PHYSICAL REVIEW B VOLUME 51, NUMBER 24 15 JUNE 1995-II

Form of kinetic energy in effective-mass Hamiltonians for heterostructures

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(Received 5 January 1995; revised manuscript received 24 January 1995)

We first prove that the class of effective-mass Hamiltonians $H = T_\alpha + V$ with $T_\alpha = \frac{1}{2} m^{\alpha} p m^{-1-2\alpha} p m^{\alpha}$, where $m = m(x)$ is a twice differentiable (C_2) function and $p = -i d/dx$ can be mapped by an unitary transformation onto the constant-mass case with still a local potential that we give explicitly. The value of α is thus irrelevant. We then consider the case when $m(x)$ is only piecewise C_2, that is, the case of heterojunctions. We show that the general connection rule for the envelope function and its derivative at an unstrained heterojunction depends on a Hermitian 2×2 matrix which is intrinsic to the junction. Hence, the latter should be described by four parameters (three in the case of time-reversal invariant systems). The parameter values may be obtained from the scattering data for Bloch waves, which can be either measured or computed. Up to two Tamm states, localized at the interface, are allowed.

I. INTRODUCTION

The advent of modern microfabrication techniques such as computer-controlled molecular-beam epitaxy has made possible the growth of crystals whose composition may be designed in an atomic layer-by-layer way, including, on one hand, graded lattices with slowly varying composition and, on the other hand, abrupt (on the atomic scale) sharp interfaces between materials of different compositions (heterojunctions). The theoretical description of electronic states in such structures in the presence of slowly varying external (usually electromagnetic) fields often relies on the effective-mass approximation. Assuming that the electronic wave function ψ is expanded on the basis of the generalized Wannier functions w of the relevant band as $\psi(\mathbf{r}) = \sum_n f(\mathbf{R}_n) w(\mathbf{r} - \mathbf{R}_n)$, this approximation is useful in circumstances when the coefficients $f(\mathbf{R}_n)$ do not change much from one site $\mathbf{R}_n$ to its neighbors. The state can then be described by the envelope function $f(\mathbf{r})$, a smooth interpolation of $f(\mathbf{R}_n)$. This envelope function is then the solution of an effective Schrödinger equation, where the (fast varying on the atomic scale) periodic potential is replaced by the constant band offset and where the electron mass in the kinetic-energy term is replaced by an effective mass. Variations in space of this effective mass require, however, modifications in the form of the kinetic energy, which we shall discuss below.

Although often crude, this approximation is useful in actual calculations of heterostructures. It is valid when the energy of the electron lies, within each piece of material through which it passes, sufficiently close to a band edge so that the band energy is a quadratic function of the quasimomentum. This requires, in particular, that the band offsets across junctions should be small compared to the bandwidths. More precisely, the envelope function should everywhere, except at sharp interfaces, vary slowly on the scale of the crystal lattice and on the scale of the extent of the Wannier functions. The potentials of the external forces included in the effective Schrödinger equation, and of the internal forces due to grading should also vary slowly on these scales. Moreover, the time interval in which the approximation may be relied upon should be small compared to the characteristic times taken by the microscopic electron wave function, whose initial value is assumed to be a packet made of states close to the parabolic band edge under consideration, to acquire a significant component outside this region under the influence of the above-mentioned forces. As in many phenomenological works dealing with semiconductor heterojunctions, we assume in the following that these conditions are satisfied.

In the case of graded composition the effective mass becomes position dependent, while the presence of sharp interfaces will lead to discontinuities. The form which the effective-mass equation should take, specifically, its kinetic energy part, has been extensively discussed.[1–18] Much of the discussion has revolved around

$$T_\alpha = \tfrac{1}{2} m^{\alpha} p m^{-2\alpha-1} p m^{\alpha} \tag{1.1}$$

and its three-dimensional, anisotropic mass equivalent.[3,6–10,12–17] In the graded case, Geller and Kohn[19] have constructed an interpolation of the Wannier basis function and shown that, within that approximation, the derivatives of the effective mass, which distinguish between various forms of type (1.1), have magnitudes within the estimated errors of the effective-mass approximation. Nevertheless, various attempts are continuing to use this form of the kinetic-energy operator to infer the discontinuities of the function and its derivative at the interface, for modeling or fitting the intrinsic properties of the interface by the parameter α.

In this paper we shall take a purely phenomenological approach. We first show that, whenever the effective mass is twice differentiable, the form (1.1) of the kinetic

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energy may be brought by an unitary transformation to the constant-mass kinetic energy plus a slowly varying local potential.

Then we turn to the general description of unstrained heterojunctions in the effective-mass approximation. In this case, when the system is invariant with respect to the discrete translations along directions parallel to the interface plane, which we assume to be parallel to a crystal plane of the crystal structures to the left/right of the interface, the components of the quasimomentum along directions parallel to the interface are conserved. We assume that the transition domain where the potential changes from the periodic form for the left crystal to the periodic one for the right is microscopic, having an extent of at most a few lattice spacings. Then, away from the interface the evanescent solutions which are needed for matching the solutions of the microscopic Schrödinger equation decay exponentially in each crystal. At a given energy and transverse quasimomentum, the general solution of the microscopic Schrödinger equation relaxes rapidly to a combination of the two asymptotic Bloch wave solutions having the same transverse quasimomentum and opposite parallel components which are allowed in the bulk by the conservation laws.[20]

Thus, from a phenomenological point of view, an unstrained interface can be described by the scattering matrix of the envelope function made of plane waves onto which the Bloch waves are mapped. The evolution of a packet of Bloch waves with a narrow energy spread and which is localized away from the interface in a bulk piece of ungraded crystal is described by the effective-mass equation in that medium,

$$-i\dot{f}=\epsilon(-i\nabla)f+Vf \ , \tag{1.2}$$

where $\epsilon(\mathbf{q})$ is the (bulk) dispersion law in the considered crystal and V is the external potential, which varies slowly on the lattice scale. If the energy is close to a band extremum, (1.2) takes the effective-mass form

$$-i\dot{f}=Hf=\left[-\frac{1}{2m}\Delta+E^0+V\right]f \ . \tag{1.3}$$

Here E^0 is the energy of the extremum and m is the effective mass, which we assumed to be isotropic for simplicity. The whole system will be described by gluing together the equations of type (1.3) which hold in each homogeneous piece. The recipe chosen must be translation invariant in the transverse direction, parallel to the interface plane. In the absence of the external potential V, the variables separate in (1.3) so that it is sufficient to consider only the one-dimensional case. We are led to the mathematical problem of constructing the self-adjoint extensions of the kinetic-energy operator T, whose action on smooth functions having a support which does not intersect the interface is

$$(Tf)(x)=-\frac{1}{2m}\frac{d^2f}{dx^2} \ , \tag{1.4}$$

if the support of f is wholly in one homogeneous piece of material. This will be done in Sec. III, where we show that the general connection rules which lead to self-adjoint operators are parametrized by a 2×2 Hermitian matrix. We will also see that the current density in the state f, defined at point x by

$$j=-\frac{i}{2m}[f^*(x)f'(x)-f'^*(x)f(x)] \ , \tag{1.5}$$

is conserved for solutions of $(T+V)f=Ef$, if T is self-adjoint. Finally, we show that up to two Tamm states, localized at the interface, may be present if the above-mentioned Hermitian matrix has negative eigenvalues.

II. CONSTRUCTION OF THE UNITARY MAPPING

We want to construct a unitary transformation which will map the Hamiltonian

$$H=T_\alpha+V \ , \tag{2.1}$$

where T_α is defined in (1.1), on the constant-mass ($=1$) Hamiltonian

$$\hat{H}=-\frac{1}{2}\frac{d^2}{dx^2}+\hat{V} \tag{2.2}$$

in the case of twice-differentiable (C_2) mass, with $0<m_1\le m(x)\le m_2<+\infty$. We start with the energy functional

$$E(f)=K(f,f)+V\int_{-\infty}^{+\infty}|f|^2dx \ , \tag{2.3}$$

where the kinetic-energy form is

$$K(f,f)=\int_{-\infty}^{+\infty}\frac{|(m^\alpha f)'|^2}{2m^{1+2\alpha}}dx \ . \tag{2.4}$$

The variational principle leads to the Schrödinger equation

$$Hf=Ef \ , \tag{2.5}$$

with H defined by (2.1) and (1.1).

Let us introduce a new coordinate:

$$Y(x)=\int_0^x m^{1/2}(\xi)d\xi \ . \tag{2.6}$$

The function $Y(x)$ is strictly monotonic and therefore invertible, Y is C_3 (three-times differentiable). The inverse transformation, $x=X(y)$, is also C_3. In differential form, we have

$$\frac{dY}{dx}(x)=m^{1/2}(x), \quad \frac{dX}{dy}(y)=m^{-1/2}[X(y)] \ . \tag{2.7}$$

Within any homogeneous piece of material, $Y(x)$ is a linear function of x, so that the mapping (2.6) amounts there to a mere change of the unit of length. We shall treat separately the kinetic energy and the potential energy. Let us start with the quadratic form (2.4) for the kinetic energy. We define a new function g by scaling f:

$$g(y)=m^{-1/4}(X(y)f(X(y))) \ . \tag{2.8}$$

The new function has the same norm as f:

$$\begin{aligned}\|f\|^2&=\int_{-\infty}^{+\infty}|f(x)|^2dx\\&=\int_{-\infty}^{+\infty}|g(y)|^2dy=\|g\|^2 \ .\end{aligned} \tag{2.9}$$

In this manner we preserve the norm and get an isometric transformation that we shall show later to be unitary.

Substituting $x = X(y)$ in (2.4), we get

$$K(f,f)=\frac{1}{2}\int_{-\infty}^{+\infty}\left| g'(y)+(\tfrac{1}{4}+\alpha)\right.$$
$$\left.\times\left[\frac{m'}{m^{3/2}}\right](X(y))g(y)\right|^2 dy, \tag{2.10}$$

and after a short calculation:

$$K(f,f)=K_1(g,g)+\frac{1+4\alpha}{8}\int_{-\infty}^{+\infty}(|g|^2)'\rho\,dy$$
$$+\frac{(1+4\alpha)^2}{32}\int_{-\infty}^{+\infty}|g|^2\rho^2 dy\ , \tag{2.11}$$

where we have defined

$$\rho(y)=m^{-3/2}(X(y))m'(X(y)) \tag{2.12}$$

and $K_1(g,g)$ is the kinetic-energy form (2.4) for unit mass, $m=1$.

Integrating by parts the second term in (2.11), taking into account that g vanishes at infinity, we have

$$K(f,f)=K_1(g,g)+\int_{-\infty}^{+\infty}\hat{V}_K|g|^2 dy\ , \tag{2.13}$$

where

$$\hat{V}_K(x)=\tfrac{1}{32}(4\alpha+1)\left[(4\alpha-1)\frac{m'}{m^3}+\left[\frac{4}{m}\right]''\right]_{X(x)}\ . \tag{2.14}$$

Finally, adding the potential energy and summing up all pieces, we see that we have transformed the variable-mass problem,

$$H=\tfrac{1}{2}m^{\alpha}pm^{-1-2\alpha}pm^{\alpha}+V\ , \tag{2.15}$$

into a fixed-mass ($=1$) problem,

$$\hat{H}=\tfrac{1}{2}p^2+\hat{V}\ , \tag{2.16}$$

where the potential $\hat{V}$ is given by

$$\hat{V}=V+\hat{V}_K\ . \tag{2.17}$$

Within any homogeneous piece of material, (2.14) vanishes and the coordinate transformation (2.6) is linear; hence $\hat{V}$ is obtained there just by changing the unit of length.

To discuss more in depth the properties of this transformation, we introduce the operator U defined by

$$(Uf)(x)=m^{-1/4}(X(x))f(X(x))\ . \tag{2.18}$$

Its adjoint is

$$(U^{\dagger}f)(x)=m^{1/4}(x)f(Y(x))\ , \tag{2.19}$$

where X and Y were defined by (2.6) and (2.7).

1. U is unitary and its domain is L^2 as can be checked immediately.

2. Let us consider the transform by U of the kinetic-energy operator T_{α} (1.1):

$$T_{\alpha U}=UT_{\alpha}U^{\dagger}\ . \tag{2.20}$$

We find after some calculations

$$(T_{\alpha U}f)(x)=-\frac{1}{2}\frac{d^2}{dx^2}f(x)+\hat{V}_K(x)f(x)\ , \tag{2.21}$$

where $\hat{V}_K(x)$ is given by (2.14).

In the case of a slowly graded lattice, when the potential (band offset) and the effective mass are slowly varying functions, each derivative introduces an additional small factor of the order of a/L—the ratio of the lattice constant a to the length L over which there is a significant variation in composition. There is then no advantage in working with any of the various forms of T_{α} which were discussed in the literature. Indeed, they are all equivalent, up to a redefinition of the potential involving second-order terms in a/L. This smallness of the difference between different choices for T_{α} was recently pointed out by Geller and Kohn.[19]

As we have seen, there is no justification for using the form (1.1) of the kinetic-energy operator in slowly graded structures. The difference between various values of α amounts in this case to adding a slowly varying potential,

$$T_{\alpha}=-\frac{d}{2dx}\frac{1}{m(x)}\frac{d}{dx}$$
$$+\frac{\alpha}{2m^3(x)}[(2+\alpha)m'^2-mm''](x)\ , \tag{2.22}$$

to the standard form of the kinetic energy. As a simple consequence of (2.22), we note that any Hamiltonian of the form $H_{\alpha}=T_{\alpha}+V_{\alpha}$ can be mapped on $H_{\beta}=T_{\beta}+V_{\beta}$ with

$$V_{\beta}=V_{\alpha}+\frac{\alpha-\beta}{2}\left[(\alpha+\beta)\frac{m'^2}{m^3}+\left[\frac{1}{m}\right]''\right]\ . \tag{2.23}$$

III. SHARP UNSTRAINED HETEROJUNCTIONS

A consequence of using (1.1) in the case of a sharp variation of m is the introduction of a family of connection rules, depending on the parameter α, for the wave function and its derivative at mass discontinuities. Let us consider only one heterojunction between slowly graded crystals in the one-dimensional case. Using the subscripts l and r for the limiting values from the left and the right, we find that the use of the form (1.1) means that

$$m_l^{\alpha}f_l=m_r^{\alpha}f_r\ , \tag{3.1}$$

$$m_l^{-1-\alpha}\left[f_l'+\alpha\frac{m_l'}{m_l}f_l\right]=m_r^{-1-\alpha}\left[f_r'+\alpha\frac{m_r'}{m_r}f_r\right]\ . \tag{3.2}$$

Introducing the 2×2 interface transfer matrix $\mathcal{T}$, which connects the left and right limit values of the function and its derivative

$$\begin{bmatrix} f_r \\ f_r' \end{bmatrix}=\mathcal{T}\begin{bmatrix} f_l \\ f_l' \end{bmatrix}\ , \tag{3.3}$$

we see that the aesthetics of choosing the kinetic energy in the form (1.1) leads to a rather particular triangular form for $\mathcal{T}$,

$$\mathcal{T}=\begin{bmatrix}(m_l/m_r)^{\alpha} & 0\\ \alpha[m_l' m_r^{1+\alpha}/m_l^{2+\alpha}-m_r'/m_l] & (m_r/m_l)^{\alpha+1}\end{bmatrix}, \tag{3.4}$$

which reduces to a diagonal one for heterojunctions between nongraded crystals. Now, since the work of Ando and Mori,[1] we know that at least for the tight-binding models considered by them this is unlikely.

Let us consider an unstrained heterojunction between two periodic (ungraded) crystals. Strictly speaking, near the interface the effective-mass approximation is not valid. Nevertheless, the evanescent solutions decay exponentially so that the solution of the Schrödinger equation relaxes quickly to a linear combination of Bloch waves—the asymptotic states allowed by the conservation laws. Since the dimensions of the domain in which the relaxation takes place are microscopic—of the order of magnitude of the lattice spacing—we may use the effective-mass approximation Schrödinger equation on each side of the interface,

$$\left[-\frac{1}{2m}\frac{d^2}{dx^2}+E^0\right]f=Ef\ , \tag{3.5}$$

and we may continue these asymptotic solutions up to the junction. There we must impose connection rules which ensure (a) self-adjointness of the Hamiltonian (this is indispensable for the quantum-mechanical interpretation of the envelope wave function) and (b) probability current conservation, $\operatorname{div}\mathbf{j}=0$ for solutions of Schrödinger's equation. The current density is defined in each component by

$$\mathbf{j}=-\frac{i}{2m}[f^*\nabla f-(\nabla f^*)f]\ . \tag{3.6}$$

As we have noted, for a nondegenerate band in the unstrained case it is sufficient to consider only the one-dimensional equation, which is equivalent to having fixed the components of the quasimomentum parallel to the interface plane. It is worth mentioning that the evanescent solutions needed for matching the microscopic wave function at the interface do not correspond to asymptotic states and must not appear in the envelope effective-mass equations. Only true asymptotic solutions, which are nonzero at large distance at least on one side of the interface, should be continued back to the interface with the help of the effective-mass equation.

Let us assume that the functions f and g are in the domain of the kinetic-energy operator T defined by fixing some connection rule for the limit values at the interface $x=0$. These relations must be linear since, if f belongs to the domain of T, then λf must also belong to it for any complex λ. Thus f and g are square integrable together with their first and second derivatives at all points except $x=0$. Multiplying (3.5) by $g^*(x)$, subtracting $(Tg)^*(x)f(x)$ from it, and integrating over the reunion of the intervals $(-\infty,0)$ and $(0,+\infty)$, where we know the action of T, we obtain

$$\int_{-\infty}^{-0}\left[\frac{g^*f''-g''^*f}{2m_l}\right](x)dx+\int_{+0}^{+\infty}\left[\frac{g^*f''-g''^*f}{2m_r}\right](x)dx=\left[\left[\frac{g_l^*f_l'-g_l'^*f_l}{2m_l}\right]-\left[\frac{g_r^*f_r'-g_r'^*f_r}{2m_r}\right]\right]\ . \tag{3.7}$$

The right-hand side in (3.7) must be zero if T is self-adjoint.

Now, we noted that the connection rule is a set of linear relations between the limiting values of the functions and their derivatives at $x=0$. It is convenient to solve them for the limiting values of the derivatives:

$$\begin{bmatrix}\dfrac{f_l'}{m_l}\\[2mm] \dfrac{f_r'}{m_r}\end{bmatrix}+\sigma_3\Lambda\begin{bmatrix}f_l\\ f_r\end{bmatrix}=0\ , \tag{3.8}$$

where σ_3 is the diagonal Pauli matrix and the matrix Λ may be readily expressed through $\mathcal{T}$ [see Eq. (3.12) below].

Substituting (3.8) and its equivalent for g into the right-hand side of (3.7) and equating the result to 0 we obtain that the kinetic-energy operator T is self-adjoint if the matrix Λ in (3.8) is Hermitian:

$$\Lambda=\Lambda^{\dagger}\ . \tag{3.9}$$

The elements of Λ satisfy the following: Λ_{11} and Λ_{22} are real and $\Lambda_{12}=\Lambda_{21}^*$. We may readily check that if f satisfies the connection rule (3.8) with a Hermitian Λ, we have

$$\left[\frac{f_l^*f_l'-f_l'^*f_l}{m_l}\right]=\left[\frac{f_r^*f_r'-f_r'^*f_r}{m_r}\right]\ , \tag{3.10}$$

so that the current density (3.6) is conserved at the heterojunction for all functions in the domain of T.

To grasp the physical meaning of the connection matrix Λ, let us write the kinetic-energy quadratic form $K(f,f)$ in this case. A straightforward calculation yields

$$\begin{aligned}K(f,f)&=(f,Tf)\\ &=\frac{1}{2m_l}\int_{-\infty}^{-0}|f'(x)|^2dx+\frac{1}{2m_r}\int_{+0}^{+\infty}|f'(x)|^2dx\\ &\quad+\sum_{\alpha,\beta=1,2}\Lambda_{\alpha\beta}f_\alpha^*f_\beta\ ,\end{aligned} \tag{3.11}$$

where we use the index 1 (2) to denote the limiting values from left (right) of the function f. Thus, if we do not constrain f and f' to be continuous at the interface, we must add to the contribution of the left and right sides to the kinetic energy the interface energy given by the last term in (3.11).

The connection rules (3.8) yield the general form that may be taken by a kinetic-energy operator which is both self-adjoint and current conserving. It allows scattering by the interface even in the case when both the effective mass and the band offset are continuous at the heterojunction. This general form depends on four real parameters at each discontinuity point. If the system is nonmagnetic, that is, time-reversal invariant, then the Hamiltonian must be real, and (3.11) forces the matrix Λ to be real. The unstrained heterojunction is described by three intrinsic parameters in this case.

The heterojunction transfer matrix $\mathcal{T}$, (3.3), may be readily expressed in terms of Λ as

$$\mathcal{T}=-\frac{1}{\Lambda_{12}}\begin{bmatrix}\Lambda_{11} & \dfrac{1}{m_l}\\ m_r\det\Lambda & \dfrac{m_r}{m_l}\Lambda_{22}\end{bmatrix}, \tag{3.12}$$

where $\det\Lambda$ is the determinant of the matrix Λ. If $\mathcal{T}$ is real, then its determinant, $\det\mathcal{T}=m_r/m_l$, is equal to the ratio of the limiting values of the masses. Otherwise this relation holds for its absolute value. This was noted by Ando and Mori,[1] who required current conservation at the heterojunction.

Inspection of (3.12) shows that it becomes meaningless if the off-diagonal element Λ_{12} vanishes. As can be readily seen, this case corresponds to a direct sum of the (independent) left and right operators, with mixed-type boundary conditions $(f_l'=-m_l\Lambda_{11}f_r,\ f_r'=m_r\Lambda_{22}f)$. Since the half-spaces to the right and the left of the junction are completely disconnected in this case, the description via $\mathcal{T}$ is meaningless. The Bloch waves undergo total reflection with a phase change at the junction. The often-assumed connection rules,

$$f_l=f_r,\quad (f'/m)_l=(f'/m)_r\ , \tag{3.13}$$

correspond to a singular limit for Λ: $\Lambda=q(1-\sigma_1)$ and $q\to+\infty$. Here σ_1 is the Pauli matrix in the standard representation. This is understandable, since in this case, (3.13), the energy associated with a discontinuity of the envelope must become infinite.

For completeness sake let us also consider the case when there is no mass discontinuity, $m_l=m_r=m_0$, which might be realized in the case of heterojunctions between quaternary compounds, where the bands might also be aligned. In quantum mechanics one often uses zero support potentials, such as δ and the so-called δ'.[21] The interface transfer matrices associated with these are triangular:

$$\mathcal{T}=\begin{bmatrix}1 & 0\\ 2m_0\lambda & 1\end{bmatrix}, \tag{3.14}$$

for a potential equal to $\lambda\delta(x)$ and

$$\mathcal{T}=\begin{bmatrix}1 & 2m_0\lambda_1\\ 0 & 1\end{bmatrix}, \tag{3.15}$$

for $\lambda_1\delta'(x)$. We remark that in the equal-mass case the general three-parameter connection rules (3.3) and (3.12) is equivalent to considering the "potential"

$$W(x)=\lambda_1\delta(x-\epsilon)+\lambda_2\delta'(x)+\lambda_3\delta(x+\epsilon)$$

and taking the limit $\epsilon\to0$.[21] However, there is no "potential" of the form $\lambda_1\delta(x)+\lambda_2\delta'(x)$ that is equivalent to the general transfer matrix $\mathcal{T}$, which depends on three parameters. Thus, the connection rules (3.3) and (3.12) constitute the adequate but not trivial generalization for the zero support potentials of quantum-mechanical textbooks.

Let us finally consider the problem of bound states at a heterojunction between nongraded materials described by a real Λ. We shall assume that the largest band offset is the left one and that the right one is zero. The other case may be brought to it by coordinate reversal; in that case, the matrix Λ is obtained by interchanging the indices 1 and 2 in the original one while the new matrix $\mathcal{T}$ is the inverse of the original one.

We are looking for solutions of the Schrödinger equation with negative energy $E<0$ which go to zero at $\pm\infty$. For $x<0$ the solution is

$$f_l(x)=\exp[\sqrt{2m_l(U+|E|)}x]\ . \tag{3.16}$$

Using the $\mathcal{T}$ matrix to obtain the function and its derivative at $x=+0$, the solution for $x>0$ is given by

$$f_r(x)=[\mathcal{T}_{11}+\mathcal{T}_{12}\sqrt{2m_l(U+|E|)}]\cosh[\sqrt{2m_r|E|}x]+\frac{\mathcal{T}_{21}+\mathcal{T}_{22}\sqrt{2m_l(U+|E|)}}{\sqrt{2m_r|E|}}\times\sinh[\sqrt{2m_r|E|}x]\ . \tag{3.17}$$

The function f_r goes to zero at $+\infty$ if the coefficient of the positive argument exponential is zero:

$$[\mathcal{T}_{11}+\mathcal{T}_{12}\sqrt{2m_l(U+|E|)}]+[\mathcal{T}_{21}+\mathcal{T}_{22}\sqrt{2m_l(U+|E|)}]/\sqrt{2m_r|E|}=0\ . \tag{3.18}$$

The discussion of the number of solutions of Eq. (3.18) is simpler in terms of the Hermitian connection matrix Λ introduced above. Using (3.12) we may transform (3.18) into an equation for $s=\sqrt{|E|}$:

$$[\sqrt{2(s^2+U)/m_l}+\Lambda_{11}](s\sqrt{2/m_r}+\Lambda_{22})=\Lambda_{12}^2\ . \tag{3.19}$$

Let us consider first the case $U=0$. Then, Eq. (3.19) becomes a simple quadratic equation:

$$s^2+(\Lambda_{11}\sqrt{m_l/2}+\Lambda_{22}\sqrt{m_r/2})s+\frac{\sqrt{m_lm_r}}{2}\det\Lambda=0\ . \tag{3.20}$$

Since its discriminant is positive,

$$(\Lambda_{11}/\sqrt{m_r}-\Lambda_{22}/\sqrt{m_l})^2+4\Lambda_{12}^2/\sqrt{m_lm_r}>0\ ,$$

it has two real distinct roots $s_1 < s_2$. Only the positive ones, for which $s = \sqrt{|E|} > 0$, correspond to bound states. The real Hermitian matrix Λ has two real eigenvalues $\lambda_1 \leq \lambda_2$. There are three possible cases: (a) $\lambda_1 > 0$. No bound states since all the coefficients in (3.20) are positive. (b) $\lambda_1 < 0 < \lambda_2$. Only one bound state since the product of the roots of (3.20) is negative. (c) $0 > \lambda_2$. Two bound states since the sum of the (real) roots of (3.20) is positive, while their product is positive.

Thus for $U=0$ the number of Tamm states bound to the interface simply coincides with the number of negative eigenvalues of the connection matrix Λ. In particular, any variation of the left and right effective masses that does not alter this latter number will not affect the former.

Let us now consider the case of $U > 0$. It is obvious that the energies of the bound states are monotonic increasing functions of U. The (positive) roots of (3.19) will be monotonic decreasing with U. In case (a) there are still no bound states. In case (c) the diagonal elements of Λ are negative, and even for $U \to +\infty$ there is a positive root of (3.19). The other Tamm state disappears into the continuum at the critical value of the band offset,

$$\sqrt{U_c} = -\sqrt{m_l/2}\left[\Lambda_{11} - \frac{\Lambda_{12}^2}{\Lambda_{22}}\right] = -\sqrt{m_l/2}[(\Lambda^{-1})_{11}]^{-1} . \tag{3.21}$$

In case (b), if $\Lambda_{22} < 0$ the Tamm state does not disappear for any $U > 0$, while for $\Lambda_{22} > 0$ it disappears for $U > U_c$. The critical value is given by the same relation (3.21). A microscopic justification of the connection rules (3.8) for heterojunctions between periodic potentials, together with some generalizations, will be presented elsewhere.[22]

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[20] We assume that at the given energy we are close to the unique minimum or maximum of a single nondegenerate band. The generalization to several bands is straightforward.

[21] We remind the reader that the so-called δ' "potential" is not the distributional derivative of $\delta(x)$.

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