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Scattering states and distribution functions for microstructures

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Orthonormality and completeness relations are found for scattering states, the states used in treatments of resonant-tunneling double barriers and other short microstructures. Explicit normalized states are used to study the density matrix and Wigner distribution function of some simple but nontrivial structures. Analytic expressions describe the quantum repulsion of a sharp barrier at distances comparable to a de Broglie wavelength. As a function of distance from the step, the zero-current density approaches its constant-potential value asymptotically as a Gaussian. We also observe that, by virtue of the exact orthogonality of scattering states, a proposed correction to Esaki and Tsu's calculation of resonant tunneling current is rigorously zero.

I. INTRODUCTION

Development of epitaxial growth techniques has led in recent years to microstructures—semiconductor devices in which the electronic potential can be controlled on practically any length scale larger than the atomic.[1] Historically, slow potential variations (those with length scales larger than an electron or a hole de Broglie wavelength) could always be treated theoretically using a semiclassical (WKB) approximation. Also, periodic potentials could be treated using Bloch states, so long as the lattice or superlattice was longer overall than a typical de Broglie wavelength (λ). In the most common microstructures, however, there is a nonrepeating (one-dimensional) potential composed of one or a few barriers and quantum wells, all in a space comparable to λ. For these "short" microstructures, the semiclassical and Bloch ideas do not suffice, and a more detailed quantum treatment is required.

Typically, these short structures are grown with flat-potential "cladding layers" on either side. It has been recognized that a natural basis of quantum states for such structures is provided by "scattering states,"[2-4] defined by boundary conditions imposed far from the structure: on one side of the structure the state is composed of an incident plane wave plus a reflected wave; in the other cladding layer there is only a transmitted wave moving away from the structure. Far from the structure, states are characterized completely by k-dependent reflection and transmission amplitudes r and t.

Scattering states are particularly convenient for the computation of transport properties; in particular, Landauer[2] showed that the resistance of a one-dimensional structure is an average of $|r|^2/|t|^2$. In general, it is clear how to perform the sum over states that corresponds to a packet initially localized and moving toward the structure. For a known potential, this is sufficient for the prediction of many quantities, like the low-field dc conductivity, which can be measured by macroscopic probes.

In more detailed studies, one wants to know the density matrix or the Wigner distribution function throughout space, often as part of a scheme to determine self-consistently the electrostatic corrections to the heterostructure potential. To perform these computations, one needs orthonormality and completeness (ONC) relations for the scattering basis. In their absence, two approaches have been used: (1) the density matrix has been evaluated in a discrete basis of localized states (e.g., see Ref. 5), or (2) the distribution function has been chosen as that sum of scattering states which gives the correct distribution function at infinity.[2-4]

A local basis is clearly inconvenient for analytical work, and in numerical work the use of a basis of local states defined on a grid leads to nonphysical features on length and momentum scales defined by the grid spacing and size. On the other hand, the usual method of applying scattering states must be considered heuristic. In particular, current-conservation arguments give correctly the probability that a state will be occupied, but they do not yield the normalization for these states and do not give the overlap integral between degenerate states. Recently, Coon and Liu[6] have noted that the usual way of writing the current, as a simple sum of contributions from individual scattering states, contains the implicit assumption that degenerate scattering states are orthogonal; they have proposed a correction to the resonant tunneling current computed by Esaki and Tsu,[3] based on the presumed nonorthogonality of degenerate scattering states.

In the present paper, we clarify the situation by deriving the ONC relations in general. The ONC relations are found by observing that scattering states are *by construction* solutions of the Lippmann-Schwinger equation, and so obey the same orthonormality relations as a related set of "unperturbed" states. Specifically, an orthogonal, normalized basis is obtained when scattering states are normalized so that the incident part of the wave function equals the incident part of a *free* state with the same momentum. This implies, *inter alia*, that degen-

erate states incident from opposite directions *are* orthogonal, so that Esaki and Tsu's original calculation is correct.

Since scattering states are eigenstates of the Hamiltonian, the Boltzmann factor is diagonal in this basis. As a result, simple expressions for the density matrix and various other quantities are recovered.

After deriving the ONC relations and some useful scattering-state sums, we treat the simple step potential as exactly as possible. This example illustrates how quantum repulsion can deplete electrons from the vicinity of a barrier, as an effect of electrostatic band bending. This confirms a conjecture that has been put forward to explain low-density regions found by numerical simulation.[5] The present results also provide a valuable test of numerical programs, and suggest some of the analytic results that are possible. Other examples are delay-time calculations for isolated wave packets. These examples utilize the Green's functions constructed from a complete basis of states, and will be described elsewhere.[7]

As noted earlier, scattering states have already been recognized as providing a natural and useful basis for the study of short structures.[2–4] Nevertheless, a formal theory of this one-dimensional scattering problem, analogous to that which exists for three-dimensional potential scattering,[8] has not been developed previously. Here we apply a single element of such a theory: the norm-preserving property of the Lippmann-Schwinger equation.[9] Other useful components of formal scattering theory are phase-shift analysis and the extension to complex energies. In a subsequent paper, we will describe how the usual treatment, based on spherically symmetric scatterers, can be modified to apply to the short microstructure geometry. In the present paper, the method used to obtain an asymptotic expansion of the density will suggest the utility of a detailed complex energy analysis.

II. MODEL AND SCATTERING STATES

We will treat electrons in the single-particle, effective-mass approximation. Each electron acts under a Hamiltonian

$$H=-\frac{\hbar^2}{2m}\nabla^2+V\ . \tag{1}$$

The potential depends on only one coordinate, x, so motion in the remaining two "perpendicular" directions is trivial. Henceforth, therefore, we regard ∇ as $\partial/\partial x$, and exclude from "energy" the kinetic contributions from momentum in the perpendicular directions.[10] Furthermore, in the usual situation of modulation doping, the carrier density is much larger in the cladding layers than in the microstructure, so the potential V approaches a constant on either side. We can thus define

$$V_{\pm}=\lim_{x\to\pm\infty}V(x)\ . \tag{2}$$

The potential drop across the structure is V_+-V_-. For the time being, we will assume that the potential achieves its limiting values at a finite distance from the structure: i.e., there exist x_-,x_+ such that $V(x)=V_-$ for $x<x_-$, $V(x)=V_+$ for $x>x_+$. Our results are essentially unchanged if the potential approaches its limiting values at positive and negative infinity sufficiently fast. This is discussed in Sec. III.

One convenient set of solutions is given by the (incoming) scattering states. Choosing a normalization prefactor that will be convenient later, we write for $k<0$ (right-incident states),

$$\psi_k(x)=\frac{1}{\sqrt{2\pi}}\begin{cases}t(k)\exp(ik'x) & \text{for } x<x_-\ ,\\ \exp(ikx)+r(k)\exp(-ikx) & \text{for } x>x_+\ ,\end{cases} \tag{3a}$$

and for $k>0$ (left-incident states),

$$\psi_k(x)=\frac{1}{\sqrt{2\pi}}\begin{cases}\exp(ikx)+r(k)\exp(-ikx) & \text{for } x<x_-\ ,\\ t(k)\exp(ik'x) & \text{for } x>x_+\ .\end{cases} \tag{3b}$$

Here and below, k' is an implicit function of k: it is the wave vector of the transmitted wave associated with an incident wave vector k. Thus for right-incident states, $k=-[(2m/\hbar^2)(E-V_+)]^{1/2}$ and $k'=-[(2m/\hbar^2)(E-V_-)]^{1/2}$, while for left-incident states, $k=[(2m/\hbar^2)(E-V_-)]^{1/2}$ and $k'=[(2m/\hbar^2)(E-V_+)]^{1/2}$.

The boundary condition expressed by (3) is that the "incoming" part of the wave function correspond to a plane wave incident from right or left. A way to incorporate this boundary condition is by using the Lippmann-Schwinger equation. Symbolically, this is

$$\psi=\psi^0+G_0(E)(V-V_0)\psi\ . \tag{4}$$

Here, ψ^0 is any solution of the Schrödinger equation for energy E and an "unperturbed" Hamiltonian

$$H_0=-\frac{\hbar^2}{2m}\nabla^2+V_0\ . \tag{5}$$

G_0 is a Green's function corresponding to this Hamiltonian. In the form given, with V_0 not necessarily zero, the solution ψ^0 is chosen to satisfy the same boundary condition that is to be imposed on the desired solution ψ. This implies that V_0 must be chosen to coincide with V at positive and negative infinity. The practical advantage of using (4) to impose the boundary conditions is that these are imposed on states of a V_0 which may be chosen to have simple solutions. For the important case of $V_-=V_+$, one can choose $V_0(x)=V_-$, and ψ^0 of the form (3) are $\psi^0_k=(1/\sqrt{2\pi})\exp(ikx)$.

It should also be noted that a range of different boundary conditions satisfied by a single ψ^0 can give rise to a corresponding range of solutions of the Lippmann-Schwinger equation. [For example, requiring that the *outgoing* part of the wave function coincide with ψ^0 gives rise to outgoing, or advanced, scattering states $\psi_k^{(-)}$, rather than the more common ingoing (retarded or casual) states (3). The two are related by $\psi_k=(\psi_{-k}^{(-)})^*$.] The choice of boundary condition corresponds to the choice of Green's function. The appropriate Green's function for incoming boundary conditions is the Fourier trans-

form of that time-domain Green's function $G_0^{(+)}(t)$ which approaches zero at large positive time.

III. ORTHONORMALITY AND COMPLETENESS

In a coordinate representation, the Lippmann-Schwinger equation (4) is realized as an integral equation. We do not propose here that scattering states be found by iterative application of the integral equation (4). It is usually more efficient in one-dimensional problems to construct linear combinations of the form (3) by integrating the differential (Schrödinger) equation directly. Once one has such a solution, however, it is clear that, since the boundary condition determines the state uniquely, it is also a solution of (4), and has any properties that can be derived formally from that equation. The property that we wish to use is that sets of solutions $\{\psi_k\}$ obey the same orthonormality relations as do the unperturbed set $\{\psi_k^0\}$ to which they are related through the Lippmann-Schwinger equation: $\langle \psi_k^0 \mid \psi_{k'}^0 \rangle = \langle \psi_k \mid \psi_{k'} \rangle$. This is proven in most elementary quantum texts.[9] More specifically, we will seek a potential V_0 and a basis of states $\{\psi_k^0\}$ which have the same incident part of the wave function as (3). Then

$$\int_{-\infty}^{\infty} dx\ \psi_k^*(x)\psi_q(x)=\delta(k-q) \tag{6}$$

will follow when one can show that the same relation holds with ψ_k replaced by ψ_k^0.

For the special case of $V_-=V_+$ we can use plane-wave states as defined earlier; these are well known to satisfy (6). In the general case we define

$$V_0(x)=V_-\Theta(-x)+V_+\Theta(x)+v\delta(x),\quad v>0\ , \tag{7}$$

where Θ is the unit step function: $\Theta(u)=1$ if $u>0$, $\Theta(u)=0$ if $u<0$. This is a family of "unperturbed" potentials parametrized by the strength v of a δ-function barrier at the origin. The states $\{\psi_k^0\}$ corresponding to a particular v satisfy a normalization condition that is independent of v, so we may select any v to confirm (6). As $v\to\infty$, the two sides $x>0$ and $x<0$ become decoupled, and $\psi_k^0=i(2/\pi)^{1/2}\Theta(-kx)\sin(kx)$ satisfies the requisite boundary condition. Then (6), with ψ_k^0 in place of ψ_k, is easily verified, completing the proof that states of the form (3) are normalized and satisfy the orthogonality relation (6).

We can put this result to immediate use. Coon and Liu[6] have redone Esaki and Tsu's[3] calculation of the current in a resonant tunneling structure. They performed the statistical average more carefully, however, constructing many-electron product states from degenerate pairs of left- and right-incident single-electron states, and found a correction to the tunneling current, expressible in terms of the degenerate-state overlap. They concluded from an estimate of this overlap that there is a significant correction. The present demonstration of orthogonality replaces this estimate with a rigorous value of zero, showing that the original result of Esaki and Tsu is correct.

One point emphasized by Coon and Liu illustrates the special utility of the orthogonality relations in tunneling problems. They noted that since the tunneling current decreases exponentially with the barrier thickness, a nonorthogonality that is exponentially small can still give rise to fractionally large effects. Thus even very good estimates of the overlap can lead to poor results, so exact results are particularly valuable.

We now seek a completeness relation to complement the orthonormality condition (6). It is then necessary to consider that for a general potential of the form chosen, there may also be bound states. By a standard argument using the Wronskian, it is known that these states are nondegenerate and mutually orthogonal.[9] Also, they all have energies below V_-, the bottom of the continuum, and so are orthogonal to all the scattering states.

The bound states and the scattering states, taken together, comprise the largest set of independent eigenstates of H that we can construct. If the Hamiltonian acted in a bounded space, Sturm-Liouville theory would guarantee that its eigenstates would form a complete basis.[9] Because the Hamiltonian is taken over an infinite space ($-\infty<x<\infty$), completeness is difficult to demonstrate rigorously. Nevertheless, it is the assumption that is usually and very successfully made in treating physical problems. It is supported by the observation that an adiabatic perturbation of the potential transforms the complete $\{\psi^0\}$ basis continuously into the combined basis of scattering and bound states. Taking the formal limit of the Sturm-Liouville result for a finite space and discrete basis, we write

$$\sum_n \psi_n(x)\psi_n^*(x')+\int_{-\infty}^{\infty} dk\ \psi_k(x)\psi_k^*(x')=\delta(x-x')\ . \tag{8}$$

Observe that the integrand in the second term on the left is discontinuous at $k=0$ if $V_-\neq V_+$.

In order to have a simple statement of the normalization condition (3), the discussion of this section has been for a potential which attains its limiting values at finite distances from the origin (at x_+ and x_-). The results hold for more general potentials, however, such as those approaching constants exponentially fast at positive and negative infinity. For these more general potentials the equalities (3) need be satisfied only asymptotically.

IV. THERMAL AVERAGES

All the single-particle information about the equilibrium system is given by the density matrix, which is a representation of the Gibbs operator $Z^{-1}\exp(-\beta H)$: $\rho(x,x')=(1/Z)\langle x \mid \exp(-\beta H) \mid x' \rangle$; Z is the partition function. We will consider the case of Boltzmann statistics. Energy eigenstates diagonalize the Gibbs operator, so we can write

$$\rho(x,x')=\frac{1}{Z}\left[\sum_n \psi_n(x)\psi_n^*(x')\exp(-\beta E_n) + \int_{-\infty}^{\infty} dk\ \psi_k(x)\psi_k^*(x')\exp[-\beta E(k)]\right]\ . \tag{9}$$

The E_n and $E(k)$ are the energies of the bound and scattering states, respectively. The scattering-state ener-

The E_n and $E(k)$ are the energies of the bound and scattering states, respectively. The scattering-state energies can be found far from the structure, where the potential is constant and the wave functions are combinations of plane waves. Thus $E(k)=(\hbar^2/2m)k^2+V_{-\sigma}$, where σ is the sign of k.

The ordinary density is just the diagonal element of the density matrix:

$$\rho(x)=\frac{1}{Z}\left[\sum_n |\psi_n(x)|^2\exp(-\beta E_n) + \int_{-\infty}^{\infty} dk\,|\psi_k(x)|^2\exp[-\beta E(k)]\right]. \quad (10)$$

The partition function Z has a physical interpretation: $Z=\exp(-\beta F)=\langle\exp(-\beta H)\rangle$. Here, because of our infinite-space normalization, the free energy F is an intensive quantity. From a thermodynamic point of view, the two cladding layers on opposite sides of the microstructure can be considered separate macroscopic systems, thermally and diffusively coupled across a negligibly short contact region ($x_-<x<x_+$).[11] In equilibrium the free energy is the same for the two systems. In either system, the microstructure is an edge effect, and the free energy takes the standard bulk value. Writing $\rho_\pm=\lim_{x\to\pm\infty}\rho(x)$, this implies

$$Z^{-1}=2\sqrt{\pi}\lambda_{\rm th}\rho_-\exp(\beta V_-)=2\sqrt{\pi}\lambda_{\rm th}\rho_+\exp(\beta V_+)\,, \quad (11)$$

where we have introduced the thermal de Broglie wavelength

$$\lambda_{\rm th}=\hbar\left[\frac{\beta}{2m}\right]^{1/2}. \quad (12)$$

Boltzmann statistics are valid when the state occupancy is low; with (11), that is $\lambda_{\rm th}\rho\ll 1$.

In the asymptotic regimes $x<x_-$ and $x>x_+$, one can express the scattering states, and thus the integral part of the density, completely in terms of the reflection and transmission amplitudes. For convenience we assume in the following that the coordinate axis is oriented so that $V_+\geq V_-$.

Before writing the density as described, it is useful to observe that at any energy, the reflection and transmission amplitudes for motion in opposite directions are related by a kind of detailed balance. To see this we note that the question only arises when both left- and right-incident states exist and have nonzero transmission amplitudes. It follows that ψ_k and ψ_k^* are linearly independent, and can be combined to form the degenerate state with incident wave vector $-k'$. Comparing the result with (3),

$$t(-k')=\frac{1-|r(k)|^2}{[t(k)]^*}\quad\text{and}\quad r(-k')=-\frac{t(k)[r(k)]^*}{[t(k)]^*}\,. \quad (13)$$

Using (13) and current continuity $[k(1-|r(k)|^2)=k'|t(k)|^2]$, and observing $kdk=k'dk'$, we find

$$\rho(x<x_-)-\rho_-=\frac{1}{Z}\left[\sum_n |\psi(x)|^2\exp(-\beta E_n)+\mathrm{Re}\left[\int_0^{\infty} dk\frac{1}{\pi}r(k)\exp[-2ikx-\beta E(k)]\right]\right] \quad (14a)$$

and

$$\rho(x>x_+)-\rho_+=\frac{1}{Z}\left[\sum_n |\psi(x)|^2\exp(-\beta E_n)+\mathrm{Re}\left[\int_{-\infty}^{0} dk\frac{1}{\pi}r(k)\exp[-2ikx-\beta E(k)]\right] + \int_0^{k_0} dk\frac{1}{2\pi}|t(k)|^2\exp[-\beta E(k)-2|k'|x]\right]. \quad (14b)$$

The third term in (14b) contains the contribution from extended states which penetrate into $x>x_+$ with imaginary wave vector k'; k_0 is that positive k corresponding to transmitted wave vector $k'=0$. There is no similar term in (14a) because $V_+\geq V_-$, so there can be no extended states in $x>x_+$ with imaginary wave vector in $x<x_-$.

In deriving the expressions (14), the terms ρ_- and ρ_+ in (14a) and (14b), respectively, were obtained by using the corresponding expressions for Z in (11). On the right-hand sides, as $x\to\pm\infty$, the sums must vanish because the bound states are normalized, and the integrals over the reflection amplitude vanish by the Riemann-Lebesgue lemma.[12] The second integral in (14b) vanishes because $|t(k)|^2$ cannot have any singularity as strong as a δ-function at $k=k_0$. The vanishing of the right-hand sides confirms that $\rho_\pm$ are in fact the limiting values of the density. Since (14a) and (14b) were derived with the use of the reciprocity relations (13), confirming the two expressions for Z in this way demonstrates that the second equality in (11) expresses the detailed balance of left- and right-directed currents. Thus, for a fixed choice of limiting potentials $V_\pm$ and temperature, any increase in reflection that tends to increase the density on one side of the microstructure is compensated by a reduced transmission of oppositely directed current.[11]

The density matrix contains all one-particle information about a statistical system; an equivalent representation of this information is contained in the Wigner distribution function, defined[13]

$$f_W(x,p)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dy\,\exp(-ipy/\hbar)\rho(x+\tfrac{1}{2}y,x-\tfrac{1}{2}y)\,. \quad (15)$$

This function is more intuitively accessible because in the classical limit it approaches the classical distribution function. In addition, expectation values of functions of position *or* momentum can be evaluated directly by integration over the distribution.

As a basis for comparison with new results, we note that for a constant potential, with a uniform density $\bar{\rho}$,

$$\rho(x,x')=\bar{\rho}\exp[-\tfrac{1}{4}(\tilde{x}-\tilde{x}')^2] \tag{16}$$

and

$$f_W(x,p)=\frac{\bar{\rho}}{\hbar\sqrt{\pi}}\lambda_{\rm th}\exp(-\tilde{p}^2)\ , \tag{17}$$

where for convenience we have defined dimensionless quantities

$$\tilde{x}=x/\lambda_{\rm th}\quad\text{and}\quad\tilde{p}=\frac{p}{\hbar}\lambda_{\rm th}\ .$$

One obtains the same effect by choosing units so that $2m=\hbar=\beta=1$.

V. ONE-STEP POTENTIALS

A. Infinite barrier

We define an infinite barrier potential to confine particles in the left half-space: $V(x)=0$ for $x<0$, ∞ for $x>0$. There can only be left-incident states, and these are clearly sine waves restricted to negative x. For this potential one can compute the density matrix exactly:

$$\rho(x,x')=\rho_-\{\exp[-\tfrac{1}{4}(\tilde{x}-\tilde{x}')^2]-\exp[-\tfrac{1}{4}(\tilde{x}+\tilde{x}')^2]\} \tag{18}$$

for $x,x'<0$, and $\rho=0$ otherwise. Immediately, we also have

$$\rho(x)=\rho_-[1-\exp(-\tilde{x}^2)]\quad\text{for } x<0\ . \tag{19}$$

Note that the density approaches its limiting value ρ_- exponentially fast. We expect to see similar behavior in the presence of a finite barrier at low temperatures—i.e., when few electrons have energies comparable to the barrier height. We confirm this explicitly below, giving a measure of how well the infinite-barrier results describe the finite-barrier situation.

Near the barrier, the density approaches zero quadratically. It is important to note that this is *not* a depletion layer in the usual sense. It is *not* caused by band bending; there are indeed no electromagnetic fields in the problem as we are treating it. The decreased density here is a "quantum repulsion." A sharp cutoff in the density at $x=0$ requires wave function components with a large momentum, while at a finite temperature only momenta of magnitude less than about $\hbar/\lambda_{\rm th}$ are available, leading to a broadened cutoff of the density on a length scale of about $\lambda_{\rm th}$. Quantum repulsion is, in a sense, complementary to barrier penetration: just as a nonzero density penetrates a finite distance into a classically forbidden region, a density deficit penetrates a finite distance into a classically allowed region. In this simplest model problem the barrier is penetrated only to an infinitesimal depth because the barrier has infinite height.

A barrier repulsion has been observed previously in numerical studies of the Wigner distribution.[5] The present analytic computation confirms the explanation given for those numerical results.

From (18), we may compute the Wigner distribution function

$$f_W(x,p)=\frac{\rho_-\lambda_{\rm th}}{2\pi\hbar}\Theta(-x)[f_W^{(1)}(x,p)-f_W^{(2)}(x,p)]\ , \tag{20}$$

where

$$f_W^{(1)}(x,p)=\sqrt{\pi}\exp(-\tilde{p}^2)[\mathrm{erf}(i\tilde{p}-\tilde{x})-\mathrm{erf}(i\tilde{p}+\tilde{x})]$$

and

$$f_W^{(2)}(x,p)=-4\tilde{x}\exp(-\tilde{x}^2)\frac{\sin(2\tilde{p}\tilde{x})}{2\tilde{p}\tilde{x}}\ .$$

We use the conventional definition of the error function:

$$\mathrm{erf}(u)\frac{2}{\sqrt{\pi}}\int_0^u dt\exp(-t^2)\ .$$

This Wigner distribution is illustrated in Figs. 1 and 2. Far from the step (large $|x|$), it approaches the free-particle Maxwellian distribution [Eq. (17)].

Near the barrier the distribution exhibits a number of nonclassical features. One such feature, as Figs. 1 and 2 make clear, is the existence of regions where the Wigner distribution is negative. These do not contradict the interpretation of f_W as a probability distribution: in order to measure a negative probability, one would have to perform a simultaneous measurement of momentum and position that violated Heisenberg's uncertainty principle.

We can investigate the oscillatory behavior analytically by regarding f_W as a function of the independent variables $\tilde{x}$ and $\xi=2\tilde{x}\tilde{p}$, and then expanding in powers of $\tilde{x}$:

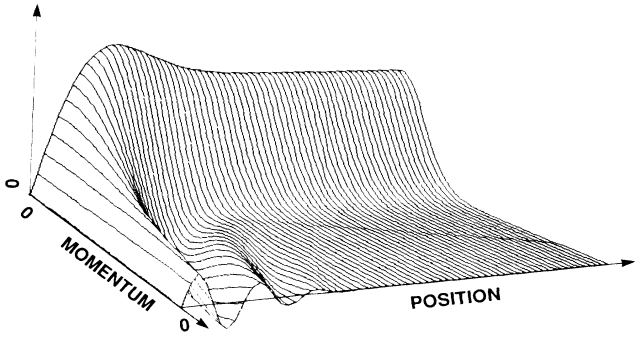

FIG. 1. The Wigner distribution function for an infinite barrier, in arbitrary units. Zero of position is at the edge of the barrier. Perspective is chosen to display quantum repulsion near the barrier.

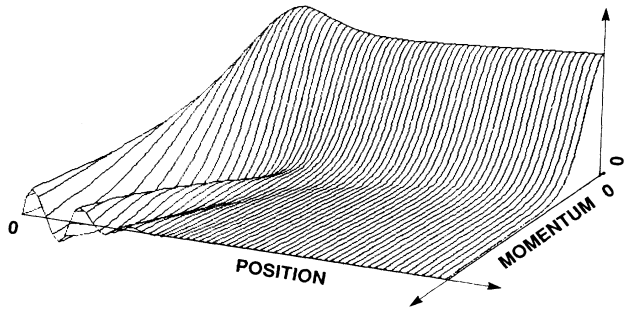

FIG. 2. The same distribution, viewed from a different perspective, chosen to display oscillations.

$$f_W(x,p)\frac{\rho_-\lambda_{\rm th}}{2\pi\hbar}\Theta(-x)4\,|\,\bar{x}\,|\left[\exp\left[\bar{x}^2\frac{d^2}{d\xi^2}\right],\right.$$
$$\left.-\exp(-\bar{x}^2)\right]\frac{\sin\xi}{\xi}.$$

For small $\bar{x}$,

$$f_W(x,p)\simeq\frac{\rho_-\lambda_{\rm th}}{2\pi\hbar}\Theta(-x)\tfrac{8}{3}\,|\,\bar{x}\,|^3 g(\xi)\,, \tag{21}$$

with

$$g(\xi)=\frac{3}{\xi^3}(\sin\xi-\xi\cos\xi)\,.$$

At $|\,\xi\,|\simeq 5.765$, g has minima which make the distribution function negative [$g(\xi)\simeq -0.086$]. Successive extrema of g, located approximately at $\pm(n^2\pi^2-3)/n\pi$, $n=3,4,\ldots$ alternate in sign.

For small ξ, $g(\xi)\simeq 1-\frac{1}{10}\xi^2$. Because $g(\xi)$ extends over a fixed range in xp, it follows that as one approaches the step, the local momentum distribution becomes broader. This has also been observed in the numerical study[5] that found barrier repulsion, and it is consistent with the explanation given earlier of quantum repulsion: only high-momentum components of the incident current can penetrate close to barrier.

We can examine this in detail by considering moments of the momentum distribution as functions of distance from the barrier. In particular,

$$\langle p^2\rangle=\frac{\int p^2 f_W(x,p)dp}{\int f_W(x,p)dp}\,,$$

which we can evaluate with (20) to find

$$\langle p^2\rangle=\left[\frac{\hbar}{\lambda_{\rm th}}\right]^2\frac{1}{2\pi}[1-\exp(-\bar{x}^2)]^{-1}\,. \tag{22}$$

Thus the root-mean-square momentum diverges as x^{-1} for small x, consistent with the factorization of f_W into x and ξ terms in (21).

B. Finite-height barrier

We now consider a more realistic version of the barrier in example A. The potential is chosen to be $V(x)=V_0\Theta(x)$, with $V_0>0$. Using the prescription given in Sec. II, it is easy to write a complete basis of normalized scattering states. Furthermore, because the potential is constant from either side of $x=0$ out to infinity, the asymptotic expressions (3) are valid everywhere except at the origin and the density may be found with expressions like (14). It suffices to state that $r(k)=(k-k')/(k+k')$ and $t(k)=2k/(k+k')$ for $k>0$, and that there are no bound states.

It is possible to perform the integration in (14a) for $x\to 0^+$ in closed form. Defining the temperature-scaled potential $\tilde{V}_0=\beta V_0$, this is

$$\rho(0)=\rho_-\left[\frac{1-\exp(-\tilde{V}_0)}{\tilde{V}_0}\right]. \tag{23}$$

Thus, as $\tilde{V}_0\to\infty$, the infinite-barrier result of $\rho(0)=0$ is approached only algebraically fast: $\rho(0)=(\rho_-/\tilde{V}_0)+O(\exp(-\tilde{V}_0))$. For small barrier heights, $\rho(0)=\frac{1}{2}(\rho_-+\rho_+)+O((\tilde{V}_0)^2)$.

In order to find the density in $x<0$, we will use expression (14a), in which, for the present case, there is no contribution from bound states. We deform the contour of integration to follow the imaginary axis to $k=i\,|\,\bar{x}\,|/\lambda_{\rm th}$ and then go to $k=\infty$. Note that the analytic continuation of $r(k)$ along the imaginary axis is real, so this part of the integration gives no contribution to the density. Evaluating the remaining integral by the method of steepest descents, we find

$$\rho(x<x_-)=\rho_-[1-\exp(-\bar{x}^2)(1-K)]\,, \tag{24}$$

where the correction is given by

$$K\sim\frac{2\bar{x}^2}{\tilde{V}_0}(U-1)+\frac{1}{2\tilde{V}_0}(2+U^{-1}+U^{-3}) \tag{25}$$

with

$$U^2=\left[1+\frac{\tilde{V}_0}{\bar{x}^2}\right].$$

[Expression (25) gives the dominant behavior as $x\to-\infty$, and the dependence on $\tilde{V}_0$ is given exactly. That is, the difference between K and the asymptotic expression on the right-hand side of (25) approaches zero as an exponential of $\bar{x}^2$.] What we may conclude from (24) and (25) about general potentials is that far from a step down, the infinite-barrier result (19) will be accurate, and that a further deviation in the density of about

$$\rho_-\exp(-\bar{x}^2)(\bar{x}^2/\tilde{V}_0)^{1/2}$$

will be associated with a V_0 that is finite but still large compared to kT.

VI. CONCLUSION

The main results of this paper, obtained in Sec. III, are the orthonormality and completeness relations [Eqs.

(6) and (8)] for a scattering-state basis. Roughly speaking, scattering states have the usual k-space normalization if they are scaled to have the same incident current as plane-wave states. The relations are valid for the one-dimensional potentials generally used to model transport in microstructures. It should be noted that they hold even when there is a potential drop across the microstructure. In this situation, k-space normalization holds with k labeling the incident momentum far from the structure.

We use the newly derived orthonormality relations to reconsider a proposed correction to Esaki and Tsu's calculation of the current in a resonant tunneling structure. The exact orthogonality of scattering states implies that the proposed correction is precisely zero.

As a first demonstration of the utility of the orthogonality and completeness relations in explicit computations, we derive general expressions for the equilibrium density matrix and obtain some analytic results for single-step potentials. These demonstrate clearly a number of nonclassical effects, and are also useful for testing numerical programs.

Far from the barrier, a Maxwellian distribution is approached. We find the density matrix in closed form for an infinite barrier and determine the asymptotic deviations from this for a finite barrier.

Near the barrier, there is a nonelectrostatic quantum repulsion and an associated broadening of the momentum distribution. Our calculations confirm the explanation put forward when these were first observed numerically. The detailed behavior demonstrates that the shape of the Wigner distribution near the barrier is a function of the form of the barrier itself, and cannot be estimated from the boundary conditions alone.

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