Modified Schrödinger equation including nonparabolicity for the study of a two-dimensional electron gas

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(Received 30 December 1992)

A modified Schrödinger equation has been obtained for calculating the energy–wave-vector dispersion relationship of the two-band Kane model and has been applied to the case of a two-dimensional electron gas. The equation is applicable when the isoenergetic surfaces are not spheres and it is expressed as an infinite series whose summation provides compact solutions. With this equation, the transverse energy levels can be obtained by using an effective mass which is independent of the transverse energy, but there is a dependence of these energy levels on the parallel energy. The boundary conditions associated with the modified Schrödinger equation have been derived by imposing the continuity of the eigenfunction and the probability current, and they have been applied to the calculation of the energy levels in an infinite and a finite square quantum well.

I. INTRODUCTION

Nonparabolicity effects in quantum wells have received a great deal of attention in recent years. The reason for this interest rests with the fact that electron levels can be some tenths of an electron volt above the bulk-conduction-band edge and therefore the $E - k$ dispersion relationship deviates from parabolic behavior. Nonparabolicity has been included in the $E - k$ dispersion relationship by expressing the energy as a series expansion in wave-vector powers:

$$
\varepsilon = \frac{\hbar^2 k^2}{2m^*} \left[ a_1 + a_2 k^2 + a_3 k^4 + a_4 k^6 + \cdots \right]
$$

or by expressing the wave vector as a series expansion in energy powers:

$$
\frac{\hbar^2 k^2}{2m^*} = \varepsilon (1 + \alpha \varepsilon + \beta \varepsilon^2 + \gamma \varepsilon^3 + \cdots),
$$

where $\varepsilon$ is the energy measured from the band edge, $k$ is the wave vector taking the coordinate origin at the band edge, and $m^*$ is the band-edge effective-mass tensor. The left-hand side of expression (2) must be interpreted as the application of the reciprocal-mass tensor to the wave vector $[k(1/m^*)k]$. If the correction due to nonparabolicity is not too large, expressions (1) and (2) are usually truncated at the second term. In the first case an equation up to order $k^4$ is obtained, which is useful because it can provide a modified Schrödinger equation directly by using the Luttinger-Kohn formulation. In this case, the correction due to nonparabolicity can be included with only one parameter, thus resulting in the well-known two-band Kane model. An expression up to order $k^4$ with additional terms that uses more than one parameter to represent the nonparabolicity corrections has also been obtained. In these models it has been questioned whether the effective mass must be dependent or independent on the energy, and there is no agreement on the mass and boundary conditions that must be used.

On the other hand, when expression (2) is truncated, the $E - k$ dispersion relationship for the two-band Kane model is expressed in the form

$$
\varepsilon (1 + \alpha \varepsilon) = \frac{\hbar^2 k^2}{2m^*}.
$$

An advantage of this model is its simplicity, since all the corrections of nonparabolicity are contained in one coefficient $\alpha$. Furthermore, the application of the effective-mass tensor remains unaltered and the correction is made on a scalar magnitude. These characteristics make this model very useful for simulation applications even for bands with nonspherical isoenergetic surfaces. The two-band Kane model, with an appropriate value for the nonparabolicity coefficient $\alpha$, is accurate enough in many cases of interest and, in any case, can be used to extract qualitative conclusions about nonparabolicity effects. Nevertheless, it is not the aim of this paper to discuss the suitability of expression (3), but to analyze some of its physical consequences in the study of a two-dimensional electron gas. One of the effects is that the parallel and transverse energies in a quantum well cannot be separated and the simple decoupling of the perpendicular and parallel motions is not possible, as pointed out by Ekemberg. This conclusion is supported by the model from expression (3) because, in this case, the energy does not depend on the wave-vector polynomial:

$$
\varepsilon = \frac{1}{2\alpha} \left[ 1 + \frac{4\alpha \hbar^2 k^2}{2m^*} \right]^{1/2} - 1.
$$

Given that the use of expression (3) is only justified when deviations from parabolicity are not too high, since large values of the moment would lead to a nonphysical description of the conduction band, it is possible to expand expression (4) in wave-vector powers up to the $k^4$ order, with a resulting expression similar to that dealt
with in Refs. 6 and 8. Nevertheless, we do not truncate this expression since we are interested in the exact model given in expression (3), and the truncation of the expansion of equation (4) prevents the further summation of the series.

In this paper we have obtained a modified Schrödinger equation according to expression (3) and have discussed the consequences of this equation. We have obtained the associated boundary conditions and applied them to the analysis of an infinite and a finite square quantum well.

II. MODIFIED SCHRODINGER EQUATION

If the $E-k$ relationship in not strictly parabolic, all the effects of the periodic potential of the lattice are not contained in the effective mass and the eigenfunctions cannot be strictly approximated by plane waves. Nevertheless, in order to obtain the relationship given in expression (3), we can modify the Schrödinger equation (instead of modifying the eigenfunctions) by substituting the quasimoment by the moment operator, $k \rightarrow i \nabla$, according to the Luttinger-Kohn approximation. To do so, the series expansion of expression (4) gives the following equation for the kinetic energy:

$$\varepsilon = \frac{1}{2\alpha} \sum_{n=1}^{\infty} \left[ \frac{1}{n} \right] \left[ 4\alpha \frac{\hbar^2}{2m^*} \right]^n.$$

By substituting the wave vector and using the effective-mass approximation, the Schrödinger equation can then be rewritten including the effects of the periodic lattice potential in the effective mass and maintaining the external potential $U(r)$:

$$\frac{1}{2\alpha} \sum_{n=1}^{\infty} \left[ \frac{1}{n} \right] \left[ -4\alpha \frac{\hbar^2}{2} \right]^{n-1} \left[ \frac{\nabla^2}{m^*} \right]^n \psi(r) + U(r)\psi(r) = \varepsilon \psi(r),$$

where $\psi(r)$ is the wave function. In this equation the reciprocal effective-mass tensor is still maintained and is applied to the nabla operator according to $\nabla^2/m^* = [\nabla(1/m^*) \nabla]$. In Eq. (6) only the band-edge mass appears, in agreement with the suggestion of Persson and Cohen that the mass present in the modified Schrödinger equation does not depend on the eigenvalues of the same equation.

When the external potential is one dimensional, $U(r) = V(z)$, we can make the ansatz equal to

$$\psi(z) = \xi(z)e^{i(k_x x + k_y y)}$$

where we have made the assumption that the $z$ axis is along one of the symmetry axes of the effective-mass tensor. $m_x$, $m_y$, and $m_z$ are the components of the effective-mass tensor along its symmetry axes. By taking into account the following equality:

$$\left[ \frac{1}{m^*} \nabla^2 \right]^{n-1} e^{i(k_x x + k_y y)} =$$

between the total energy and the parallel energy

$$\varepsilon_z \equiv \varepsilon - \varepsilon_{||},$$

so that the one-dimensional Schrödinger equation reduces to

$$\frac{1}{2\alpha} \sum_{n=1}^{\infty} \left[ \frac{1}{n} \right] \left[ -4\alpha \frac{\hbar^2}{2} \right]^{n-1} \sum_{l=1}^{n} \left[ \frac{1}{m^*} \frac{\partial^2 \xi(z)}{\partial z^2l} \right]_{l=1}^{n} \left[ \frac{k_x^2}{m_x} - \frac{k_y^2}{m_y} \right]_{n-1} =$$

By changing the summation order, according to $\sum_{n=1}^{\infty} \sum_{l=1}^{n} = \sum_{l=1}^{\infty} \sum_{n=l}^{\infty}$, making the substitution $n-l = r$ and using the equalities

$$\left[ \frac{1}{n} \right] \left[ \frac{1}{r} \right] = \left[ \frac{1}{l} \right] \left[ \frac{1}{r} \right]$$

We can also define the transverse energy as the difference and

$$\varepsilon_{\perp} = \frac{k_x^2}{m_x} + \frac{k_y^2}{m_y}.$$
\[
\sum_{r=0}^{\infty} \frac{1}{r!} \left( \frac{k^2}{m_x + \frac{k^2}{m_y}} \right)^r = \left( 1 + 4\alpha \frac{\mathbf{r}^2}{2m_x(1 + 2\alpha \varepsilon_\parallel)} \right)^{-1/2}.
\]

Equation (14) is the modified one-dimensional Schrödinger equation that allows the determination of \( \varepsilon_z \) for a fixed parallel energy. It reduces to the normal Schrödinger equation in the \( \alpha = 0 \) limit.

In the special case where \( V(z) \) is uniform, we can obtain an analytical solution for Eq. (14). We have considered two cases.

(a) \( \varepsilon_z > V \): The solution of Eq. (14) is
\[
\tilde{\zeta}(z) = Ae^{ik_z z} + Be^{-ik_z z}
\]
and we obtain the following expression for the energy:
\[
(\varepsilon_z - V)[1 + 2\alpha \varepsilon_\parallel + \alpha(\varepsilon_z - V)] = \frac{\mathbf{r}^2k_z^2}{2m_z}.
\]

(b) \( \varepsilon_z < V \): This is a special case of interest for determining appropriate boundary conditions. In this case we could also solve Eq. (14) taking the solution given by
\[
\tilde{\zeta}(z) = Ae^{\varepsilon_z z} + Be^{-\varepsilon_z z}
\]
and deriving a relation between \( \varepsilon_z \) and \( \kappa_z \). Nevertheless, it has been claimed that different Hamiltonians are required to describe wave functions in a quantum well and wave functions extending into a barrier. When the energy is lower than the potential, the energy \( \varepsilon_z \) in expression (14) must be substituted by \( V - \varepsilon_z \), and \( ik_z \) must be changed for the reciprocal-penetration length \( \kappa_z \). Therefore, instead of Eq. (14) we would obtain
\[
(\varepsilon_z - V)[1 + 2\alpha \varepsilon_\parallel + \alpha(\varepsilon_z - V)] = \frac{\mathbf{r}^2k_z^2}{2m_z}.
\]

Equation (18) also reduces to the normal Schrödinger equation in the \( \alpha = 0 \) limit, and the left-hand side can be interpreted as minus the kinetic energy. When the function given in expression (17) is substituted into Eq. (18), a relation between \( \kappa_z \) and the energy is obtained:
\[
(V - \varepsilon_z)[1 + 2\alpha \varepsilon_\parallel + \alpha(V - \varepsilon_z)] = \frac{\mathbf{r}^2k_z^2}{2m_z}.
\]
FIG. 1. Ground-state level of an infinite well with \(\alpha = 0.7\) and a ground-state level in the parabolic case of \(\varepsilon_{00} = 100\) meV (this corresponds to a well width about 74 Å for \(m_z = 0.067 m_0\)) represented vs parallel energy. Curve (1) corresponds to expression (22), where all the terms of expression (6) have been considered, and curve (2) shows the values of the ground-state level with only the first two terms of the series.

IV. BOUNDARY CONDITIONS

When nonparabolic corrections are included, there exist different ways of introducing boundary conditions.\(^1\)\(^7\)

The boundary conditions that we have applied are a continuity of the envelope function \(\zeta(z)\) and a continuity of the probability current \(j(z)\).\(^4\) To do this, it has been necessary to obtain an expression for the probability current in the nonparabolic case with the two-band Kane model. We have distinguished between the following two cases.

(a) \(\varepsilon_z > V\): We started with the continuity equation written as

\[
\frac{dj}{dz} = \frac{i}{\hbar} \left( \xi^* H \xi - \xi H \xi^* \right) .
\] (26)

We substituted the Hamiltonian \(H\) by the modified Hamiltonian given in Eq. (14) and we have the next equality:

\[
\xi^* \frac{d^{2l+1} \xi}{dz^{2l+1}} - \xi \frac{d^{2l+1} \xi^*}{dz^{2l+1}} = \frac{d}{dz} \sum_{k=0}^{2l-1} (-1)^k \frac{d^{k+1} \xi}{dz^{k+1}} \frac{d^{2l-k-1} \xi^*}{dz^{2l-k-1}} ,
\] (27)

obtaining an expression for \(j\) that verifies expression (26):

\[
j = \frac{i}{\hbar} \frac{1 + 2 \alpha \varepsilon_z}{2 \alpha} \sum_{l=1}^{\infty} \left[ \frac{1}{l} \left( -4 \alpha \frac{\hbar^2}{2 m_z (1 + 2 \alpha \varepsilon_z)^2} \right)^l \right] \times \sum_{k=0}^{2l-1} (-1)^k \frac{d^{k+1} \xi}{dz^{k+1}} \frac{d^{2l-k-1} \xi^*}{dz^{2l-k-1}} .
\] (28)

If the terms in the summation for \(k\) in expression (28) are separated in two different summations, one of them for even \(k\) and the other for odd \(k\), the two resulting summations are conjugate (and with opposite signs). Thus we can ensure the continuity of expression (28) if we impose the continuity of one of the summations. The magnitude whose continuity we have imposed is

\[
j_z = \frac{i}{\hbar} \frac{1 + 2 \alpha \varepsilon_z}{2 \alpha} \sum_{l=1}^{\infty} \left[ \frac{1}{l} \left( -4 \alpha \frac{\hbar^2}{2 m_z (1 + 2 \alpha \varepsilon_z)^2} \right)^l \right] \times \sum_{k=0}^{l-1} \frac{d^{k+1} \xi}{dz^{k+1}} \frac{d^{2l-k-1} \xi}{dz^{2l-k-1}} .
\] (29)

Expression (29) gives an interesting result in the case where the solution of Eq. (14) takes the form of expression (15). In this case all the terms of the summation for \(k\) index in expression (29) are the same. Using the equality

\[
2l \begin{pmatrix} \frac{1}{2} \\ l \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} \\ l-1 \end{pmatrix} ,
\] (30)

we obtain

\[
j_z = \frac{\hbar}{2i m_z (1 + 2 \alpha \varepsilon_z)} \left[ 1 + 4 \alpha \frac{\hbar^2 k_z^2}{2 m_z (1 + 2 \alpha \varepsilon_z)^2} \right]^{-1/2} \xi \frac{d \xi}{dz} .
\] (31)

Since we also impose the continuity of \(\xi^*\), the continuity of the probability current is guaranteed if the expression

\[
\frac{1}{m_z (1 + 2 \alpha \varepsilon_z)} \left[ 1 + 4 \alpha \frac{\hbar^2 k_z^2}{2 m_z (1 + 2 \alpha \varepsilon_z)^2} \right]^{-1/2} \frac{d \xi}{dz}
\] (32)

is continuous.

(b) \(\varepsilon_z < V\): In this case, we substitute \((-H)\) in the continuity equation (26) according to Eq. (18), obtaining

\[
j = -\frac{i}{\hbar} \frac{1 + 2 \alpha \varepsilon_z}{2 \alpha} \sum_{l=1}^{\infty} \left[ \frac{1}{l} \left( \frac{\hbar^2}{2 m_z (1 + 2 \alpha \varepsilon_z)^2} \right)^l \right] \times \sum_{k=0}^{l-1} \frac{d^{k+1} \xi}{dz^{k+1}} \frac{d^{2l-k-1} \xi}{dz^{2l-k-1}} ,
\]

and in the case of the solution of Eq. (18) taking the form of expression (17), the function whose continuity we have to impose is

\[
\frac{1}{m_z (1 + 2 \alpha \varepsilon_z)} \left[ 1 + 4 \alpha \frac{\hbar^2 k_z^2}{2 m_z (1 + 2 \alpha \varepsilon_z)^2} \right]^{-1/2} \frac{d \xi}{dz} .
\] (33)

V. FINITE SQUARE WELL

We have also applied the equations obtained to the case of a finite square well

\[
V(z) = \begin{cases} 0 & \text{for } |z| < w \\ U_0 & \text{otherwise} . \end{cases}
\] (34)

By solving Eqs. (14) and (18) we find two types of functions.

(a) Even eigenfunctions:

\[
\xi(z) = \begin{cases} A \cos(k_z z) & \text{for } |z| < w \\ B e^{-k_z z} & \text{for } z > w \\ B e^{k_z z} & \text{for } z < -w . \end{cases}
\] (35)
We have substituted expression (35) in Eqs. (14) and (18), obtaining
\[
e_{z} = \frac{1+2\alpha_{w}e_{\parallel}}{2\alpha_{w}} \left[ \frac{\hbar^{2}k_{z}^{2}}{1+4\alpha_{w}m_{w}(1+2\alpha_{w}e_{\parallel})^{2}} \right]^{1/2} - 1
\]
and
\[
U_{0} - e_{z} = \frac{1+2\alpha_{b}e_{\parallel}}{2\alpha_{b}} \times \left[ \frac{\hbar^{2}k_{z}^{2}}{1+4\alpha_{b}m_{b}(1+2\alpha_{b}e_{\parallel})^{2}} \right]^{1/2} - 1
\]
where \(\alpha_{w}\) and \(m_{w}\) are, respectively, the nonparabolicity coefficient and the \(z\)-directed effective mass in the well, and \(\alpha_{b}\) and \(m_{b}\) are the values of these two coefficients in the barrier (\(|z| > w\)). If the continuity of function \(\xi(z)\) and the functions given in expressions (31) and (33) is imposed, the following result is obtained:
\[
tg(k_{z}w) = \frac{m_{w}k_{z}}{m_{b}} \left[ \frac{\hbar^{2}k_{z}^{2}}{1+2\alpha_{w}m_{w}(1+2\alpha_{w}e_{\parallel})^{2}} \right]^{1/2} \times \left[ \frac{1+2\alpha_{w}m_{w}(1+2\alpha_{w}e_{\parallel})^{2}}{1+2\alpha_{b}m_{b}(1+2\alpha_{b}e_{\parallel})^{2}} \right].
\]

(b) Odd eigenfunctions:
\[
A \sin(k_{z}z) \quad \text{for} \quad |z| < w
\]
\[
B e^{-k_{z}z} \quad \text{for} \quad z > w
\]
\[
B e^{k_{z}z} \quad \text{for} \quad z < -w.
\]

The relation between \(k_{z}, \kappa_{z}\), and the energy is given by expressions (36) and (37), respectively. The application of the boundary conditions gives, in this case
\[
-tg^{-1}(k_{z}w) = \frac{m_{w}k_{z}}{m_{b}} \left[ \frac{\hbar^{2}k_{z}^{2}}{1+2\alpha_{w}m_{w}(1+2\alpha_{w}e_{\parallel})^{2}} \right]^{1/2} \times \left[ \frac{1+2\alpha_{w}m_{w}(1+2\alpha_{w}e_{\parallel})^{2}}{1+2\alpha_{b}m_{b}(1+2\alpha_{b}e_{\parallel})^{2}} \right].
\]

In order to illustrate the results of the model, we have applied expressions (35)-(40) to a two-dimensional electron gas contained in a quantum well with the conduction-band step and effective masses typical of the Al_{0.35}Ga_{0.65}As/GaAs structure: \(\Delta E_{C} = 0.3\) eV, \(m_{w} = 0.067m_{0}\), and \(m_{b} = 0.09m_{0}\), where \(m_{0}\) is the free-electron mass, but for different values of the nonparabolicity coefficients. The values obtained for the ground- and first excited-state levels, \(e_{z} = E_{0}\) and \(e_{z} = E_{1}\), as a function of \(\alpha_{w}\) are represented in Figs. 2(a) and 2(b), respectively. The minima of the subbands (\(e_{z} = 0\)) are shown for \(\alpha_{w} = 0\) (dashed line) and \(\alpha_{b} = \alpha_{w}\) (dotted line). The curves shown in solid lines correspond to the values of \(e_{z}\) obtained with \(\alpha_{b} = \alpha_{w}\) and \(e_{z} = 0.3\) eV. In Fig. 3 the deviations of \(E_{0}\) and \(E_{1}\) from the parabolic case are plotted against the width of the well \(2w\) for \(\alpha_{w} = 0.7\) eV. The three cases shown correspond to \(\alpha_{b} = 0\) and \(e_{z} = 0\) (dashed line), \(\alpha_{b} = \alpha_{w}\) and \(e_{z} = 0\) (dotted line), and \(\alpha_{b} = \alpha_{w}\) and \(e_{z} = 0.3\) eV (solid line). Only for \(E_{0}\) in the case \(\alpha_{b} = 0\) do we obtain an increase in the transverse energy produced by the nonparabolicity, as found by Nelson, Miller, and Kleinman.\(^{5}\) In the remaining cases we always find a decrease in \(e_{z}\), as in the infinite well case. This result might be different if we use Eq. (14) for \(e_{z} < V\) and different boundary conditions, but the dependence of \(e_{z}\) on the parallel energy is maintained in any case. The equation can easily

FIG. 2. Values of the ground- and first excited-state levels vs the coefficient of nonparabolicity in the well \(\alpha_{w}\) obtained for a quantum well with the following characteristics: \(\Delta E_{C} = 300\) meV, \(m_{w} = 0.067m_{0}\), and \(m_{b} = 0.09m_{0}\). The ground-state level \(e_{z} = E_{0}\) is shown in (a) and the first excited-state level \(e_{z} = E_{1}\) is shown in (b). The three curves have been obtained with \(\alpha_{b} = 0, e_{z} = 0\) (dashed line); \(\alpha_{b} = \alpha_{w}, e_{z} = 0\) (dotted line); and \(\alpha_{b} = \alpha_{w}, e_{z} = 0.3\) eV (solid line).

FIG. 3. Values for the deviation of the ground- and first excited-state levels from the parabolic case vs the width of the well, obtained for a quantum well with the same characteristics as that in Fig. 2. The deviation of the ground-state level is shown in (a) and the deviation of the first excited-state level is shown in (b). The three curves have also been obtained with \(\alpha_{b} = 0, e_{z} = 0\) (dashed line); \(\alpha_{b} = \alpha_{w}, e_{z} = 0\) (dotted line); and \(\alpha_{b} = \alpha_{w}, e_{z} = 0.3\) eV (solid line).
be applied to a well or a barrier with arbitrary shapes if they are approximated by stepped potentials, as done in Ref. 11.

VI. CONCLUSIONS

We have obtained a modified Schrödinger equation that gives the energy–wave-vector dispersion relationship of the two-band model of expression (3). The equation contains infinite terms which are all maintained in order to achieve compact solutions by summing the series. With this equation the transverse energy levels can be obtained by using an effective mass which is independent of the transverse energy, but there is a dependence of these energy levels on the parallel energy. This dependence must be taken into account when the model of expression (3) is used in transport simulations of a two-dimensional electron gas. The boundary conditions associated with the modified Schrödinger equation have been derived by imposing the continuity of the probability current and they have been applied to the calculation of the energy levels in a finite square quantum well. Only for the ground-state level, when the nonparabolicity of the barrier is ignored, have we obtained an increase in the transverse energy produced by the nonparabolicity. In all other cases we always find a decrease in the transverse energy. The equation can easily be applied to a well or a barrier with arbitrary shapes using the formalism of step potentials.

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