Properties of the Landauer resistance of finite repeated structures

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Several properties of the Landauer resistance of finite repeated structures are derived. A theorem relating the energies of unity transmission through a finite repeated structure to the band structure of an infinite superlattice formed by periodic repetition of the finite structure [Vezzetti and Cahay, J. Phys. D **19**, L53 (1986)] is generalized to the case of structures with spatially varying effective mass. We also establish a *sum rule* for the Landauer resistances of periodic structures formed by periodically repeating a basic subunit. Finally, we derive an analytical expression for the "boundary resistance" of a structure, as introduced by Azbel and Rubinstein in connection with pseudolocalization, and prove several properties of this quantity.

I. INTRODUCTION

The Landauer formula[1] for calculating the resistance of a dissipationless mesoscopic structure has been used quite widely in the study of quantum transport phenomena. The formula relates in a simple way the resistance of a structure (in the linear-response regime) to the probability of transmission of an electron through the structure. The usefulness of the formula lies in the fact that it reduces the problem of quantum mechanically calculating resistance—a rather difficult problem—to a much simpler problem of calculating just the transmission probability. In this paper, we prove several interesting properties of the Landauer resistance (i.e., the resistance in the linear-response regime) of a finite repeated structure such as a semiconductor superlattice. These properties are all derived from the properties of the transmission coefficient of an electron through a periodic potential of finite spatial extent.[2–5]

In Sec. II of this paper, we first employ a transfer-matrix technique to derive a general expression for the transmission probability of an electron through an arbitrary potential profile. We then extend this result in Sec. III to calculate the transmission probability $|T_N|^2$ of an electron through N subunits of a finite repeated structure. Using this expression, we extend an earlier result[5] relating the energies of unity transmission through a finite repeated structure to the energy–wave-vector relation for an infinite structure formed by periodically repeating the basic subunit of the finite structure. In Sec. IV, we prove a set of theorems that establish interesting and useful relationships between the transmission probabilities (and hence the Landauer resistances) associated with the subunits of a finite repeated structure. These theorems are all illustrated with numerical examples dealing with compositional and effective-mass superlattices. In Sec. V, we establish a *sum rule* for the Landauer resistances of periodic structures formed by successively repeating a basic subunit, and in Sec. VI, we derive an exact analytical expression for the "boundary resistance" of a structure as introduced by Azbel and Rubinstein in connection with pseudolocalization. Finally, in Sec. VII, we summarize our conclusions.

II. TRANSMISSION OF AN ELECTRON THROUGH AN ARBITRARY POTENTIAL

In this section, we first derive an expression for the transmission coefficient of an electron through an arbitrary *one-dimensional* potential of finite spatial extent. For the sake of generality, we allow for spatial variation of the electron's effective mass but assume it varies only in one direction. The time-independent Schrödinger equation describing the steady-state (ballistic) motion of an electron through such a potential is

$$-\frac{\hbar^2}{2m^*(z)}\frac{\partial^2\psi}{\partial x^2}-\frac{\hbar^2}{2m^*(z)}\frac{\partial^2\psi}{\partial y^2}-\frac{\hbar^2}{2}\frac{\partial}{\partial z}\left[\frac{1}{m^*(z)}\frac{\partial\psi}{\partial z}\right]+E_c(z)=E\psi\ , \quad (1)$$

where $E_c(z)$ is the one-dimensional potential that varies in the z direction and $m^*(z)$ is the spatially varying effective mass. In a semiconductor heterostructure, $E_c(z)$ is the conduction-band edge profile which incorporates any band bending due to space charges, variations due to compositional inhomogeneity, and also variations due to any external electric field.

Because the Hamiltonian in Eq. (1) is invariant in the x and y directions, the transverse wave vector $\mathbf{k}_t$ is a good quantum number. Furthermore, since the z component of the electron's motion is decoupled from the transverse motion in the x-y plane, the wave function ψ can be written as

$$\psi=\phi(z)e^{i\mathbf{k}_t\cdot\rho}\ , \quad (2)$$

where $\mathbf{k}_t=(k_x,k_y)$ and $\boldsymbol{\rho}=(x,y)$.

The z component of the wave function $\phi(z)$ now satisfies the Schrödinger equation

$$\frac{d}{dz}\left[\frac{1}{\gamma(z)}\frac{d\phi}{dz}\right]+\frac{2m_c^*}{\hbar^2}\{E_p+E_t[1-\gamma(z)^{-1}]-E_c(z)\}\phi(z)=0\ , \quad (3)$$

where m_c^* is the effective mass of the electrons in the "contacts" sandwiching the region of interest (m_c^* is spatially invariant within the contacts and isotropic), $\gamma(z)=m^*(z)/m_c^*$, $E_t=\hbar^2k_t^2/2m_c^*$, and E_p is the kinetic energy associated with the z component of the motion in the contacts ($E_p=\hbar^2k_z^2/2m_c^*$).

The above equation cannot be solved exactly for an arbitrary potential $E_c(z)$. However, an approximate solution can be found by approximating the potential profile by a series of potential steps[6] (see Fig. 1) or by using a piecewise linear approximation for the potential.[7] In the former scheme, the region over which the potential varies is broken down into a finite number of intervals. Within each interval the potential and the effective mass are assumed to be *constant*. In that case, the wave function and its first derivative at the left and right edges of an interval are related through a so-called "transfer matrix," characteristic of that interval, whose elements do not depend on the z coordinate and can be determined analytically.

The transfer matrix for the nth interval $[z_{n-1},z_n]$ is defined according to

$$\begin{bmatrix}\frac{1}{\gamma(z_n^-)}\frac{d\phi}{dz}(z_n^-)\\ \phi(z_n^-)\end{bmatrix}=\begin{bmatrix}W_{11}^{(n)}W_{12}^{(n)}\\ W_{21}^{(n)}W_{22}^{(n)}\end{bmatrix}\begin{bmatrix}\frac{1}{\gamma(z_{n-1}^+)}\frac{d\phi}{dz}(z_{n-1}^+)\\ \phi(z_{n-1}^+)\end{bmatrix}, \quad (4)$$

where $W_{ij}^{(n)}$ are the elements of the transfer matrix, and z_{n-1}^+ and z_n^- stand for $z_{n-1}+\epsilon$ and $z_n-\epsilon$, respectively, with ϵ being a vanishingly small positive quantity. Explicit expressions for the elements of the transfer matrix are given in the Appendix.

Assuming continuity of $\phi(z)$ and $[1/\gamma(z)]/(d\phi/dz)$ everywhere in the structure, the overall transfer matrix $W^{\rm tot}$ describing the entire region $[0,L]$ (see Fig. 1) can be found by simply cascading (multiplying) the individual transfer matrices for the individual intervals:

$$W^{\rm tot}=W^{(N)}\cdots W^{(1)}\ , \quad (5)$$

where $W^{(n)}$ is the transfer matrix for the nth interval as defined in Eq. (4).

The overall transfer matrix $W^{\rm tot}$ relates the wave functions and their first derivatives at the left and right contacts:

$$\begin{bmatrix}\frac{1}{\gamma(L^+)}\frac{d\phi}{dz}(L^+)\\ \phi(L^+)\end{bmatrix}=W^{\rm tot}\begin{bmatrix}\frac{1}{\gamma(0^-)}\frac{d\phi}{dz}(0^-)\\ \phi(0^-)\end{bmatrix}. \quad (6)$$

In Eq. (6), $\phi(0^-)$ and $\phi(L^+)$ are the electronic states inside the left and right contacts. They are given by[1,6–10]

$$\phi(z)=\begin{cases}e^{ik_0z}+Re^{-ik_0z}, & z<0\\ Te^{ik_0(z-L)}, & z>L\end{cases} \quad (7)$$

where k_0 $[=(2m_c^*E_p/\hbar)^{1/2}]$ is the z component of the electron's wave vector in the contact and R and T are the overall reflection and transmission coefficients through the region $[0,L]$. Using these scattering states for the wave functions at $z=0^-$ and $z=L^+$ and noting that, by definition, $\gamma(L^+)=\gamma(0^-)=1$, we obtain from Eq. (6)

$$T\begin{bmatrix}ik_0\\ 1\end{bmatrix}=W^{\rm tot}\begin{bmatrix}ik_0(1-R)\\ 1+R\end{bmatrix}. \quad (8)$$

Equation (8) finally gives us the two equations for the two unknowns T and R. From these two equations T and R can be found by straightforward algebra. Eliminating R gives

$$T=\frac{2ik_0(W_{11}^{\rm tot}W_{22}^{\rm tot}-W_{12}^{\rm tot}W_{21}^{\rm tot})}{ik_0(W_{11}^{\rm tot}+W_{22}^{\rm tot})+(W_{21}^{\rm tot}k_0^2-W_{12}^{\rm tot})}\ , \quad (9)$$

where $W_{ij}^{\rm tot}$ are the elements of the matrix $W^{\rm tot}$ that are found from Eq. (5).

Since $W^{\rm tot}$ is a unimodular matrix,[5] the term within parentheses in the numerator of Eq. (9) is unity. In addition (see the Appendix), $W_{ij}^{\rm tot}$ is always purely real. Therefore Eq. (9) gives

$$|T|^2=\frac{4k_0^2}{k_0^2(W_{11}^{\rm tot}+W_{22}^{\rm tot})^2+(W_{21}^{\rm tot}k_0^2-W_{12}^{\rm tot})^2}\ . \quad (10)$$

The above equation gives us a general expression for the transmission probability of an electron through an arbitrary potential. The transmission probability $|T|^2$ is, of course, related to the reflection probability $|R|^2$ according to the relation $|T|^2+|R|^2=1$ as required by current conservation.

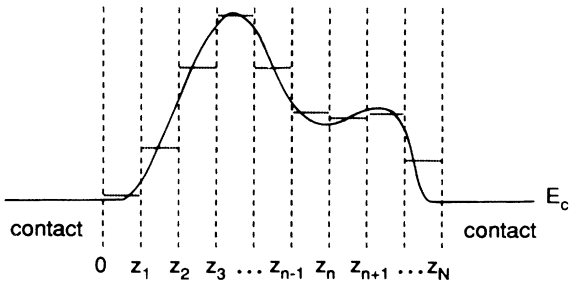

FIG. 1. An arbitrary potential profile approximated by a series of potential steps. Within each interval, the potential and effective mass are assumed to be spatially invariant.

III. TRANSMISSION OF AN ELECTRON THROUGH A FINITE REPEATED STRUCTURE

Having found a general expression for $|T|^2$, we now proceed to evaluate the transmission probability (and hence the Landauer resistance) associated with a finite repeated structure formed by the periodic repetition of a structure with arbitrarily varying potential.

Consider the potential profile in Fig. 2 formed by the

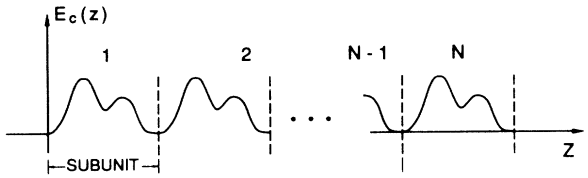

FIG. 2. The potential profile for a finite repeated structure formed by periodic repetition of a region with arbitrarily varying potential.

periodic repetition of an arbitrary potential. Every "period" in this structure has the same transfer matrix (say $\underline{W}$) characterizing that period and the grand overall transfer matrix $\underline{W}^{\text{tot}}$ describing the entire structure is, as before, obtained by cascading the transfer matrices for the individual periods. It is easy to see that for a structure with N periods with each period identical,

$$\underline{W}^{\text{tot}}=(\underline{W})^N \tag{11}$$

As shown in Ref. 10, the elements of the matrix $\underline{W}^{\text{tot}}$ can be expressed in terms of the elements of the matrix $\underline{W}$:

$$\underline{W}^{\text{tot}}=\underline{W}\frac{\sin(N\theta)}{\sin\theta}-\mathbf{I}\frac{\sin[(N-1)\theta]}{\sin\theta}\ , \tag{12}$$

where $\underline{I}$ is a 2×2 identity matrix and θ depends on the eigenvalues of the matrix $\underline{W}$ and is given by

$$\exp(i\theta)=\lambda_1=\lambda_2^{-1}=\frac{\text{Tr}(\underline{W})}{2}+\left[\left[\frac{\text{Tr}(\underline{W})}{2}\right]^2-1\right]^{1/2}\ , \tag{13}$$

where $\lambda_{1,2}$ are the eigenvalues of the 2×2 matrix $\underline{W}$ and the second equality follows from the fact that the matrix $\underline{W}$ is unimodular.

We can now find the overall transmission probability $|T_N|^2$ through a periodic structure with N periods. For this, we use Eq. (10) with the elements of $\underline{W}^{\text{tot}}$ now given by Eq. (12). This gives

$$|T_N|^2=\left\{[\sin^2(N\theta)]\left[\left[\frac{k_0^2W_{21}-W_{12}}{2k_0\sin\theta}\right]^2-1\right]+1\right\}^{-1}\ , \tag{14}$$

which is our main result.

The two- and four-probe (2-p and 4-p) Landauer resistances for a strictly one-dimensional repeated structure can now be found easily by substituting Eq. (14) for the transmission probability $|T_N|^2$ in the single-channel Landauer formula:

$$\begin{aligned}R_L^{2\text{-p}}&=\frac{h}{2e^2}\frac{1}{|T_N|^2}\\&=\frac{h}{2e^2}\left\{[\sin^2(N\theta)]\left[\left[\frac{k_0^2W_{21}-W_{12}}{2k_0\sin\theta}\right]^2-1\right]+1\right\},\\R_L^{4\text{-p}}&=\frac{h}{2e^2}\frac{1-|T_N|^2}{|T_N|^2}=R_L^{2\text{-p}}-\frac{h}{2e^2}\ ,\end{aligned} \tag{15}$$

where k_0 is the wave vector of the incident electron.

IV. TRANSMISSION THEOREMS FOR A FINITE REPEATED STRUCTURE

We now prove a set of theorems related to transmission through finite repeated structures. First, we prove a theorem that relates the energies of unit transmission (i.e., the values of the incident energy for which the transmission coefficient is exactly unity) through a finite repeated one-dimensional structure, to the band structure of the associated infinite lattice formed by periodic repetition of the one-dimensional structure. This theorem was stated for the first time in Ref. 5. A more detailed proof is given here with generalization to the case of a structure with a variable effective mass.

Theorem I. The transmission coefficient of a particle through a periodic structure, formed by N repetitions of a basic subunit, reaches unity at the following energies: (a) energies at which the transmission through the basic subunit is unity, and (b) $N-1$ energies in each energy band of the lattice formed by infinite periodic repetition of the basic subunit, where these $N-1$ energies are given by $E=E_i(k=\pm n\pi/NL)(n=1,2,3,\ldots,N-1$, and L is the length of a period). Here $E_i(k)$ is the energy–wave-vector relation (or the dispersion relation) for the ith band of the infinite lattice.

Part (a) of the theorem is actually fairly obvious. All it states is that by connecting identical structures of transmission unity, one always obtains unit transmission through the composite structure. Although this is intuitive, we prove it nevertheless for the sake of completeness. For this, we first note from Eq. (14) that the transmission $|T_N|^2$ through N periods reaches unity when the term within the large square brackets vanishes. The term within the large square brackets vanishes when

$$\left[\frac{k_0^2W_{21}-W_{12}}{2k_0\sin\theta}\right]^2=1\ . \tag{16}$$

We now show that this corresponds to the condition that $|T_1|^2$ (i.e., the transmission through *one* period, or the basic subunit) is unity. Substituting $N=1$ in Eq. (14), we get that the condition for unit transmission through one subunit is given by

$$1=|T_1|^2=\left\{[\sin^2(\theta)]\left[\left[\frac{k_0^2W_{21}-W_{12}}{2k_0\sin\theta}\right]^2-1\right]+1\right\}^{-1}\ , \tag{17}$$

which, after simplification, reduces exactly to Eq. (16). This proves the first part of the theorem, viz., that the energies of unit transmission through one period are also the energies of unit transmission through all the N periods.

To prove the second part of the theorem, we note from Eq. (14) that the transmission $|T_N|^2$ also reaches unity for those values of θ that satisfy the conditions

$$\sin(N\theta)=0, \quad \sin(\theta)\neq 0 ; \tag{18}$$

i.e.,

$$\theta=\pm\frac{\pi}{N},\pm\frac{2\pi}{N},\pm\frac{3\pi}{N},\ldots,\pm\frac{(N-1)\pi}{N} . \tag{19}$$

We now have to prove that the above values of θ also correspond to the wave vectors $k=\pm n\pi/NL$ where L is the period. For this, we first apply the Bloch theorem to the infinite structure. The Bloch theorem gives

$$\phi(z+L)=\phi(z)\exp(ikL) , \tag{20}$$

where k satisfies the relation[11]

$$\det[W_{ij}-\delta_{ij}\exp(ikL)]=0 . \tag{21}$$

In the above equation, W_{ij} is the ijth element of the transfer matrix W describing one period and δ_{ij} is a Kronecker delta. From Eq. (21) we immediately see that $\exp(ikL)$ is the eigenvalue of the 2×2 unimodular matrix $\underline{W}$ and hence

$$\exp(ikL)=\lambda_1=\lambda_2^{-1}=\frac{\mathrm{Tr}(\underline{W})}{2}+\left[\left[\frac{\mathrm{Tr}(\underline{W})}{2}\right]^2-1\right]^{1/2} . \tag{22}$$

The right-hand sides of Eqs. (13) and (22) are identical so that their left-hand sides must also be identical. Therefore

$$\exp(ikL)=\exp(i\theta) , \tag{23}$$

or

$$kL=\theta(\mathrm{mod}2\pi) . \tag{24}$$

Consequently whenever $k=\pm n\pi/NL$, the quantity $\theta=\pm n\pi/N$. Thus the energies corresponding to $k=\pm\pi/NL,\pm 2\pi/NL,\pm 3\pi/NL,\ldots,\pm[(N-1)\pi]/NL$ are the energies corresponding to $\theta=\pm\pi/N$, $\pm 2\pi/N,\pm 3\pi/N,\ldots,\pm[(N-1)\pi]/N$, which, in turn, are the energies corresponding to unity transmission through the finite repeated structure with N periods as previously noted. Stated in other words, this means that the energies associated with unity transmission through an N-period structure are the band energies $E(k_n)$ corresponding to the wave vectors $k_n=\pm n\pi/NL$ in an infinite repeated structure. This gives us the $E(k_n)$-versus-k_n relation and proves the theorem.

The usefulness of theorem I lies in the fact that by evaluating the energies of unit transmission through a *finite* structure [which we can do from Eq. (14)], we can calculate the band structure of an *infinite* superlattice formed by the periodic repetition of the finite structure.

The locations of the band edges can be found directly from the following property, which we prove: The states characterized by wave vectors k for which $|\mathrm{Tr}(\underline{W})|>2$ are the evanescent states corresponding to the "stop band" of a finite repeated structure. The states characterized by wave vectors k for which $|\mathrm{Tr}(\underline{W})|<2$ are the propagating states corresponding to the "pass band" of the finite repeated structure.

To prove the property, we invoke Eq. (22). If $|\mathrm{Tr}(\underline{W})|>2$, then the right-hand side of Eq. (22) is purely real and *greater than unity*. In that case, the wave vector k must be purely imaginary which means that the state is an evanescent state corresponding to the "stop band" of the finite repeated structure. On the other hand, if $|\mathrm{Tr}(\underline{W})|<2$, the right-hand side of Eq. (22) becomes complex which permits k to be real. In the latter case, the state is a propagating state corresponding to the "pass band" of the structure. The values of wave vector k for which $|\mathrm{Tr}[\underline{W}]|=2$ evidently correspond to the edges between the pass bands and the stop bands.

Theorem II. At the energies of unity transmission through a finite repeated structure with N periods, the following equality holds: $|T_{N_1}|^2=|T_{N_2}|^2$ whenever $N_1+N_2=N$. Here $|T_{N_1}|^2$ and $|T_{N_2}|^2$ are the transmission probabilities through two subsections with N_1 and N_2 periods respectively.

As stated in the proof of theorem I, the transmission $|T_N|^2$ through N periods reaches unity under two conditions: (a) when the transmission through *each* of the N periods is unity, and (b) when

$$\theta=\pm\frac{n\pi}{N} \quad (n=1,2,3,\ldots,N-1) . \tag{25}$$

In case (a), the proof of theorem II is trivial. If the transmission through *each* period is unity, then, of course, the transmission through any arbitrary number of periods is also unity. In that case, obviously,

$$|T_{N_1}|^2=|T_{N_2}|^2=1 , \tag{26}$$

regardless of what N_1 and N_2 might be. This proves the theorem for case (a).

The proof for case (b) proceeds as follows. We first note that

$$\begin{aligned}\sin N_1\theta=\sin(N-N_2)\theta&=\sin(\pm n\pi-N_2\theta)\\&=(-1)^{2n+1}\sin N_2\theta ,\end{aligned} \tag{27}$$

where we used Eq. (25) to obtain the second equality. Using the above equality in Eq. (14), we immediately see that

$$|T_{N_1}|^2=|T_{N_2}|^2 \tag{28}$$

which proves case (b).

Theorem III. At the energies of unity transmission ($|T_N|^2=1$) through a finite repeated structure with N periods, the following equality holds: $|T_{N+M}|^2=|T_{N-M}|^2$ for all M such that $1\leq M<N$.

The proof of this theorem is very similar to that of theorem II and is therefore not presented.

A. Numerical examples

To illustrate theorem I, we show in Fig. 3 the construction of the energy-band diagram of an infinitely repeated structure whose basic subunit is shown in the inset. The points Q,Q' are the two lowest energies at which the transmission through two subunits is unity, whereas the points P,P' and R,R' are the two lowest energies for which the transmission through three subunits is unity. These points are on the two lowest-energy bands. Other points on the energy-band diagram can be found similarly by steadily increasing the number of periods and searching for the energies of unit transmission. Finally, the points P_1,P_2 and Q_1,Q_2 correspond to the band edges and are found from the condition $|\mathrm{Tr}(\underline{W})|=2$.

To illustrate theorems II and III, we provide the following numerical examples.

Example 1. We have calculated the transmission $|T_N|^2$ [using Eq. (14)] through a compositional superlattice consisting of rectangular wells and barriers in which the barrier and well thicknesses are 50 Å. The effective mass was assumed to be $0.067m_0$ everywhere and the barrier height was taken to be 0.3 eV. Figure 4 shows the transmission coefficient through one, two, and three barriers in the vicinity of the lowest resonant energy through two barriers. (Resonant transmission through two barriers has been studied extensively in connection with the double-barrier resonant tunneling diode.[8,12]) Figure 4 is a clear illustration of theorem III. It shows that when the transmission through two barriers is unity, the transmission through three barriers is equal to the transmission through one barrier, i.e., $|T_{N+M}|^2=|T_{N-M}|^2$ with $N=2$ and $M=1$. Figure 4 also shows that whenever $|T_3|^2=1$, $|T_1|^2=|T_2|^2$, illustrating theorem II for the case $N_1=1$, $N_2=2$.

Example 2. In Fig. 5 we show the transmission through an effective-mass superlattice[13] in which the conduction-band edges in the different layers are assumed to be aligned but the effective masses are different. We assume effective masses of $0.039m_0$ and $0.073m_0$, respectively, in two alternating layers. (These correspond to the effective masses of $In_{0.72}Ga_{0.28}As_{0.86}P_{0.14}$ and InP.[14]) The transmissions through one, two, and three layers were calculated from Eq. (14) at the resonant energy through three layers. Clearly, when $|T_3|^2=1$, $|T_1|^2=|T_2|^2$. This illustrates theorem II. Also when $|T_2|^2=1$, $|T_1|^2=|T_3|^2$ as stated in theorem III.

Theorem IV. If the Fermi energy of a finite repeated one-dimensional structure lies at the boundary between a "pass band" and a "stop band," then the four-probe Landauer resistance of N periods of the structure is equal to N^2 times the four-probe Landauer resistance of one period. This means that the four-probe Landauer resistance increases with the structure's length as L^2 instead

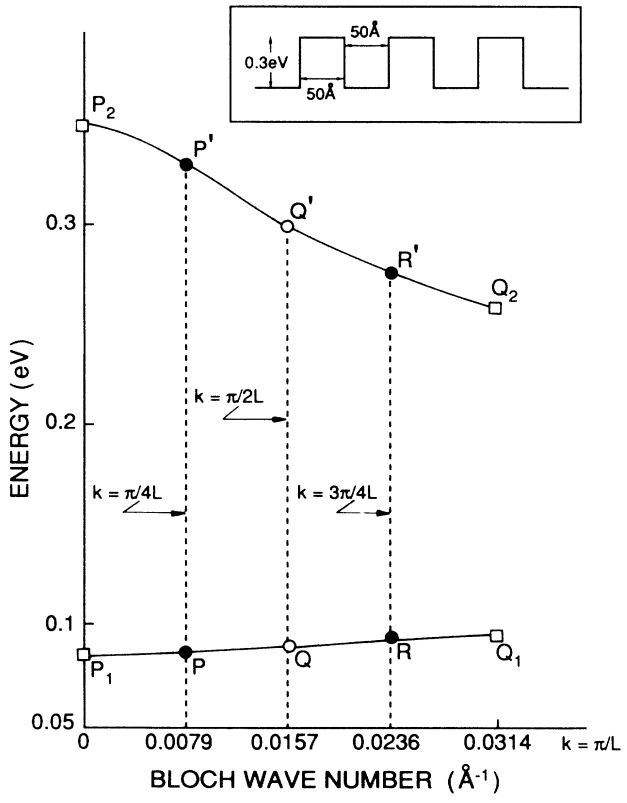

FIG. 3. Energy-band diagram of an infinitely repeated structure whose basic subunit is shown in the inset. The conduction band is constructed by numerically evaluating the energies at which the transmission through increasing number of periods go to unity. The points Q,Q' correspond to the two lowest energies at which transmission through two subunits is unity, whereas the points P,P' and R,R' correspond to the lowest energies for which transmission through three subunits is unity. The points P_1,P_2 and Q_1,Q_2 correspond to the band edges and are found from the condition $\mathrm{Tr}[\underline{W}]=2$.

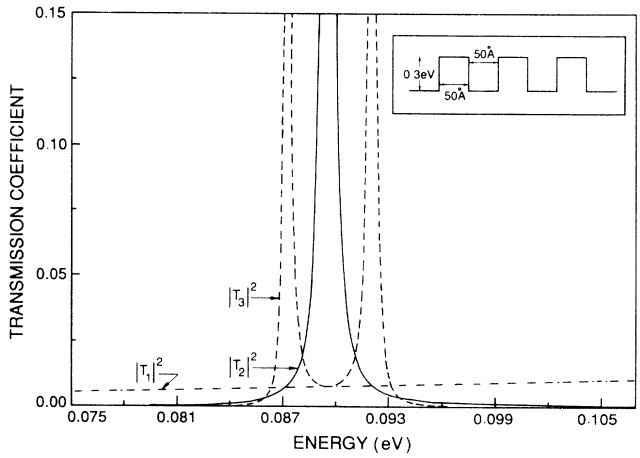

FIG. 4. Transmission coefficients through a periodic structure formed by repeating the subunit shown in the inset. The subunit consists of a GaAs well and an $Al_{1-x}Ga_xAs$ barrier both 50 Å thick. The barrier height is 0.3 eV and the effective mass is assumed to be $0.067m_0$ everywhere. Note that when $|T_3|^2=1$, $|T_1|^2=|T_2|^2$. Also whenever $|T_3|^2=1$, $|T_1|^2=|T_2|^2$. These illustrate theorems II and III, respectively.

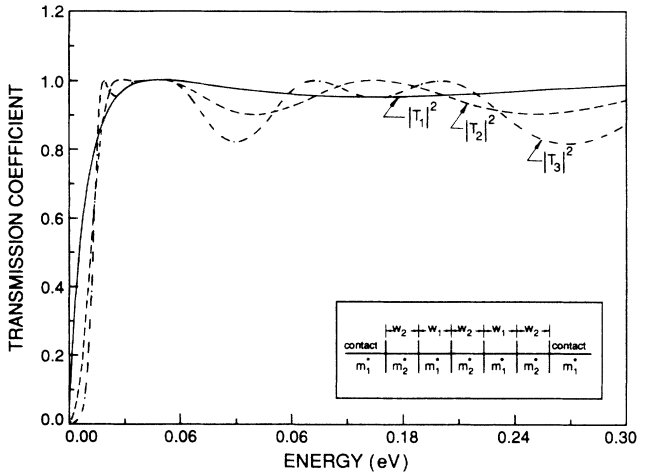

FIG. 5. Transmission coefficient through an effective-mass superlattice. The inset shows the superlattice composed of alternating layers of InP with effective mass $m_1^* = 0.073 m_0$ and $In_{0.72}Ga_{0.28}As_{0.86}P_{0.14}$ with effective mass $m_2^* = 0.039 m_0$. Each layer is 50 Å thick. These figures also illustrate theorems II and III. Note that as stated in theorem II, when $|T_3|^2 = 1$, $|T_1|^2 = |T_2|^2$. Also when $|T_2|^2 = 1$, $|T_1|^2 = |T_3|^2$ illustrating theorem III.

of as L in violation of Ohm's law.

To prove the theorem, we first show that the energies at the boundaries between the pass bands and stop bands of a structure correspond to $\theta = \pm n\pi$, where θ is defined from Eq. (13).

To show this, we first recast Eq. (13) as

$$\exp(i\theta) = \cos\theta + i\sin\theta = \frac{\mathrm{Tr}(\underline{W})}{2} + i\left[1 - \left(\frac{\mathrm{Tr}(\underline{W})}{2}\right)^2\right]^{1/2} . \quad (29)$$

Recalling that at the boundaries (band edges) $|\mathrm{Tr}(\underline{W})| = 2$, we see from the above equation that at the band edges, $\sin\theta = 0$ so that $\theta = \pm n\pi$.

We now obtain a general expression for the four-probe Landauer resistance of one period. Using Eq. (10) for the transmission $|T|^2$ through one period, we obtain

$$\begin{aligned} R_L^{4\text{-p}}(1) &= \frac{h}{2e^2}\frac{1-|T|^2}{|T|^2} \\ &= \frac{h}{2e^2}\left[\frac{(W_{11}+W_{22})^2 + (k^2 W_{21} - W_{12})^2}{4k^2} - 1\right] \\ &= \frac{h}{2e^2}\left[\frac{4k^2\cos^2\theta + (k^2 W_{21} - W_{12})^2}{4k^2} - 1\right] \\ &= \frac{h}{2e^2}\left[\frac{(k^2 W_{21} - W_{12})^2 - 4k^2\sin^2\theta}{4k^2}\right] , \end{aligned} \quad (30)$$

where we used Eq. (29) to substitute for $(W_{11} + W_{22})$ in terms of $\cos\theta$.

From Eq. (15) we also find that the Landauer resistance of N periods is

$$\begin{aligned} R_L^{4\text{-p}}(N) &= \frac{h}{2e^2}\left[\left(\frac{\sin(N\theta)}{\sin\theta}\right)^2 \frac{(k^2 W_{21} - W_{12})^2 - 4k^2\sin^2\theta}{4k^2}\right] \\ &= \left(\frac{\sin(N\theta)}{\sin\theta}\right)^2 R_L^{4\text{-p}}(1) . \end{aligned} \quad (31)$$

At the band edges when $\theta = \pm n\pi$, the above expression becomes

$$R_L^{4\text{-p}}(N) = \lim_{\theta \to \pm n\pi}\left(\frac{\sin(N\theta)}{\sin\theta}\right)^2 R_L^{4\text{-p}}(1) = N^2 R_L^{4\text{-p}}(1) , \quad (32)$$

which proves theorem IV. It also shows that since the resistance of N periods is N^2 times (instead of N times) the resistance of one period, the four-probe Landauer resistance increases with the square of the structure's length instead of with its length. This deviation from Ohmic behavior was pointed out in Ref. 15 where it was demonstrated for a periodic array of "δ potentials." In the present treatment, we have generalized it to any arbitrary potential profile.

The L^2 dependence of the resistance is an interesting feature. It is well known that in the pass band, where the states are extended, the resistance should be Ohmic and increase linearly with L, while in the stop band, where the states are localized, it should increase exponentially with L. The fact, that at the boundaries between the pass bands and stop bands the resistance increases as the *square* of L, can be used to identify the onset of *metal-insulator transition*[16] which occurs when the Fermi energy of a system crosses the boundary between a pass band and stop band.

It is also interesting to note from Eq. (31) that the Landauer resistance at the band edges goes to zero when

$$k^2 W_{21} - W_{12} = 0 . \quad (33)$$

The above condition is in general not satisfied for any arbitrary potential. Specific cases when this condition is satisfied are discussed in Ref. 17.

V. SUM RULE FOR FOUR-PROBE LANDAUER RESISTANCES

In this section, we prove the following "sum rule" for the four-probe Landauer resistances associated with the subunits of a repeated one-dimensional structure.

The four-probe Landauer resistances of the various subunits of a repeated one-dimensional structure obey the following equality when evaluated at the energies of unit transmission through the structure corresponding to case (b) of theorem I:

$$\sum_{n=1}^{n=N-1} \frac{R_L^{(n)}(1)}{\sum_{m=1}^{m=N-1} R_L^{(n)}(m)} = 1 , \quad (34)$$

where $R_L^{(n)}(m)$ is the four-probe Landauer resistance of a subunit with m periods evaluated at the nth resonant energy (energy of unit transmission). The summation is carried out over all the $N-1$ resonant energies corresponding to case (b) of theorem I.

To prove the sum rule, we make use of Eq. (31). This equation is valid for all N. Replacing N by a running index m and then summing over m, we obtain

$$\sum_{m=1}^{m=N} \sin^2(m\theta) = \sum_{m=1}^{m=N} \frac{R_L(m)}{R_L(1)} \sin^2\theta \ . \tag{35}$$

Note that in the above equation we dropped the superscript "4-p" from $R_L^{4\text{-p}}$ for the sake of brevity. We will follow this convention in all following equations with the tacit understanding that the resistance being referred to is the four-probe rather than the two-probe resistance.

Making use of the trigonometric identity[18]

$$\sum_{m=1}^{m=N} \sin^2(m\theta) = \frac{N}{2} - \frac{1}{2} \frac{\sin(N\theta)\cos[(N+1)\theta]}{\sin\theta} \ , \tag{36}$$

and recalling from Eq. (18) that at the energies of unity transmission through N periods (i.e., at the resonant energies), $\sin(N\theta)=0$, we get from the above identity that at *any* resonant energy

$$\sum_{m=1}^{m=N} \sin^2(m\theta_r) = \frac{N}{2} \ , \tag{37}$$

where θ_r is a resonant value of θ, i.e., $\theta_r = n\pi/N$ where $n = 1,2,3,\ldots,N-1$.

Using the above result to substitute for the left-hand side in Eq. (35) we obtain

$$\begin{aligned} \frac{N}{2} &= \frac{\sum_{m=1}^{m=N} R_L^{(n)}(m)}{R_L^{(n)}(1)} \sin^2(\theta_r) \\ &= \frac{\sum_{m=1}^{m=N-1} R_L^{(n)}(m)}{R_L^{(n)}(1)} \sin^2(\theta_r) \\ &= \frac{\sum_{m=1}^{m=N-1} R_L^{(n)}(m)}{R_L^{(n)}(1)} \sin^2\left[\frac{n\pi}{N}\right] , \end{aligned} \tag{38}$$

where, in deriving the second equality above, we used the fact that at the energy of unity transmission through N periods, the Landauer resistance of N periods is zero, i.e., $R_L^{(n)}(N)=0$.

From Eq. (38), we obtain (by summing over the index n)

$$\begin{aligned} \frac{N}{2} \sum_{n=1}^{n=N-1} \frac{R_L^{(n)}(1)}{\sum_{m=1}^{m=N-1} R_L^{(n)}(m)} &= \sum_{n=1}^{n=N-1} \sin^2\left[\frac{n\pi}{N}\right] \\ &= \sum_{n=1}^{n=N} \sin^2\left[\frac{n\pi}{N}\right] - \sin(\pi) \\ &= \sum_{n=1}^{n=N} \sin^2(n\theta_{r1}) \ , \end{aligned} \tag{39}$$

where θ_{r1} is the value of θ_r at the first resonance, i.e., $\theta_{r1}=\pi/N$.

Comparing Eqs. (37) and (39), we finally obtain Eq. (34) which is the sum rule.

TABLE I. The sum of the three A's is unity, which satisfies Eq. (34) and, hence, the "sum rule." Note that the energies in the first column correspond to points R', Q', and P' in Fig. 3. $A \equiv (1-|T_1|^{-2})/(3-|T_1|^{-2}-|T_2|^{-2}-|T_3|^{-2})$.

Energy (eV) for which $\lvert T_4\rvert^2=1$	$\lvert T_1\rvert^2$	$\lvert T_2\rvert^2$	$\lvert T_3\rvert^2$	A
0.2798	0.1751	0.095 95	0.1751	0.2499
0.3009	0.023 57	1.0	0.023 57	0.5
0.3304	0.3477	0.2105	0.3477	0.2499

In Table I we provide a numerical example of the sum rule for the case $N=4$ and for the potential profile shown in the inset of Fig. 3. The right-hand side of Eq. (34) does become equal to unity within the numerical accuracy available.

VI. BOUNDARY RESISTANCE OF A FINITE REPEATED ONE-DIMENSIONAL STRUCTURE

While studying pseudolocalization, Azbel and Rubinstein[19] introduced the concept of the "boundary resistance" of a finite repeated one-dimensional structure. The "boundary resistance" of a structure with M periods is the limiting value of the "average resistance" of the structure defined as

$$R_{\text{av}}^{M} = \frac{1}{M} \sum_{m=1}^{m=M} R_L^{4\text{-p}}(m) \ , \tag{40}$$

where $R_L^{4\text{-p}}(m)$ is the four-probe Landauer resistance of a section composed of m subunits.

Reference 19 showed that in the case of uniformly spaced δ scatterers, the average resistance evaluated at the *resonant energies* of the structure converges to a nonzero constant value independent of the number of periods M (or the length of the structure), provided M is sufficiently large. This constant value was termed the "boundary resistance" since it arises from the effects of the boundaries that break the translational invariance of the structure. In this section we derive, for the first time, an *analytical* expression for the boundary resistance. We then prove two properties—one associated with the boundary resistance, and the other associated with the average resistance evaluated at the energies corresponding to the edges between the pass bands and stop bands of an infinitely periodic structure.

Property 1. The boundary resistance of a periodic structure is indeed independent of the number of periods M (or the length of the structure) and depends only on the potential profile within any one period.

The above result was demonstrated from numerical simulations (but not proved analytically) in Ref. 19 for the specific case of a periodic array of "δ-potentials." In this paper, we provide an *analytical* proof of this property which is valid for any arbitrary shape of the periodic potential.

Property 2. The average resistance of a periodic struc-

ture, evaluated at the edges between the "pass bands" and "stop bands" increases with the *square* of the length of the structure if the number of periods is large.

We first derive an analytical expression for the boundary resistance.

At the resonant energies [for case (b) of theorem I] we have from Eq. (38),

$$\sin^2(\theta_r)=\frac{(M/2)R_L(1)}{\sum_{m=1}^{m=M} R_L(m)} . \tag{41}$$

Therefore using Eq. (41) in Eq. (40) we obtain

$$R_{\rm av}^{M}(\text{resonance})=\frac{1}{2\sin^2(\theta_r)}R_L(1) . \tag{42}$$

Finally, using Eq. (30) to replace $R_L(1)$ in the above equation, we obtain

$$R_{\rm av}^{M}(\text{resonance})=\frac{h}{4e^2}\left[\left[\frac{k^2W_{21}-W_{12}}{2k\sin(\theta)}\right]^2-1\right]_{\text{resonance}} , \tag{43}$$

where the quantity in the right-hand side is evaluated at any one of the resonant energies for a structure with M periods.

We now have to prove that the right-hand side is independent of M if M is sufficiently large, i.e., if $M\gg 1$. This will prove property I.

Referring back to Eq. (14), we see that resonance conditions ($T_M=1$) are reached when either the term within the square brackets in the equation above reaches zero[20] or when $\sin(N\theta)=0$.

Case 1. For the former case, i.e., when the term within the square brackets is zero in Eq. (14), $R_{\rm av}^{M}$(resonance) is identically zero as seen from Eq. (43) and hence obviously independent of M. Thus, we have proved property 1 for this special case.

Case 2. When $\sin(N\theta)=0$ but the term within the large curly braces is nonzero, the value of $R_{\rm av}^{M}$(resonance) is not zero. The dependence of this nonzero value on the number of periods M enters through only four quantities—the matrix elements W_{21} and W_{12}, and also k_r^M ($=n\pi/ML$) and θ_r^M ($=n\pi/M$), where the last two quantities are the resonant values of the wave vector and the corresponding resonant values of θ for a structure with M periods. To prove property 1, we have to merely show that (1) the matrix elements W_{21} and W_{12} are continuous functions of energy, and (2) the difference between k_r^M and k_r^{M+1}, and also θ_r^M and θ_r^{M+1}, and hence $R_{\rm av}^{M}$(resonance) and $R_{\rm av}^{M+1}$(resonance), decreases continuously with increasing value of M. The former fact, namely that the matrix elements are continuous functions of energy, is obvious from the derivation of these elements given in the Appendix. The latter fact follows from the inequality

$$k_r^{M+1}-k_r^M=\frac{n}{L}\left[\frac{1}{M+1}-\frac{1}{M}\right]<\frac{1}{ML} , \tag{44}$$

$$\theta_r^{M+1}-\theta_r^M=n\pi\left[\frac{1}{M+1}-\frac{1}{M}\right]<\frac{\pi}{M} . \tag{45}$$

Hence the differences go to zero as $1/M$ which proves property 1.

We now proceed to prove property 2. When the Landauer resistances are evaluated at the edges between a pass band and a stop band,

$$\begin{aligned} R_{\rm av}^{M}(\text{band edges})&=\frac{1}{M}\sum_{m=1}^{m=M}R_L(m)\\ &=\frac{1}{M}\sum_{m=1}^{m=M}m^2R_L(1)\\ &=\frac{(M+1)(2M+1)}{6}R_L(1)\\ &\approx\frac{M^2}{3}R_L(1)\quad\text{if } M\gg 1 , \end{aligned} \tag{46}$$

where we used theorem IV to arrive at the second equality.

Hence the average resistance, evaluated at the band edges, increases as the square of the length of the structure when the number of periods in the structure is large. This proves property 2.

VII. CONCLUSION

In this paper we have proved several theorems related to the Landauer resistances of finite repeated structures. Of particular importance is the theorem that relates the energies of unity transmission through a finite, repeated one-dimensional structure to the energy–wave-vector dispersion relation for the associated infinite lattice formed by periodic repetition of the structure. This theorem is valid even for a structure with spatially varying effective mass and is therefore very useful in calculating the energy–wave-vector dispersion relation for any infinitely repeated structure.

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APPENDIX

In a region where both E_c and γ are constant (spatially invariant), the Schrödinger equation becomes [see Eq. (3)]

$$\frac{d}{dz}\left[\frac{1}{\gamma}\frac{d\phi}{dz}\right]+\frac{2m_c^*}{\hbar^2}\left[E-\frac{E_t}{\gamma}-E_c\right]\phi(z)=0 . \tag{A1}$$

To define the transfer matrix through a section of length L where both E_c and γ are constant, we look at solutions $u(z)$ of Eq. (A1) which satisfy the boundary conditions

$$u_1(0)=0, \quad u_1'(0)=1 , \tag{A2}$$

and

$$u_2(0)=1, \quad u_2'(0)=0 , \tag{A3}$$

where the prime denotes first derivative with respect to space. The solutions $u_{1,2}(z)$ are linearly independent solutions (their Wronskian is unity) and a general solution of Eq. (A1) can be written as

$$\phi(z)=A_1u_1(z)+A_2u_2(z) . \tag{A4}$$

The transfer matrix W is defined as follows:

$$\begin{bmatrix} \frac{\phi'}{\gamma}(L) \\ \phi(L) \end{bmatrix} = W \begin{bmatrix} \frac{\phi'}{\gamma}(0+) \\ \phi(0+) \end{bmatrix} . \tag{A5}$$

Using Equations (A2)–(A5), we obtain

$$W=\begin{bmatrix} u_1'(L) & \frac{u_{2'}}{\gamma}(L) \\ \gamma u_1(L) & u_2(L) \end{bmatrix} . \tag{A6}$$

The explicit forms for $u_{1,2}(z)$ are the following.

Case a. If $E > E_t/\gamma + E_c$,

$$u_1(z)=\frac{\sin\beta z}{\beta} , \tag{A7}$$

$$u_2(z)=\cos\beta z , \tag{A8}$$

where

$$\beta^2=\frac{2m^*}{\hbar^2}\left[E-\frac{E_t}{\gamma}-E_c\right] . \tag{A9}$$

Case b. If $E < E_t/\gamma + E_c$,

$$u_1(z)=\frac{\sinh(\kappa z)}{\kappa} , \tag{A10}$$

$$u_2(z)=\cosh(\kappa z) , \tag{A11}$$

where

$$\kappa^2=\frac{2m^*}{\hbar^2}\left[\frac{E_t}{\gamma}+E_c-E\right] . \tag{A12}$$

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