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LETTER TO THE EDITOR

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 used, our relativistic approach demonstrates that the two results are coincident if the BenDaniel–Duke prescription for the kinetic-energy operator is implemented. Applications for semiconductor heterostructures are discussed.

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 semiconductor heterostructures is to decide how to write out the Hamiltonian operator. This problem arises from the 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 KEO, all having the generic form proposed by von Roos [2]

$$\hat{T} = \tfrac{1}{4}(m^{\alpha}(x)\hat{p}m^{\beta}\hat{p}m^{\gamma}(x) + m^{\gamma}(x)\hat{p}m^{\beta}\hat{p}m^{\alpha}(x)) \tag{1}$$

where $\alpha + \beta + \gamma = -1$, but the problem was not resolved because there is no first principle to fix only one operator.

This ambiguity indicates that the Schrödinger equation is not rigorously suitable in the effective-mass aproximation with position-dependent effective mass. It is reasonable to try another equation that represents the same physics as 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 the Dirac equation, the KEO and the mass term appear separately, so there is no ordering problem in this context.

Obviously the considerations of this Letter only concern the mathematical issues related to 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 Letter we use a numerical method (multistep potential approximation [4]) which has been applied to solve the Schrödinger equation for an arbitrary potential profile. Here

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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 α, β and γ. For a KEO in the Schrödinger equation of the form suggested by BenDaniel and Duke ($\beta = -1$, $\gamma = 0$) [5], we conclude that the two 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 subjected to an arbitrary one-dimensional potential well $V(z)$. The time-independent Dirac equation is written as (in units with $\hbar = c = 1$) [8]

$$(\alpha \hat{p} + \beta m(z))\Psi = (E - V(z))\Psi \tag{2}$$

where $\hat{p} = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z}$ is the momentum operator, E is the electron energy, α and β are 4×4 matrices given by

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

where I is the 2×2 identity matrix and σ^3 is a 2×2 Pauli matrix defined as

$$\sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4}$$

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

$$V(z) = V(z_i) = V_i \qquad \text{and} \qquad m(z) = m(z_i) = m_i \qquad \text{for} \quad z_i \leqslant z < z_{i+1}. \tag{5}$$

The wavefunction of the electron in Dirac's equation with no spin flip in the ith interval is

$$\psi_i(z) = A_i \mathrm{e}^{\mathrm{i}p_i z} \begin{pmatrix} 1 \\ 0 \\ \frac{p_i}{E - v_i + m_i} \\ 0 \end{pmatrix} + B_i \mathrm{e}^{-\mathrm{i}p_i z} \begin{pmatrix} 1 \\ 0 \\ \frac{-p_i}{E - v_i + m_i} \\ 0 \end{pmatrix} \tag{6}$$

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 wavefunction 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 wavefunction requires that

$$M(E)_{22} = 0. \tag{8}$$

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

Note that this numerical method is especially convenient for treating wells and barriers with arbitrary profiles and it is nothing other 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

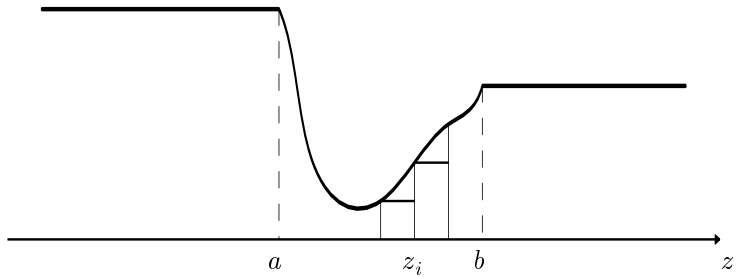

Figure 1. Generic profile of a one-dimensional quantum potential well. We split the interval $[a, b]$ into N infinitesimal intervals of length $\Delta z = (b - a)/N$.

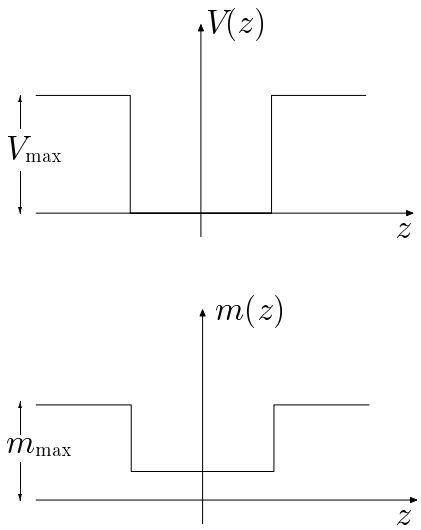

Figure 2. Potential well and effective mass, as a function of the position, for an abrupt heterostructure.

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 figure 2. The electron effective mass is $0.67m_0$ and $0.86m_0$ for GaAs and $Al_{0.3}Ga_{0.7}$As respectively (m_0 is the free electron mass) (figure 2). In the Schrödinger equation we use the von Ross operator [2] considering several values of the α parameter. Note that for abrupt heterojunctions only Hamiltonians with $\alpha = \gamma$ are viable, due to continuity conditions across the heterojunction [9]. As we can see in figure 3 there is an extraordinary coincidence between the results from the Dirac and Schrödinger equations for $\alpha = 0$. As a matter of fact, this is expected since the maximum value of the energy involved is 3 eV. Further, this result strongly supports the prescription of BenDaniel and Duke [5] 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 those regions (denoted by a)

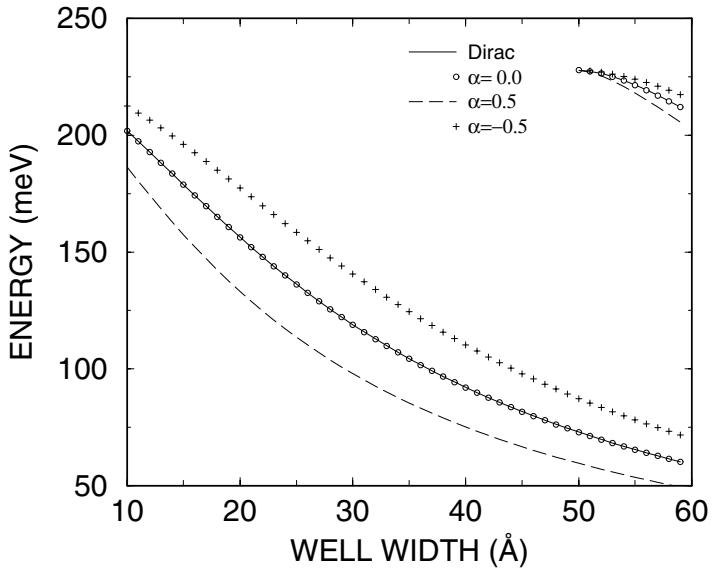

Figure 3. Eigenenergies in the conduction band of GaAs/$Al_{0.3}Ga_{0.7}As$, with a conduction band offset of 0.6 versus the well width (abrupt heterojunction). The chosen value for a is 20% of the well width. The solid curve shows the calculations performed using the Dirac equation. The broken curve shows the calculations for the Schrödinger equation using the BenDaniel–Duke prescription ($\alpha = 0$). The ++ curve denotes calculations using the Zhu–Kroemer prescription ($\alpha = -0.5$).

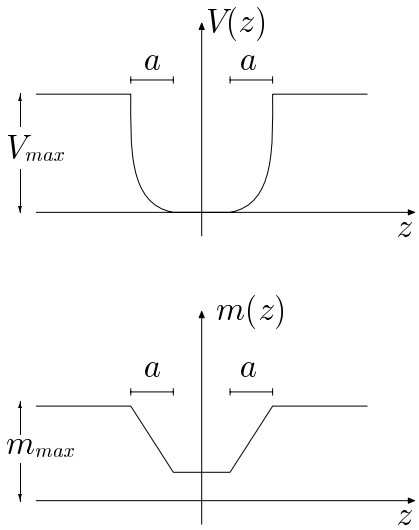

Figure 4. Potential well and effective mass, as a function of the position, for a nonabrupt heterostructure (a denotes the transition region).

as shown in figure 4. There the potential is given by

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

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 [6, 7]).

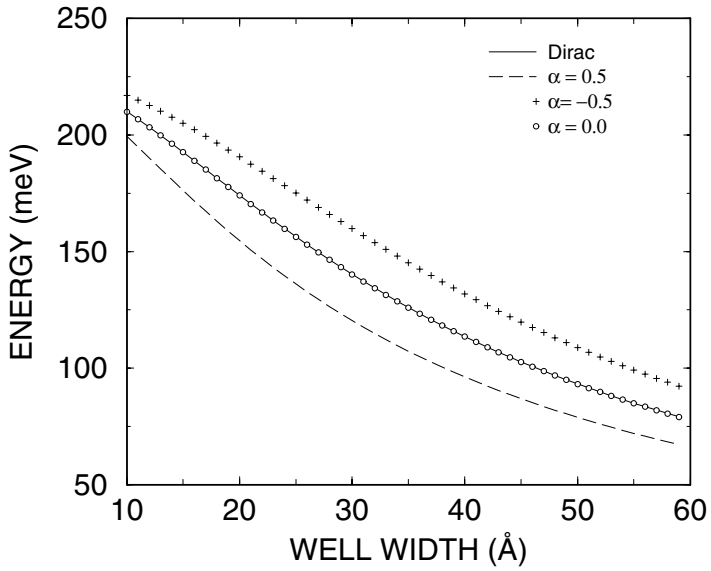

Figure 5. Eigenenergies in the conduction band of GaAs/$Al_{0.3}Ga_{0.7}As$, with a conduction band-offset of 0.6 versus the well width (nonabrupt heterojunction). The chosen value for a is 20% of the well width. The solid curve shows the calculations performed using the Dirac equation and the broken curve shows the calculations for the Schrödinger equation using the BenDaniel–Duke prescription ($\alpha = \gamma = 0$). The ++ curve denotes calculations using the Zhu–Kroemer prescription ($\alpha = \gamma = -0.5$).

Again, we use our relativistic method and the Schrödinger equation with the BenDaniel–Duke prescription ($\alpha = \gamma = 0$). Once more, as we can see in figure 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 KEO 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 on in the introduction, we claim attention for the coincidence shown above. Therefore, we believe that, after exhaustive and appropriate considerations of the effective-mass approximation, band structures and the periodic potential, the relativistic approach constructed here 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

$$-\frac{\mathrm{d}}{\mathrm{d}z}\left[\frac{1}{p(z)}\frac{\mathrm{d}f}{\mathrm{d}z}\right] + q(z)f(z) = \lambda w(z)f(z). \tag{10}$$

Here f is an eigenfunction, λ 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 a corresponding Dirac equation to avoid ordering problems.

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