Model effective-mass Hamiltonians for abrupt heterojunctions and the associated wave-function-matching conditions

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We consider a class of Hermitian effective-mass Hamiltonians whose kinetic energy term is $(m^{\alpha}\hat{p}m^{\beta}\hat{p}m^{\gamma}+m^{\gamma}\hat{p}m^{\beta}\hat{p}m^{\alpha})/4$ with $\alpha+\beta+\gamma=-1$. We apply these Hamiltonians to an abrupt heterojunction between two crystals and seek the matching conditions across the junction on the effective-mass wave function (ψ) and its spatial derivative ($\dot{\psi}$). For $\alpha\neq\gamma$ we find that the wave function must vanish at the junction thus implying that the junction acts as an impenetrable barrier. Consequently, the only viable cases are for $\alpha=\gamma$ where we show that $m^{\alpha}\psi$ and $m^{\alpha+\beta}\dot{\psi}$ must be continuous across the junction.

I. INTRODUCTION

Effective-mass theory (EMT) has been used to calculate physical quantities in crystals when the desired accuracy did not justify the use of a more complete theory.[1] Although originally[2] developed to treat impurities in an otherwise perfect crystal, EMT has been extended to crystals whose chemical composition changes from region to region—the so-called graded crystals.[3–6] The new feature appearing in these latter applications is that the effective mass, which depends on the local crystalline properties, varies with position. When the grading is slow the effective-mass equation can be derived in a reasonably satisfactory way starting from a Bloch- or Wannier-function formalism. When the grading is abrupt, as in a heterojunction, no satisfactory derivation of EMT exists.

One of the problems in using EMT in graded crystals, where the carrier mass is position dependent, is to decide how to write the Hamiltonian. No derivation exists which leads to a unique form for the kinetic energy operator. Several expressions were suggested and arguments were put forward to support them. These expressions include

$$\hat{T}=\left[\frac{1}{m}\hat{p}^{2}+\hat{p}^{2}\frac{1}{m}\right]\Big/4$$

by Gora and Williams,[3]

$$\hat{T}=\left[\hat{p}\frac{1}{m}\hat{p}\right]\Big/2$$

by von Roos,[6] and

$$\hat{T}=\left[\frac{1}{\sqrt{m}}\hat{p}^{2}\frac{1}{\sqrt{m}}\right]\Big/2$$

by Zhu and Kroemer,[7] all of which have the general form

$$\hat{T}=\tfrac{1}{4}(m^{\alpha}\hat{p}m^{\beta}\hat{p}m^{\gamma}+m^{\gamma}\hat{p}m^{\beta}\hat{p}m^{\alpha}),\quad \alpha+\beta+\gamma=-1\ , \qquad (1)$$

suggested by von Roos.[6]

These operators are Hermitian, but none have been derived uniquely within the context of a single-particle theory. Actually, in slowly graded crystals the distinction between the different operators in Eq. (1) is not important, since the derivations of EMT there are valid only when the chemical composition changes appreciably over a distance that is large in comparison to a lattice constant; all operators of the type in Eq. (1) are equivalent in that limit.[8]

In treatments of abrupt heterojunctions the situation is more confused. Instead of trying to derive the correct form of the kinetic energy operator (if indeed one exists) from a single-particle theory, attention has been directed at the closely related problem of determining the matching conditions on the effective-mass wave function and its derivative across the heterojunction. The two problems are related. Away from the junction the effective mass is constant, and thus Eq. (1) simplifies to standard form in these regions. Only at the junction does the specific form of Eq. (1) become important, and only then to determine the matching conditions which follow uniquely from it. There is no agreement in the literature, however, as to what the matching conditions should be. Some workers such as Zhu and Kroemer[7] suggest matching conditions that involve a free parameter to be determined by experiment in individual cases. Thus the question of just how to treat abrupt heterojunctions in EMT is still open.

The purpose of the present work is to study Hamiltonians constructed using the kinetic energy operator of Eq. (1) when applied to abrupt heterojunctions. That is, we adopt an effective-mass Hamiltonian based on Eq. (1) and determine the matching conditions on the wave function. Our result is that only single-term Hamiltonians with $\alpha=\gamma$ are viable, and for them both $m^{\alpha}\psi$ and $m^{\alpha+\beta}\dot{\psi}$ must be continuous across the abrupt heterojunction. We are thus able to reject certain model Hamiltonians for abrupt heterojunctions that might otherwise seem possible. Our discussion is limited to one dimension, but can be generalized to three dimensions.

II. MODEL HAMILTONIAN

We consider an abrupt heterojunction located at $x=0$ between two crystals. The parameters relating to the crystal lying in the region $x<0$ ($x>0$) will be denoted by the subscript $-(+)$. The Hamiltonian we adopt uses the kinetic energy operator of Eq. (1) and leads to the eigenvalue problem

$$\tfrac{1}{4}(m^{\alpha}\hat{p}m^{\beta}\hat{p}m^{\gamma}+m^{\gamma}\hat{p}m^{\beta}\hat{p}m^{\alpha})\psi+V\psi=E\psi \ , \tag{2}$$

with $\alpha+\beta+\gamma=-1$. Here both m and V are allowed to have finite discontinuities at $x=0$, but are well behaved otherwise.

Equation (2) is readily rewritten as ($\partial_x\equiv\partial/\partial x$)

$$m^{\alpha}\partial_x m^{\beta}\partial_x m^{\gamma}\psi+m^{\gamma}\partial_x m^{\beta}\partial_x m^{\alpha}\psi=-k^2\psi+U\psi\equiv R(x) \ , \tag{3}$$

and we model m and U as[9]

$$m^{\sigma}(x)=m_-^{\sigma}+(\Delta m^{\sigma})\Theta(x)=m_+^{\sigma}-(\Delta m^{\sigma})\Theta(-x) \ , \tag{4}$$

$$U(x)=U_-+(\Delta U)\Theta(x)=U_+-(\Delta U)\Theta(-x) \ , \tag{5}$$

with

$$\Theta(x)=\begin{cases}1 & \text{for } x>0 \ ,\\ 0 & \text{for } x<0 \ .\end{cases}$$

In passing, we note that the Hamiltonian of Eq. (2) is Hermitian and is consistent with a conserved current which can be written in the standard form

$$j(x)=\frac{\hbar}{2i}\left[\psi^*\frac{1}{m}\partial_x\psi-\psi\frac{1}{m}\partial_x\psi^*\right] . \tag{6}$$

The problem now is to determine how ψ and $\partial_x\psi\equiv\dot{\psi}$ at $x=0^-$ are related to their values at $x=0^+$, i.e., the matching conditions.

We proceed first to integrate Eq. (3) from some fixed point $x_0<0$ to an arbitrary point x [using $\dot{\Theta}(x)=\delta(x)$]:

$$m^{\alpha+\beta}\partial_x m^{\gamma}\psi+m^{\beta+\gamma}\partial_x m^{\alpha}\psi=[(\Delta m^{\alpha})(m^{\beta}\partial_x m^{\gamma}\psi)_0+(\Delta m^{\gamma})(m^{\beta}\partial_x m^{\alpha}\psi)_0]\Theta(x)+\int_{x_0}^{x}dx'R(x')+2\frac{1}{m_-}\dot{\psi}(x_0) \ , \tag{7}$$

and then we proceed to integrate Eq. (7) over the same range,

$$\begin{aligned}2m^{\alpha+\beta+\gamma}\psi=&[(\Delta m^{\alpha+\beta})(m^{\gamma}\psi)_0+(\Delta m^{\gamma+\beta})(m^{\alpha}\psi)_0]\Theta(x)+[(\Delta m^{\alpha})(m^{\beta}\partial_x m^{\gamma}\psi)_0+(\Delta m^{\gamma})(m^{\beta}\partial_x m^{\alpha}\psi)_0]\Theta(x)x\\&+\int_{x_0}^{x}dx'\int_{x_0}^{x'}dx''R(x'')+2\frac{1}{m_-}\psi(x_0)+2\frac{1}{m_-}\dot{\psi}(x_0)(x-x_0) \ ,\end{aligned} \tag{8}$$

where $(\ )_0$ indicates that the quantity in parentheses is to be evaluated at $x=0$.

We now impose the reasonable requirement that $\psi(x)$ be finite everywhere.[10] Inspection of Eq. (8) shows that we must then have

$$(\Delta m^{\alpha+\beta})(m^{\gamma}\psi)_0+(\Delta m^{\gamma+\beta})(m^{\alpha}\psi)_0 \ \text{ finite} \ , \tag{9}$$

and

$$(\Delta m^{\alpha})(m^{\beta}\partial_x m^{\gamma}\psi)_0+(\Delta m^{\gamma})(m^{\beta}\partial_x m^{\alpha}\psi)_0 \ \text{ finite} \ . \tag{10}$$

Because of Eq. (10), we can conclude from Eq. (7) that

$$m^{\alpha+\beta}\partial_x m^{\gamma}\psi+m^{\gamma+\beta}\partial_x m^{\alpha}\psi \ \text{ is finite for all } x \ ,$$

or, upon dividing by m^{β}, that

$$m^{\alpha}\partial_x m^{\gamma}\psi+m^{\gamma}\partial_x m^{\alpha}\psi \ \text{ is finite for all } x \ , \tag{11}$$

from which we can also conclude that $\partial_x\psi$ is finite for all $x\neq0$ (recall that m^{σ} is constant except at $x=0$). The subscripts 0 can then be removed from the quantities in Eq. (10), and we are led to

$$(\Delta m^{\alpha})m^{\beta}\partial_x m^{\gamma}\psi+(\Delta m^{\gamma})m^{\beta}\partial_x m^{\alpha}\psi \ \text{ is finite for all } x \ . \tag{12}$$

Through the use of Eqs. (4), (11), and (12) it is easy to show that

$$m_-^{\alpha}m^{\beta}\partial_x m^{\gamma}\psi+m_-^{\gamma}m^{\beta}\partial_x m^{\alpha}\psi \ \text{ is finite for all } x \ , \tag{13}$$

and

$$m_+^{\alpha}m^{\beta}\partial_x m^{\gamma}\psi+m_+^{\gamma}m^{\beta}\partial_x m^{\alpha}\psi \ \text{ is finite for all } x \ . \tag{14}$$

For Eqs. (13) and (14) to be true we need

$$m^{\beta}\partial_x m^{\gamma}\psi \ \text{ and } \ m^{\beta}\partial_x m^{\alpha}\psi \ \text{ to be finite for all } x \ ,$$

or

$$\partial_x m^{\gamma}\psi \ \text{ and } \ \partial_x m^{\alpha}\psi \ \text{ to be finite for all } x \ ,$$

or, upon integrating from $-\epsilon$ to $+\epsilon$ and taking the limit $\epsilon\to0$,

$$m_-^{\gamma}\psi(0^-)=m_+^{\gamma}\psi(0^+) \ \text{ and } \ m_-^{\alpha}\psi(0^-)=m_+^{\alpha}\psi(0^+) \ ,$$

which in turn implies

$$\psi(0^-)=\psi(0^+)=0 \ \text{ if } \alpha\neq\gamma \ ,$$

or (15)

$$m^{\alpha}\gamma \ \text{ continuous at } x=0 \text{ if } \alpha=\gamma \ .$$

In the event that $\alpha=\gamma$, we return to Eq. (3), which now becomes

$$2m^{\alpha}\partial_x m^{\beta}\partial_x m^{\alpha}\psi=-k^2\psi+U\psi \ . \tag{16}$$

The right-hand side of Eq. (16) is finite for all x, having possibly a step discontinuity at $x=0$. This left-hand side must be similarly well behaved. This implies that

$$\partial_x m^{\beta}\partial_x m^{\alpha}\psi \ \text{ is finite for all } x \ ,$$

which, by integrating from $-\epsilon$ to $+\epsilon$ and taking the limit $\epsilon \to 0$, leads to the conclusion that $m_{-}^{\beta+\alpha}\dot{\psi}(0^-) = m_{+}^{\beta+\alpha}\dot{\psi}(0^+)$ or that

$$m^{\alpha+\beta}\dot{\psi} \text{ is continuous at } x=0 \; . \tag{17}$$

In the event that $\alpha \neq \gamma$, we have from Eqs. (6) and (15) that the conserved current $j(0^{\pm})=0$. This allows only separate standing waves in the regions $x<0$ and $x>0$, corresponding to the presence of an impenetrable barrier at $x=0$. Since this is unphysical for our model heterojunction, we must conclude that any viable Hamiltonian of the form given in Eq. (2) must have $\alpha=\gamma$.

We may now inquire if a kinetic energy operator of the form

$$\hat{T} = \tfrac{1}{4}(m^{\alpha_1}\hat{p}m^{\beta_1}\hat{p}m^{\alpha_1} + m^{\alpha_2}\hat{p}m^{\beta_2}\hat{p}m^{\alpha_2}) \tag{18}$$

is possible. However, by considerations paralleling those above, we are led to the conclusion that $\psi(0^+)=\psi(0^-)=0$ if $\alpha_1 \neq \alpha_2$, and so we must reject unphysical Hamiltonians constructed using Eq. (18) as being unphysical.

III. CONCLUSIONS

We have investigated model effective-mass Hermitian Hamiltonians for abrupt heterojunctions that involve as part of the kinetic energy operator terms of the form $m^{\alpha}\partial_x m^{\beta}\partial_x m^{\gamma}\psi$ with $\alpha+\beta+\gamma=-1$. Our conclusion is that only single-term forms with $\alpha=\gamma$ are viable candidates, and that for them the matching conditions are continuity of $m^{\alpha}\psi$), and $m^{\alpha+\beta}\dot{\psi}$. These conditions in turn imply continuity of $\psi\dot{\psi}/m = (m^{\alpha}\psi)(m^{\alpha+\beta}\dot{\psi})$, and therefore could follow from a demand that the current be continuous across the heterojunction. In the three-dimensional case the matching conditions are continuity of $m^{\alpha}\psi$ and $m^{\alpha+\beta}\nabla_n\psi$ across the junction, where ∇_n denotes the derivative normal to the junction.

It is interesting that kinetic energy operators such as

$$\frac{1}{4}\left[\frac{1}{m}\hat{p}^2 + \hat{p}^2\frac{1}{m}\right]$$

which seem reasonable *a priori* are not acceptable in treating abrupt heterojunctions, since they have the effect of presenting an impenetrable barrier at the junction. Our work still leaves open the question of whether they are valid in situations where the grading is not abrupt, but gradual.

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[5]C. M. van Vliet and A. H. Marshak, Phys. Rev. B 26, 6734 (1982).

[6]O. von Roos, Phys. Rev. B 27, 7547 (1983).

[7]Q.-G. Zhu and H. Kroemer, Phys. Rev. B 27, 3519 (1983).

[8]R. A. Morrow, Phys. Rev. B (to be published).

[9]We take both m and U to be constant away from $x=0$ for convenience. It is actually only important to rule out discontinuities in m away from $x=0$.

[10]Certainly, ψ must be finite for $x \neq 0$. The assumption that $\psi(0)$ is finite is justified *a posteriori* by finding such a solution, and by demonstrating through simple Wronskian arguments that it is unique.