

LETTER TO THE EDITOR

The effective-mass Hamiltonian for abrupt heterostructures

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Abstract. The effective-mass Hamiltonian $H = \frac{1}{2}m^\alpha \mathbf{p} m^\beta \mathbf{p} m^\alpha + V_c + v$ for non-homogeneous semiconductors is studied. Here m is the position-dependent effective mass, $2\alpha + \beta = -1$, V_c is the position-dependent conduction band edge and v is a localised potential. Through an exact model calculation we show that when effective-mass theory is applicable, $\alpha = 0$ and $\beta = -1$.

Effective-mass theory is an important and extensively used tool for the determination of electronic properties of semiconductors. The theory is well established [1] for homogeneous materials with small perturbations—such as a shallow impurity potential $v(\mathbf{r})$ —added. With the recent interest in superlattices and quantum wells, effective-mass theory has also been applied to non-uniform materials in which the carrier effective mass depends on position. Examples include determination of electronic levels in heterojunctions [2], superlattices [3] and quantum wells [4], determination of band offsets across heterojunctions [5], and treatments of exciton binding energies [6]. Immediately two questions arise: Is effective-mass theory applicable in these situations? And if so, what is the effective-mass Hamiltonian?

The effective-mass Hamiltonian must clearly incorporate the spatial variation of the conduction band edge $V_c(\mathbf{r})$. More intriguing is the question of the kinetic-energy term since the momentum operator \mathbf{p} and the effective mass $m(\mathbf{r})$ do not commute. We consider effective-mass Hamiltonians of the general form [7]

$$H_0 = \frac{1}{2}m^\alpha \mathbf{p} m^\beta \mathbf{p} m^\alpha + V_c(\mathbf{r}). \quad (1)$$

With $2\alpha + \beta = -1$, this constitutes a one-parameter class of Hermitian Hamiltonians for the inhomogeneous material.

In applications, the spatial variation of m is either neglected [8], or, most commonly, the form (1) with $\alpha = 0$ and $\beta = -1$ is postulated [9]. The choice $\alpha = -\frac{1}{2}$, $\beta = 0$ is also seen [10], as well as [11] $\frac{1}{4}p^2 m^{-1} + \frac{1}{4}m^{-1}p^2$ for the kinetic term, a choice outside (1) and with inherent difficulties [7]. No fundamental derivation of (1), specifying α , exists [12].

In slowly graded crystals the distinction between the different operators (1) is rather unimportant, and we therefore focus on *abrupt* heterostructures. For an abrupt heterostructure, the electron wavefunction $\psi(\mathbf{r})$ must satisfy the conditions

$$m^\alpha \psi(\mathbf{r}) = \text{continuous} \quad m^\beta \nabla(m^\alpha \psi) = \text{continuous} \quad (2)$$

at the boundary between two homogeneous regions [7]. It is easy to see that (2) is consistent with the Schrödinger equation based on (1).

It is natural to believe that the value of β is universal. If so, one strategy to determine its value could be via a well selected experiment. Our strategy is different. We determine β by comparing, for a test case, exact results with effective-mass results, parametrised by β . The questions of the validity of effective-mass theory, and of the universality of the result, can to some extent be looked into by varying the parameters of the model.

As a test case we use a heterostructure consisting of two homogeneous regions 1 and 2 (figure 1), and we consider energy levels for an electron bound in a potential well $v(x)$ localised near the boundary between material 1 and material 2 (figure 1). For analytic convenience, each of the homogeneous materials is a one-dimensional Kronig–Penney lattice and the local potential is taken to be a square well:

$$H = \frac{p^2}{2m} - \frac{\hbar^2}{ma} \sum_{n=-\infty}^{+\infty} \alpha(n)\delta(x - na) + V_1\theta(x) + V_2\theta(-x) + v(x) \quad (3)$$

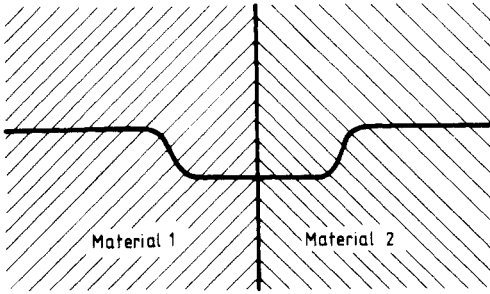


Figure 1. A localised potential in a heterostructure.

where $\theta(x)$ is the Heaviside step function

$$\alpha(n) = \begin{cases} \alpha_1 & \text{for } n > 0 \\ \frac{1}{2}(\alpha_1 + \alpha_2) & \text{for } n = 0 \\ \alpha_2 & \text{for } n < 0 \end{cases} \quad (4)$$

and

$$v(x) = \begin{cases} -V_0 & \text{for } -s_2a \leq x \leq s_1a \\ 0 & \text{otherwise} \end{cases} \quad (5)$$

with integer well width parameters s_1 and s_2 . The lattice constant is a .

Each of the homogeneous materials has two independent parameters: the dimensionless strength parameter α_r and an adjustable energy constant V_r .

The exact evaluation proceeds by standard transfer-matrix techniques. Let ψ_n and ψ'_n refer to the wavefunction and its derivative immediately to the right of the n th δ -well. Since the potential is constant between the δ -wells, the transfer matrix \mathbf{T} is of the usual Kronig–Penney form [13]

$$X_n = \mathbf{T}X_{n-1}$$

with

$$X_n = \begin{pmatrix} \psi_n \\ a\psi'_n \end{pmatrix}$$

and

$$\mathbf{T}(Q) = \begin{pmatrix} \cos Q & Q^{-1} \sin Q \\ -Q \sin Q - 2\alpha(n) \cos Q & \cos Q - 2\alpha(n)Q^{-1} \sin Q \end{pmatrix}. \tag{6}$$

Here Q is determined by the energy E and the constant potential:

$$Q = \begin{cases} q_1 \equiv [2ma^2(E - V_1)/\hbar^2]^{1/2} & \text{for } n \geq s_1 \\ Q_1 \equiv [2ma^2(E - V_1 + V_0)/\hbar^2]^{1/2} & \text{for } 1 \leq n < s_1 \\ Q_2 \equiv [2ma^2(E - V_2 + V_0)/\hbar^2]^{1/2} & \text{for } -s_2 < n \leq 0 \\ q_2 \equiv [2ma^2(E - V_2)/\hbar^2]^{1/2} & \text{for } n \leq -s_2. \end{cases} \tag{7}$$

Transforming to the right we have

$$X_{n+s_1} = \mathbf{T}^n(q_1)\mathbf{T}^{s_1}(Q_1)X_0 = \mathbf{S} \begin{pmatrix} \lambda_1^n & 0 \\ 0 & \lambda_2^n \end{pmatrix} \mathbf{S}^{-1}\mathbf{T}^{s_1}(Q_1)X_0 \tag{8}$$

where $\mathbf{T}(q_1)$ has been diagonalised with eigenvalues λ_1 and λ_2 . The wavefunction vanishes for $n \rightarrow \infty$ if and only if the energy is in a forbidden gap of material 1. Then one eigenvalue (λ_2 , say) is less than unity in magnitude, and the initial vector X_0 must be chosen so that there is no increasing part. With $|\lambda_1| > 1$ the upper component of $\mathbf{S}^{-1}\mathbf{T}^{s_1}(Q_1)X_0$ must vanish, i.e.

$$(\mathbf{S}^{-1}\mathbf{T}^{s_1}(Q_1))_{11}\psi_0 + (\mathbf{S}^{-1}\mathbf{T}^{s_1}(Q_1))_{12}a\psi'_0 = 0. \tag{9}$$

This determines ψ'_{0+}/ψ_0 in terms of \mathbf{S} and $\mathbf{T}(Q_1)$.

Transforming towards $n = -\infty$ instead, an analogous condition on ψ'_{0-}/ψ_0 is obtained. Finally the difference $(\psi'_{0+} - \psi'_{0-})/\psi_0$ is given by the strength of the δ -function well at the origin.

The resulting condition for the bound states can, after considerable algebra, be written in the following compact form [14]:

$$\sum_{r=1}^2 Q_r \frac{\sin U_r}{\sin Q_r} \tan(s_r U_r + \delta_r) = 0 \tag{10}$$

where

$$\tan \delta_r = -\frac{q_r}{\sin q_r} \frac{\sin Q_r}{Q_r} \frac{\sinh u_r}{\sin U_r}. \tag{11}$$

Here U_r and u_r are positive auxiliary variables defined through

$$\cos U_r = |\cos Q_r - (\alpha_r/Q_r) \sin Q_r| \tag{12}$$

$$\cosh u_r = |\cos q_r - (\alpha_r/q_r) \sin q_r|. \tag{13}$$

Note that when $s_1 = s_2 = 0$, V_0 drops out of the equation, as it must, leaving a condition for Tamm states at the interface. Another special case is the homogeneous

limit ($\alpha_1 = \alpha_2, V_1 = V_2$). Then (10) depends upon s_1 and s_2 only through the combination $s_1 + s_2$, and can be written as

$$\tan(s_1 U + s_2 U + 2\delta) = 0 \quad \tan \delta = -\frac{q}{\sin q} \frac{\sin Q}{Q} \frac{\sinh u}{\sin U}. \quad (14)$$

We now turn to the effective-mass treatment. We denote the conduction band edges and the effective masses of the materials by V_{c1}, V_{c2} , and m_1, m_2 , respectively. Since the potential energy is piece-wise constant the effective-mass Schrödinger equation

$$-\frac{1}{2}\hbar^2(m(x))^\alpha (d/dx)(m(x))^\beta (d/dx)(m(x))^\alpha \psi = (E - V_c(x) - v(x))\psi$$

is satisfied by

$$\psi(x) = \begin{cases} \exp(\bar{q}_2 x/a) & x < -s_2 a \\ \cos(\bar{Q}_2 x/a + c_2) & -s_2 a < x < 0 \\ \cos(\bar{Q}_1 x/a + c_1) & 0 < x < s_1 a \\ \exp(-\bar{q}_1 x/a) & s_1 a < x. \end{cases}$$

Here

$$\bar{q}_r = [2m_r a^2 (V_{cr} - E)/\hbar^2]^{1/2} \quad \bar{Q}_r = [2m_r a^2 (E - V_{cr} + V_0)/\hbar^2]^{1/2}. \quad (15)$$

Connecting the wavefunction and its derivative at $x = -s_2 a, 0$ and $s_1 a$ in accordance with the boundary condition (2), we readily obtain the following implicit equation for the bound-state energies E :

$$\sum_{r=1}^2 m_r^{-\beta} \bar{Q}_r^{-1} \tan(s_r \bar{Q}_r + \eta_r) = 0 \quad (16)$$

where

$$\tan \eta_r = \bar{Q}_r / \bar{q}_r. \quad (17)$$

When the actual values for the effective masses m_r and band edges V_{cr} are inserted, the two results (10) and (12) of the exact and the effective-mass calculations can be compared. They are clearly different equations for the bound-state energies, but the question is whether there are conditions under which they are essentially in agreement. For *homogeneous* materials the effective-mass approximation becomes accurate for a sufficiently shallow local potential v , and consequently we will consider this limiting case of the exact expression (10).

It is well known that the conduction band edge for the n th gap in a homogeneous Kronig–Penney lattice is located at $q^* = n\pi$, corresponding to the energy

$$V_{cr} = n^2 \pi^2 \hbar^2 / 2a^2 m + V_r \quad (r = 1, 2). \quad (18)$$

The other inputs in the effective-mass theory, the effective masses m_r at the bottom of the conduction bands, are determined by the expansion of the dispersion relation $\cos(k + n\pi) = \cos q - (\alpha_r/q) \sin q$ around $q = q^*$:

$$E(q) - V_{cr} = \hbar^2 k^2 / 2a^2 m_r + o(k^2). \quad (19)$$

Since the auxiliary variable u_r , equation (13), vanishes at the band edge, we can expand the energy in u_r ; and the similarity between (13) and the dispersion relation shows that the quadratic contribution is governed by the effective mass:

$$E - V_{cr} \approx -\hbar^2 u_r^2 / 2a^2 m_r. \tag{20}$$

The factor $\sin q_r$ in the exact expression (11) also vanishes at the band edge, and a similar expansion yields

$$\sin q_r \approx (-1)^{n+1} u_r^2 m / 2n\pi m_r. \tag{21}$$

Take first the case with no offset, i.e. $V_1 = V_2$, and consequently $q_1 = q_2$, $Q_1 = Q_2$. For small V_0 , the bound-state energies are close to the band edge and the expansions (20) and (21) apply. Moreover, since $Q^2 - q^2 \propto V_0$, Q and q differ only slightly for the case where V_0 is small and consequently U_r can also be considered to be small. Comparison between (12) and (13) then yields an expansion

$$\sin Q_r \approx (-1)^n U_r^2 m / 2n\pi m_r \tag{22}$$

near the band edge. We now insert (21) and (22) into the exact condition (10) and (11), and take u_r and U_r (but not necessarily $s_r U_r$) to be small quantities. The result is

$$\sum_{r=1}^2 m_r U_r^{-1} \tan(s_r U_r + \delta_r) = 0 \tag{23}$$

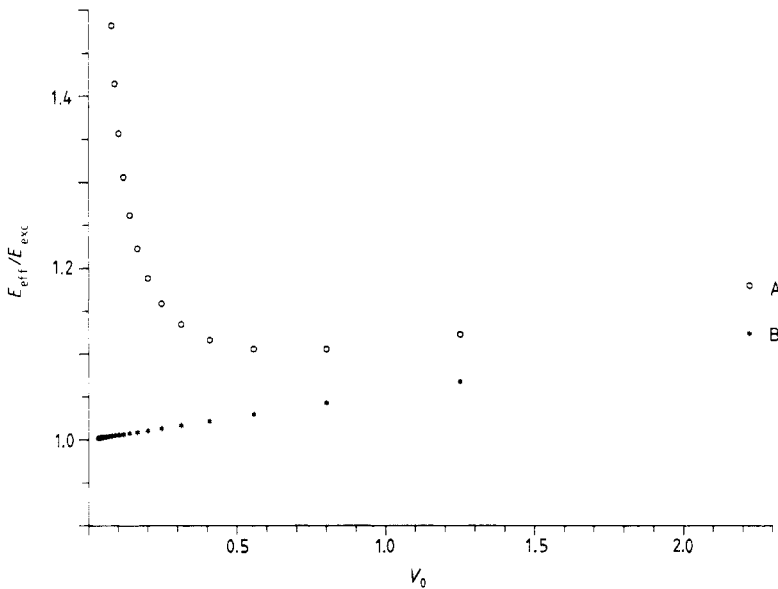


Figure 2. A comparison of the binding energies E_{eff} , E_{exc} determined via the effective-mass calculation, equation (16) with $\beta = -1$, and by the exact method, equation (10), respectively. We consider the lowest gap ($n = 1$), and have taken $\alpha_1 = 0.5$, $\alpha_2 = 1$. (The resulting effective masses are $m_1 \approx 0.05m$ and $m_2 \approx 0.1m$.) The square well is symmetrically situated ($s_1 = s_2 = s$), with a depth chosen to be $V_0 = 20/s^2$ (which yields precisely one bound state). Data points corresponding to $s = 3, 4, 5, \dots$ are shown. Potential energies are given in units of $\hbar^2/2ma^2$. A: with offset ($V_{c1} - V_{c2} = 0.5$); B: without offset ($V_{c1} = V_{c2}$).

with

$$\tan \delta_r = U_r/u_r. \quad (24)$$

This condition for the bound-state energies is, except for notation ($U_r \rightarrow \bar{Q}_r$, $u_r \rightarrow \bar{q}_r$, $\delta_r \rightarrow \eta_r$), *exactly* the effective-mass relation (16) with, most importantly, $\beta = -1$.

With a non-negligible offset present, a bound-state energy cannot be close to the conduction band edge of *both* materials, and the asymptotic analysis given above cannot be carried through. As a consequence, effective-mass theory will *not* be asymptotically exact (for a shallow local potential) in such cases. (This does not of course exclude the possibility that the effective-mass approximation may give a qualitatively correct and quantitatively reasonable description.) Figure 2 shows explicitly that in the presence of an offset, the ratio of the effective-mass binding energy to the exact binding energy does not approach unity in the shallow-potential limit, in contrast to the zero-offset case with $\beta = -1$.

In conclusion we have shown that when the effective-mass treatment is applicable, the Hamiltonian (1) with $\alpha = 0$ and $\beta = -1$ should be used.

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