Form of the quantum kinetic-energy operator with spatially varying effective mass

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Through a nonrelativistic limit of the Dirac Hamiltonian and considering the spatial dependence of the particle mass in the Foldy-Wouthuysen transformation, it is shown that the quantum kinetic-energy operator with spatially varying effective mass has the form $\frac{1}{4}\{\hat{p}[1/\sqrt{m(\mathbf{r})}]\hat{p}[1/\sqrt{m(\mathbf{r})}]+[1/\sqrt{m(\mathbf{r})}]\hat{p}[1/\sqrt{m(\mathbf{r})}]\hat{p}\}$. However, the transmission properties of an electron through a $GaAs/Al_xGa_{1-x}As$ heterojunction calculated both with this form and the BenDaniel and Duke operator $\hat{p}[m(\mathbf{r})]^{-1}\hat{p}/2$, the most used kinetic-energy operator, differ at most by 1% if the existence of interface regions as thin as two GaAs lattice units is taken into account. [S0163-1829(97)02903-2]

The effective-mass theory is very useful in condensed-matter physics. Initially proposed to describe impurities in crystals,[1–3] it is nowadays a key element in the study of semiconductor heterostructures.[4,5] To take into account the spatial variation of the semiconductor type, effective-mass Hamiltonians are constructed based on kinetic-energy operators (KEO's) with a position-dependent carrier effective mass, $m=m(\mathbf{r})$. Several KEO's were proposed,[6–10] all of them special cases of the most general von Roos form[11] given by

$$\tfrac{1}{4}[m^{\alpha}(\mathbf{r})\hat{p}m^{\beta}(\mathbf{r})\hat{p}m^{\gamma}(\mathbf{r})+m^{\gamma}(\mathbf{r})\hat{p}m^{\beta}(\mathbf{r})\hat{p}m^{\alpha}(\mathbf{r})], \quad (1)$$

where $\hat{p}=(\hbar/i)\boldsymbol{\nabla}$ is the carrier momentum operator, the parameters α, β, and γ satisfy the relation $\alpha+\beta+\gamma=-1$. The hermiticity condition of the Hamiltonian, current-density conservation, comparison between experiments and theoretical results,[12–17] and condensed-matter first-principle theories[18,19] were unable to indicate conclusively a unique form for the KEO with a position-dependent effective mass, i.e., the exact values for the parameters α, β, and γ in Eq. (1). The question of the exact form of the KEO is still an open problem.

It was suggested that all KEO's are equivalent if the spatial variation of the semiconductor alloy in the interface region is smooth.[15–17,19] However, this suggestion does not minimize the problem related with the KEO ambiguous definition. In fact, some results show that the influence of the KEO form on the properties of semiconductor heterostructures is important.[12–15] In particular, a limit of the order of 100 Å for the $GaAs/Al_{0.3}Ga_{0.7}As$ interface was obtained recently for the equivalence of several KEO's with respect to electron transmission phenomena.[20] This very large interface width is of the order of the semiconductor dimensions that Wolfe, Holonyak, and Stillmann[21] have suggested for the validity of the effective-mass approximation based on simple arguments related to the Heisenberg uncertainty principle.

The purpose of this paper is to present a scheme to obtain unambiguously the Schrödinger equation with spatially varying particle mass. This is accomplished through the nonrelativistic limit of the Dirac Hamiltonian performed by means of a Foldy-Wouthuysen transformation that considers the spatial dependence of the particle mass. At this point, it is worth highlighting that the famous original publications of Schrödinger allow us to ponder the assumption of a particle mass that is position dependent.[22–24] This possible dependence seems never to be considered.

A way to solve the ambiguity in the KEO definition was proposed early by Liu.[25] By considering the following time-independent Lagrangian for a single band envelope wave function (a Schrödinger-like field),

$$L=-\frac{\hbar^2}{2m(\mathbf{r})}\boldsymbol{\nabla}\Psi^*\cdot\boldsymbol{\nabla}\Psi-\Psi^*V\Psi, \quad (2)$$

he obtained with the Euler-Lagrange equations the BenDaniel and Duke Hamiltonian ($\beta=-1$, $\gamma=0$).[6] Since some other forms for the Lagrangian can be chosen, it is argued here that the method proposed by Liu[25] does not allow an unambiguous KEO definition. In fact, if $L=-(\hbar^2/2)\boldsymbol{\nabla}[\Psi^*/\sqrt{m(\mathbf{r})}]\cdot\boldsymbol{\nabla}[\Psi/\sqrt{m(\mathbf{r})}]-\Psi^*V\Psi$, the Zhu and Kroemer Hamiltonian ($\alpha=-1/2$, $\beta=0$) (Ref. 7) is obtained; if $L=-(\hbar^2/4)\{\boldsymbol{\nabla}\Psi^*\cdot\boldsymbol{\nabla}\Psi[1/m(\mathbf{r})]+[1/m(\mathbf{r})]\boldsymbol{\nabla}\Psi^*\cdot\boldsymbol{\nabla}\Psi\}-\Psi^*V\Psi$, the Gora and Williams[8] and/or Bastard[9] Hamiltonian ($\alpha=-1$, $\gamma=0$) is obtained; if $L=-(\hbar^2/4)\{[1/\sqrt{m(\mathbf{r})}]\boldsymbol{\nabla}[\Psi^*/\sqrt{m(\mathbf{r})}]\cdot\boldsymbol{\nabla}\Psi+\boldsymbol{\nabla}[\Psi^*/\sqrt{m(\mathbf{r})}]\boldsymbol{\nabla}[\Psi/\sqrt{m(\mathbf{r})}]\}-\Psi^*V\Psi$, the Li and Kuhn Hamiltonian[10] ($\alpha=0$, $\gamma=-1/2$) is obtained.

The point of departure in this paper to solve the KEO ambiguity problem is to consider the following Lagrangian for the Dirac equation (that is more fundamental than the Schrödinger equation):[26]

$$\mathcal{L}=\overline{\Psi}[\gamma^{\mu}p_{\mu}-m(\mathbf{r})]\Psi, \quad (3)$$

where $p_{\mu}=(\hbar c/i)\partial_{\mu}$, γ are the Dirac matrices,

$$\gamma^0=\beta=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \quad \gamma^j=\alpha_i=\begin{pmatrix}\sigma_i & 0\\ 0 & \sigma_i\end{pmatrix},$$

and σ_i ($i=1, 2, 3$) are the Pauli matrices.[26]

The choice of the Dirac equation circumvents problems related with the noncomutativity of the momentum operator

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and the particle mass. By using the Euler-Lagrange equations, the following Hamiltonian is obtained:

$$\mathcal{H}=\alpha\hat{p}+m(\mathbf{r})\beta. \tag{4}$$

The differential equations for the spinors of the above Hamiltonian are coupled through the operator $\Omega_1=\alpha\hat{p}$. Since $m(\mathbf{r})\beta$ is considered as the dominant term in the nonrelativistic limit, $\mathcal{H}$ can be transformed into a new Hamiltonian $\mathcal{H}'$ through the following Foldy-Wouthuysen transformation:[27]

$$\mathcal{H}'=\exp(iS)\ \mathcal{H}\ \exp(-iS). \tag{5}$$

In the case of a constant mass, it is obtained that $H'=\Sigma_{n=0}^{\infty}(1/n!)T^n$, where $T_0=\mathcal{H}$ and $T_n=[iS,T_{n-1}]$. For a spatially varying effective mass, since $m(\mathbf{r})$ does not commute with $\hat{p}$, there are two possibilities for the operator S:

$$S_1=-\frac{i}{2}\frac{1}{\sqrt{m(\mathbf{r})}}\beta\Omega_1\frac{1}{\sqrt{m(\mathbf{r})}}, \tag{6}$$

$$S_2=-\frac{i}{4}\left[\frac{1}{m(\mathbf{r})}\beta\Omega_1+\beta\Omega_1\frac{1}{m(\mathbf{r})}\right]. \tag{7}$$

By using the expansion $\mathcal{H}'=\mathcal{H}+i[S,\mathcal{H}]-i/2[S,[S,\mathcal{H}]]+\cdots$ and disregarding terms $\mathcal{O}(1/m^3(\mathbf{r}))$, it is straightforward to show that both operators S_1 and S_2 gives the following form for the transformed Hamiltonian in the nonrelativistic limit:

$$\mathcal{H}'=\frac{1}{4}\left[\hat{p}\frac{1}{\sqrt{m(\mathbf{r})}}\hat{p}\frac{1}{\sqrt{m(\mathbf{r})}}+\frac{1}{\sqrt{m(\mathbf{r})}}\hat{p}\frac{1}{\sqrt{m(\mathbf{r})}}\hat{p}\right]. \tag{8}$$

The scheme used here indicates conclusively that $\alpha=0$ and $\gamma=-1/2$ in Eq. (1). Hence, the ambiguity problem in the KEO with spatially varying effective mass seems to be solved.

The Hamiltonian of Eq. (8) was proposed early by Liu and Kuhn[10] as one of the possible forms for the KEO. They named it *redistributed* since the mass operators are redistributed among the momentum terms. However, the BenDaniel and Duke[6] KEO $\hat{p}[m(\mathbf{r})]^{-1}\hat{p}/2$ is the most used for calculations of semiconductor heterostructure properties, although recent works have suggested that other operators are more suitable—see Ref. 12, for example.

To have an idea of the role of the KEO's choice on the theoretical calculations of transmission properties in semiconductor heterostructures, the transmission coefficient of an electron through a $GaAs/Al_{0.3}Ga_{0.7}As$ heterojunction is performed taking into account the KEO's of BenDaniel and Duke[6] (T_{BD}), Zhu and Kroemer[7] (T_{ZK}), Gora and Williams[8] or Bastard[9] ($T_{GW/B}$), and Li and Kuhn[10] (T_{LK}). The interface potential description of Freire, Auto, and Farias,[30] and the numerical method of Ando and Itoh[31] is used in the calculations.

Figure 1 shows that the electron transmission is sensitive to the KEO's form, principally when abrupt interfaces are considered. For abrupt interfaces and an electron with low energy, the differences between T_{LK} and $T_{GW/B}$ (T_{BD} or T_{ZK}) can be as high as 30% (15%) (see the inset in Fig. 1). When

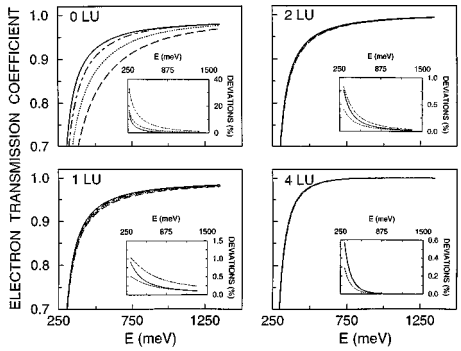

FIG. 1. Transmission coefficients of electrons through $GaAs/Al_{0.3}Ga_{0.7}As$ heterojunctions with interface widths of zero, one, two, and four GaAs lattice units (LU). The following KEO's are considered: BenDaniel and Duke (Ref. 6), T_{BD} (solid); Zhu and Kroemer (Ref. 7), T_{ZK} (dashed); Gora and William (Ref. 8), or Bastard (Ref. 9), $T_{GW/B}$ (dotted dashed); and Li and Kuhn (Ref. 10), T_{LK} (dotted). The insets show the relative deviations $(T_{LK}-T_{BD})/T_{LK}$ (solid), $(T_{LK}-T_{GW/B})/T_{LK}$ (dotted dashed), and $(T_{LK}-T_{ZK})/T_{LK}$ (dashed). An electron band offset of 0.6 is always used.

the interface width or the electron energy increases, the differences between the transmission coefficients decrease to less than 1%. Consequently, the KEO's of BenDaniel and Duke,[6] Zhu and Kroemer,[7] Gora and Williams,[8] or Bastard,[9] and Li and Kuhn (redistributed)[10] are all equivalent for interface widths at least of four GaAs lattice units. It is worth mentioning that it was shown by Ribeiro Filho *et al.*[20] that KEO's with $\alpha=-2.0$, -1.0, -0.5, 0.0, 0.5, 1.0, 2.0 are all equivalent only when the transition region (where the effective mass is position dependent) is of the order of sixteen GaAs lattice units.

In conclusion, we have shown a way to solve the ambiguity problem of the form of the quantum kinetic-energy operator with spatially varying effective mass. $\alpha=0$ and $\gamma=-1/2$ were obtained by making the nonrelativistic limit of the Dirac Hamiltonian through a Foldy-Wouthuysen transformation that has considered the spatial dependence of the particle mass. Theoretical calculations of semiconductor heterostructures properties with BenDaniel and Duke[6] and Li and Kuhn[10] KEO's will give very approximately the same results with respect to semiconductor heterostructures properties only when the interface widths are large. In $GaAs/Al_xGa_{1-x}As$ systems, this means at least interface widths thicker than or of the order of two GaAs lattice parameters, the width of interfaces that are actually grown.[28,29] Finally, the present results suggest that no experiment can be performed nowadays on semiconductor samples to determine the KEO form in systems with spatially varying effective mass since the actual interface widths preclude this possibility.

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