( p_i = \sqrt{(E - V_i)^2 - m_i^2} \). The bound state conditions are given by \( |E - V_0| < m_0 \) and \( |E - V_{N+1}| < m_{N+1} \). By imposing the continuity of the wave function at each \( z = z_i \), we have a matrix \( M(E) \) which relates the coefficients in the region where \( z < a \) with the region where \( z > b \).

\[ \begin{pmatrix} A_{N+1} \\ B_{N+1} \end{pmatrix} = M(E) \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} \tag{7} \]

The finiteness of the wave function requires that

\[ M(E)_{22} = 0 \tag{8} \]

So, the solution of (8) gives us the energy levels.

Note that this numerical method is specially convenient for treating wells and barriers with arbitrary profiles and it is nothing else than an extension of the transfer-matrix method for relativistic theories. To the best of our knowledge, this is the first numerical analysis for evaluating energy levels in an relativistic equation with mass position-dependent and arbitrary potential. However, our main point here is to demonstrate that the Dirac equation can be used to obtain unambiguously results in situations where the Schrödinger equation depends on ordering problems.

As an illustration, we applied the method described above for an electron in a one-dimensional GaAs/Al\(_{0.3}\)Ga\(_{0.7}\)As heterostructure. For the sake of comparison with previous results we take a square well, as sketched in fig. 2. The electron effective mass is 0.67\( m_0 \) and 0.86\( m_0 \) for GaAs and Al\(_{0.3}\)Ga\(_{0.7}\)As respectively (\( m_0 \) is the free electron mass)(Fig. 2). In the Schrödinger equation we use the von Ross operator considering several values of the \( \alpha \) parameter. Note that for abrupt heterojunctions only Hamiltonians with \( \alpha = \gamma \) are viable, due to continuity conditions across the heterojunction. As we can see in fig. 3 there is an extraordinary coincidence between the results from the Dirac and from the Schrödinger equations for \( \alpha = 0 \). As a matter of fact, this is expected since the maximum value of the energy involved is 3eV. Further, this result strongly supports the prescription of BenDaniel and Duke for the Schrödinger context.

As a second illustration consider the conduction-band structure of a GaAs/Al\(_{0.3}\)Ga\(_{0.7}\)As system with nonabrupt interface and assume that the effective mass changes linearly at the transition regions while the potential well varies quadratically in that regions (denoted by \( a \)) as it is shown in fig. 4. There the potential is given by

\[ V(z) = C \left[ \epsilon_1 \chi(z) + \epsilon_2 \chi(z)^2 \right], \tag{9} \]

where \( C = 0.6 \) is the conduction band offset and \( \epsilon_1 = 0.3, \epsilon_2 = 0.7 \) are constants associated with the compositional dependence of the energy-gap difference between GaAs and AlGaAs (experimental parameters and details concerned can be seen in refs. [6,7]).
Again, we use our relativistic method and the Schrödinger equation with the BenDaniel and Duke prescription ($\alpha = \gamma = 0$). Once more, as we can see in fig. 5, a complete coincidence between the relativistic and non-relativistic results is obtained.

In conclusion, we have shown that a relativistic method can be successfully used to overcome the ordering problem of the kinetic energy operator in non-relativistic models. Since the range of energy involved is extremely low (comparing to electron rest mass), the numerical results are perfectly coincident in both cases.

It is worthwhile to mention that, notwithstanding the Wannier-Slater theorem commented in the introduction, we claim attention for the coincidence shown above. Therefore, we believe that, after exhaustive and appropriate considerations about effective-mass approximation, band structures and the periodic potential, the relativistic approach constructed here it could be used to calculate physical parameters in the theory of abrupt and nonabrupt semiconductor heterostructures.

Moreover, the relativistic treatment developed here can be applied to all physical systems described by a Sturm-Liouville eigenvalue equation (within an appropriate range of energy), namely

\[
- \frac{d}{dz} \left[ \frac{1}{p(z)} \frac{df}{dz} \right] + q(z)f(z) = \lambda w(z)f(z).
\]  

(10)

Here $f$ is an eigenfunction, $\lambda$ is an eigenvalue and $p, q,$ and $w$ describe particular properties of the system. For example, this equation can describe the motion of electrons or phonons along the growth axis of a [100] zinc-blende heterostructure [10]. Thereby, the equation (10) can always be replaced by an correspondent Dirac equation for avoid ordering problems.

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**FIGURE CAPTIONS**

Figure 1: Generic profile of a one-dimensional quantum potential well. We split up the interval \([a, b]\) into \(N\) infinitesimal intervals of length \(\Delta z = (b - a)/N\).

Figure 2: Potential well and effective mass, as a function of the position, for an abrupt heterostructure.

Figure 3: Eigenenergies in the conduction band of the GaAs/Al\(_{0.3}\)Ga\(_{0.7}\)As, with a conduction band-offset of 0.6 vs the well width (abrupt heterojunction). The chosen value for \(a\) is 20\% of the well width. Solid line shows the calculations performed using the Dirac equation. Dotted line shows the calculations for Schrödinger equation using the BenDaniel-Duke prescription (\(\alpha = 0\)). The + + curve denotes calculations using the Zhu and Kroemer prescription (\(\alpha = -0.5\)).

Figure 4: Potential well and effective mass, as a function of the position, for a nonabrupt heterostructure (\(a\) denotes the transition region).

Figure 5: Eigenenergies in the conduction band of the GaAs/Al\(_{0.3}\)Ga\(_{0.7}\)As, with a conduction band-offset of 0.6 vs the well width (nonabrupt heterojunction). The chosen value for \(a\) is 20\% of the well width. Solid line shows the calculations performed using the Dirac equation and dotted line shows the calculations for Schrödinger equation using the BenDaniel-Duke prescription (\(\alpha = \gamma = 0\)). The + + curve denotes calculations using the Zhu and Kroemer prescription (\(\alpha = \gamma = -0.5\)).
\[ V(z) \]

\[ m(z) \]

\[ V_{\text{max}} \]

\[ m_{\text{max}} \]
