Quantum mechanics with coordinate-dependent mass

A. V. Kolesnikov† and A. P. Silin‡
† Fakultät für Physik und Astronomie,
Ruhr-Universität Bochum,
Universitätsstr. 150, Bochum, Germany
‡ Tamm Theoretical Department of the
Lebedev Physical Institute, RAS,
Leninskii pr. 53, 117924, Moscow, Russia

Abstract

We study a motion of quantum particles, whose properties depend on one coordinate so that they can move freely in the perpendicular direction. A rotationally-symmetric Hamiltonian is derived and applied to study a general interface formed between two semiconductors. We predict a new type of electron states, localized at the interface. They appear whenever the two bulk dispersions intersect. These shallow states lie near the point of intersection and are restricted to a finite range of perpendicular momentum. The scattering of carriers by the interface is discussed.
I. INTRODUCTION

Highly developed methods of crystal growth allow building of mesoscopic systems with spatially varying parameters. The motion of carriers in such a system is described within the effective mass theory (EMT) by a quantum equation. Depending on the semiconductors chosen, this can be either Schrödinger-like for wide-gap materials, or Dirac-like or more complicated for narrow-gap semiconductors. Thus, there is a way to realize in practice the quantum mechanics with parameters depending on coordinates. All information about the periodic quickly varying potential of the lattice is contained in the effective mass or the “velocity of light” – the interband matrix element.

The foundation of the phenomenological EMT is based on the envelope function approximation (EFA). The total wave function is represented as the product of the Bloch function and a slowly varying envelope function; it is the latter which enters the quantum equation. The commonly used heuristic EFA exploits the fact that the interband matrix element does not change much in many important for practice III-V semiconductors. This leads to a reasonable assumption that the Bloch function can be chosen to be identical through the whole system. The resulting EMT is equivalent to the conventional quantum mechanics, e.g. the envelope function should be continuous at any heterojunction. However, the interband matrix element does vary for different semiconductors. Recently, a new exact version of the EFA was suggested, where only the total wave function has to be continuous and the envelope function does not need necessarily to fulfill this requirement.

In Ref. first evidence indicated the existence of new interface states, impossible in the conventional quantum mechanics. The further investigation revealed a novel effect for the coordinate-dependent two-band Dirac Hamiltonian: A localization can occur at a step-like potential (junction), provided that the free motion along the junction is accounted for. The envelope wave function was shown to be discontinuous for these states. In the present paper, we study an arbitrary junction of two wide-gap semiconductors. Also here, the free motion along the junction leads to binding in its perpendicular direction.

Although graded crystals with very different dependences of the effective mass $m(z)$ on the coordinate $z$ can be grown, the most attention has been drawn to abrupt heterostructures. This is probably because one does not need to use a Hamiltonian with coordinate-dependent kinetic term (see below). Instead, a problem of choosing the matching conditions (MC), connecting the wave functions on either side of a junction, is met. Usually they are derived from the requirements of the continuity of the probability and its current at the junction. These requirements, although being correct, are not constructive. Indeed, they are meaningless for matching of exponentially growing or decaying solutions as their current vanishes. On the other hand, incident and scattered waves appear in the propagating case. Two continuity equations are not enough to fix the MC and two constants of the scattering problem.

An alternative approach of deriving the MC directly from the Hamiltonian is suggested in Ref. The abrupt junction can be treated as a limiting case of a smooth one, when its “smoothness” length tends to zero. For the graded case, the Hermitian Dirac operator is derived and from it the MC are extracted. Apart of appealing to intuition, such a method is shown to be equivalent to the conventional scheme. The Dirac Hamiltonian is convenient to handle with, because it contains first-order derivatives, so that it can be easily
symmetrized and it is originally rotationally-symmetric. In the present paper, we follow the above-described approach and develop an effective way to derive Hermitian, rotationally-invariant one-band Schrödinger Hamiltonian. The MC depend on the free motion, since it is incorporated in the Hamiltonian.

The paper is organized as follows: In Sec. II, we derive the Hamiltonian and obtain from it the matching conditions. In Sec. III, the dispersion of the interface states localized at the heterojunction is found and the scattering of the carriers by the junction is discussed. Sec. IV summarizes the results.

II. ROTATIONALLY-SYMMETRIC SCHRODINGER HAMILTONIAN

We study a junction of two semiconductors with the effective masses \( m_i \) and the bandgaps \( 2\Delta_i \), dependent on one coordinate \( z, i = 1 \) for \( z < 0 \) and \( i = 2 \) for \( z > 0 \) (see Fig. 1). Since all parameters depend on \( z \) only, the free motion in the perpendicular direction \( x \) has a good quantum number \( k_\perp \) so that the wave function is \( \psi \sim \exp(ik_\perp x) \). (Hereinafter we put \( \hbar = 1. \)) Let us start with the case of vanishing free motion \( k_\perp = 0 \); we consider \( k_\perp \neq 0 \) later. The problem one immediately meets while studying a graded crystal with some function \( m(z) \) is that the kinetic term \( T = \partial_z^2/2m \) is not Hermitian. Its most general form, after symmetrization, was found\(^3\) to equal

\[
T = m^\alpha \partial_z m^\beta \partial_z m^\alpha/2 = \frac{1}{2m} \left[ \partial_z^2 - \frac{m'}{m} \partial_z + \alpha \beta \left( \frac{m'}{m} \right)^2 + \alpha \frac{m''}{m} \right], \tag{2.1}
\]

with constants \( \alpha \) and \( \beta \) such that \( 2\alpha + \beta = -1 \). Note the appearance of singular terms for abrupt junctions \( m'' \sim \delta'(z)\Delta_m \) and \( (m')^2 \sim \delta^2(z)(\Delta_m)^2 \), where \( \delta(z) \) is the Dirac delta-function and \( \Delta_m = m_2 - m_1 \). These singularities lead to a discontinuity of the wave function. Representing the wave function \( \psi(z) = \varphi(z)f(z) \) as a product of the continuous part \( f(+0) = f(-0) \) and the function \( \varphi(z) \), which jumps at the junction, \( \Delta_\varphi = \varphi(+0) - \varphi(-0) \), one obtains \( \psi' \simeq f\Delta_\varphi \delta(z) \) and \( \psi'' \simeq f\Delta_\varphi \delta'(z) + 2\Delta_\varphi \delta(z)f' \). Substituting these expressions into Eq. (2.1) and selecting the singular contributions, proportional to \( \delta'(z) \) and \( \delta^2(z) \), one finds that all the singularities in Eq. (2.1) are compensated under the following conditions: \( \Delta_\varphi /\varphi + \alpha \Delta_m /m = 0 \) and \( \alpha \beta (\Delta_m) /m - \Delta_\varphi /\varphi = 0 \). These give either \( \beta = -1 \) or \( \alpha = 0 \). Recalling that \( 2\alpha + \beta = -1 \), one notices that both possibilities lead to the same effective Hamiltonian \( T(z) = \partial_z (1/2m) \partial_z \), acting on the continuous function \( f(z) \). This form was already derived in many works\(^4\), where arguments different from ours were used.

The next step is to incorporate the free motion along the surface. Up to our knowledge, the Hermitian rotationally-symmetric form of the Schrödinger Hamiltonian has not been written yet. The only form, being simplified for \( k_\perp = 0 \) to the one-dimensional case, recovering the Laplace operator for constant \( m \), and invariant with respect to orthogonal rotations involving \( z \) and \( x \) is given by

\[
T = (\partial_z - i\lambda \partial_x) \frac{1}{2m} (\partial_z + i\lambda \partial_x), \tag{2.2}
\]

where \( \lambda = \pm 1 \). The physical meaning of the value \( \lambda \) will be elucidated later, from the comparison of the one-band and the two-band Hamiltonians. The appearance of \( \lambda \) is due
to the fact that the axial symmetry possessed by the heterojunction is broken as soon as \( k_\perp \neq 0 \). Two signs of \( \lambda \) formally account for two possible ways of writing the kinetic form symmetrically. Acting by the operator \( T \) on the function \( f = g(z) \exp(ik_\perp x) \), we derive the eigenvalue equation for the energy \( \epsilon \) and half the energy gap, \( \Delta(z) \), playing the role of the potential at \( k_\perp = 0 \):

\[
\left( \frac{1}{2m} \frac{\partial^2}{\partial z^2} - \frac{m'}{2m^2} \partial_z + \lambda \frac{m'}{2m^2} k_\perp - \frac{k_\perp^2}{2m} - \Delta + \epsilon \right) g = 0 .
\] (2.3)

The presence of the third term in Eq. (2.3), originating from the mixed derivative \( \partial_z(1/m) \partial_x \) in Eq. (2.2), will be crucial for the following discussion. Let us search for solutions of Eq. (2.3) in the form \( g = \exp[\int dz \kappa(z)] \). Far from the junction, \( z \to \pm \infty \), the second and the third terms of Eq. (2.3) vanish. The remaining terms determine the values \( \kappa_i = \pm \sqrt{2m_i(\Delta_i - \epsilon) + k_\perp^2} \), nothing else but the (imaginary) wave numbers of the two bulk semiconductors. The terms \( \kappa'/2m - \kappa m'/2m^2 + \lambda k_\perp m'/2m^2 \) prevail at the junction. To avoid unphysical discontinuities in the abrupt case, we require \( [(\kappa - \lambda k_\perp)/m]' = 0 \), recovering thus the matching conditions

\[
[(\kappa - \lambda k_\perp)/m]_1 = [(-\kappa - \lambda k_\perp)/m]_2 .
\] (2.4)

The sign of \( \kappa_1 \) and \( \kappa_2 \) is chosen in the way to ensure a localized wave function. For the case \( m = \text{const} \), these matching conditions coincide with those of Bastard\(^3\) and do not depend on \( k_\perp \).

III. INTERFACE STATES

If the energy \( \epsilon \) is measured from \( (\Delta_1 + \Delta_2)/2 \), one rewrites \( \kappa_i^2 = k_\perp^2 - 2m_i(\epsilon \pm \Delta) \), where the sign “+” corresponds to \( i = 1 \), “−” to \( i = 2 \) and \( \Delta = (\Delta_1 - \Delta_2)/2 \). Equation (2.4), together with the bulk values of \( \kappa_i \), yields

\[
\epsilon(k_\perp) = -P(m_1 + m_2) + \lambda 2k_\perp \sqrt{P} ,
\] (3.1)

where \( P = |\Delta/(m_2 - m_1)| \). To obtain Eq. (3.1) one squares Eq. (2.4), therefore it should be found which branch of Eq. (3.1) in which region represents the solution of Eq. (2.4) and corresponds to localized interface states. A simple analysis reveals that the states are localized in the region \( k_{\perp\min} < k_\perp < k_{\perp\max} \), between minimal and maximal values of \( k_{\perp\min}^2 = 4m_1^2 P \). At \( k_{\perp\max} \), the curve \( \epsilon(k_\perp) \) is tangential to the bulk dispersions \( \epsilon_i = \mp \Delta + k_\perp^2 / 2m_i \). The necessary condition for the interface states to exist is \( (m_1 - m_2)(\Delta_1 - \Delta_2) > 0 \), i.e. the bulk dispersions must intersect. The dispersion \( \epsilon(k_\perp) \), Eq. (3.1), and the bulk dispersions \( \epsilon_i \) are shown in Fig. 2 for the following parameters: \( \Delta_1 = 1.2 \text{ eV}, \Delta_2 = 1.4 \text{ eV}, m_1 = 0.01 m_0, m_2 = 0.02 m_0 \) (\( m_0 \) is the free mass of the electron).

It follows from Eq. (2.4) that \( \lambda k_\perp(m_2 - m_1) \) is positive. Recalling that the signs of \( \lambda \) “+” and “−” originate from two possible ways of writing the Hamiltonian (2.2), we conclude that the opposite signs in Eq. (2.4) correspond to localized states for positive and negative \( k_\perp \). That is, if \( m_2 > m_1 \), then \( k_\perp > 0 \) is localized for \( \lambda = +1 \) in Eq. (2.2) and \( k_\perp < 0 \) is localized for \( \lambda = -1 \). The signs in Eq. (3.1) have to be chosen accordingly.
Since both values of $\lambda = \pm 1$ are equivalent, the degeneracy of bulk dispersion of the Schrödinger Hamiltonian with respect to the sign of $k_\perp$ is preserved for the localized states: $\epsilon(k_\perp) = \epsilon(-k_\perp)$. This differs for the two-band model with the non-relativistic Dirac Hamiltonian $\mathcal{H}$, where the eigenvalues of energy $\epsilon$ are classified (apart of momentum $k_\perp$) by eigenvalues of helicity $\lambda = \pm 1$. Here, the initial degeneracy of the bulk dispersion is lifted for the interface states: $\epsilon_\lambda(k_\perp) = \epsilon_{-\lambda}(-k_\perp)$. It is not difficult to check that the Klein-Gordon equation, obtained in the two-band model, contains the kinetic term analogous to Eq. (2.2). Thus, the value $\lambda$ in Eq. (2.2) corresponds to helicity in the two-band model. In discussing further similarities of the one- and two-band description, it is worth noticing following: Although qualitatively the dispersion of the interface states is similar in both models, corresponding to localized states between tangency points with the two bulk dispersions, the dispersion in the two-band model is nonlinear due to different bulk spectrum.

Let us now briefly discuss the scattering of carriers by the interface. Like for the bound states, it is convenient to represent the wave function in the form $g(z) = \exp[\pm i \int dz \kappa(z)]$. Then for $z < 0$ it will be the sum of incident and reflected waves $g = \exp[i \int dz \kappa_1(z)] + B \exp[-i \int dz \kappa_1(z)]$ and for $z > 0$ the transmitted wave is $g = A \exp[i \int dz \kappa_2(z)]$, where $\kappa_i^2 = 2m_i(\epsilon \pm \Delta) - k_\perp^2$. The condition of continuity of the wave function $g$ yields $1 + B = A$ and the analog of Eq. (2.4) reads $[(k_\perp + i\kappa)/m + B(k_\perp - i\kappa)/m]_1 = A[(k_\perp + i\kappa)/m]_2$. The transmission coefficient $D(\epsilon) = |A|^2\kappa_2/\kappa_1$ is given by

$$D(\epsilon) = 4\kappa_1\kappa_2m_2^2/[k_1^2(m_1 - m_2)^2 + (\kappa_1m_2 + \kappa_2m_1)^2].$$

Far away from the point of intersection, $k_\perp^2 \ll 4m_1m_2P$ or $k_\perp^2 \gg 4m_1m_2P$, function $D(\epsilon)$ vanishes as square root as the energy tends to its threshold value (one of the bulk dispersions): $D(\epsilon) \sim \kappa_i$. On the other hand, near the point of intersection, $k_\perp^2 \approx 4m_1m_2P$, the function $D(\epsilon)$ vanishes linearly: $D(\epsilon) \sim \epsilon - (m_1 + m_2)P$. This behaviour is typical for the conventional quantum mechanics: the coefficient of penetration $D(\epsilon)$ is governed by the asymptotic behavior of the potential $U(z)$ only. If the value $U(+\infty) - U(-\infty)$ is zero than $D(\epsilon)$ is linear at the penetration threshold. In the opposite case it vanishes as square root.

**IV. CONCLUSIONS**

It is worth emphasizing that it is the free motion along the junction, which leads to the effects discussed. Although for $k_\perp = 0$ we have a step-like potential $U(z) = \Delta_i$, its role for $k_\perp \neq 0$ is taken over by some more complicated function $U^\pm(z, k_\perp)$. Substituting into Eq. (2.3) $g(z) = m^{1/2}y(z)$, we obtain a Schrödinger equation for the function $y(z)$ with the potential

$$U^\pm(z, k_\perp) = 3m^2/8m^3 - m''/4m^2 - \lambda k_\perp m'/2m^2 + k_\perp^2/2m + \Delta.$$

The potential $U^\pm$ for $m(z) = (m_1 + m_2)/2 + (m_2 - m_1) \tan(z/l)/2$ with the smoothness parameter $l$ is presented in Fig. 3 as a function of $z$ for several values of $k_\perp$ and $l$. The asymptotic behavior of the potential is preserved for any smooth $m(z)$, $U(\pm\infty) = \Delta_i + k_\perp^2/2m_i$. If the bulk dispersions intersect, then at $k_\perp$, corresponding to the point of intersection, we
have no step in the potential any more: \( U(+\infty) = U(-\infty) \). As it is known from quantum mechanics, any potential with this property and containing a well, has at least one localized level. This level becomes shallow, if the potential changes rapidly, \( l \to 0 \), (e.g. a \( \delta \)-function). For the abrupt potential, the part of the well is played by the matching conditions Eq. (2.4). For \( k_\perp \neq 0 \) and small \( \kappa_i \), i.e. near the intersection point of the bulk dispersions, Eq. (2.4) has a solution, describing a shallow level. The scattering by the junction is interpreted analogously.

The states considered lie above the band edge, being embedded in the continuum spectrum. However, they are real localized states, not resonant ones, since they lie in the energy gap of the whole system: Their energies are below the bulk dispersions, corresponding to the same value of \( k_\perp \). Naturally, many-particle effects, due to e.g. impurities and the boundary roughness could strongly affect these states. However, qualitatively it is clear that as long as these can be treated as elastic scatterer, the states preserve because in our analysis the absolute value of \( k_\perp \) was essential, but not its direction.

In summary, we have derived a rotationally-invariant effective one-band Hamiltonian, which mass depends on one coordinate. We applied it to derive the matching conditions for a single general junction of two semiconductors. They depend on the free motion along the junction, due to its mixing with the motion in the direction of growth. If the bulk dispersions of the two semiconductors intersect, then shallow localized states occur. The problem studied can be classified as an example of weak localization. The essential condition for the existence of the states, the intersection of the bulk dispersion curves, holds for a large variety of semiconductors. Although more investigation is needed to understand in detail the many-particle effects, we believe that the states are not crucially sensitive to them.

V. ACKNOWLEDGEMENTS

We are indebted to K. B. Efetov and S. G. Tikhodeev for useful discussions. APS was supported in part by the Russian Foundation for the Fundamental Research under projects No. 96-02-16701, 97-02-16346, by Russian Science Ministry under project No. 97-1087, INTAS 96-0398. AVK acknowledges a support from the Sonderforschungsbereich 237 “Unordnung und grosse Fluktuationen”.

6
REFERENCES

1 G. Bastard, J. A. Brum, and R. Ferreira, *Solid State Physics* Vol. 44 ed. H. Ehrenreich and D. Turnbull (Academic Press, London) (1991).
2 G. Bastard, *Wave mechanics applied to semiconductor heterostructures* (Les Éditions de Physique, Les Ulis) (1996).
3 D. L. Partin and J. Hermans, *Handbook of semiconductors*, ed. S. Mahajan, Vol. 3a, (North-Holland, Amsterdam) (1994).
4 M. G. Burt, *Semicond. Sci. Technol.*, 2 460 (1987); 3 739 (1988); 3 1224 (1988); *J. Phys.: Cond. Matter*, 4 6651 (1992).
5 S. G. Tikhodeev, *Solid State Commun.*, 78 339 (1991).
6 A. V. Kolesnikov, R. Lipperheide, A. P. Silin and U. Wille *Euro. Phys. Lett.*, 43 331 (1998).
7 R. A. Morrow and K. R. Brownstein, *Phys. Rev. B*, 30 678 (1984).
8 R. A. Morrow, *Phys. Rev. B*, 35 8074 (1987).
9 G. T. Einevoll and P. G. Hemmer, *J. Phys. C*, 21 L1193 (1988).
10 I. Galbraith and G. Duggen, *Phys. Rev. B*, 38 10057 (1988).
11 J. Thompson, G. T. Einevoll, and P. C. Hemmer, *Phys. Rev. B*, 39 12783 (1989).
12 A. Brezini and N. Zekri, *Sol. State Commun.*, 86 613 (1993).
13 G. Bastard, *Phys. Rev. B*, 24 (1981) 5693; *ibid.*, 25 (1982) 7584.
14 A. V. Kolesnikov and A. P. Silin *J. Phys.: Cond. Matt.*, 9 10929 (1997).
15 L. D. Landau and E. M. Lifshitz, *Quantum Mechanics*, Pergamon Press, Oxford (1977).
FIGURE CAPTIONS

Figure 1. Band-edge profile of an heterojunction. The energy gap is shaded. Because of symmetry, only the region of energy near the conduction bands is studied.

Figure 2. Dispersion $\epsilon(k_{\perp})$, Eq. (3.1), of the system shown in Fig. 1 (solid curve; for parameters, see text). Dotted curves: bulk dispersions $\epsilon_{1,2}(k_{\perp})$. Energy is measured from the middle of the bandgap. States are localized between tangency points $k_{i\perp}$ with the two bulk dispersions (heavy solid line). It is understood that similar curves occurs for $k_{\perp} < 0$ and near the valence band.

Figure 3. Effective potential $U^\pm$, Eq. (4.1), of the smooth junction; for parameters: 1) $k_{\perp} = 10^6$ cm$^{-1}$, $l = 1.5 \times 10^5$ cm$^{-1}$; 2) $k_{\perp} = 5 \times 10^6$ cm$^{-1}$, $l = 1.5 \times 10^5$ cm$^{-1}$; 3) $k_{\perp} = 5 \times 10^6$ cm$^{-1}$, $l = 10^5$ cm$^{-1}$; 4) $k_{\perp} = 6.2 \times 10^6$ cm$^{-1}$, $l = 1.5 \times 10^5$ cm$^{-1}$. Note appearance of a barrier for $\lambda = -1$, $U^-$ (curve 5); parameters are the same as for curve 2.
Figure 1
Figure 2
Figure 3