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Density of states, electron-transport mechanisms, and chemical potentials in the presence of inelastic processes

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We present a formulation for the estimation of the density of states for quantum structures, such as the quantum wire and the single- and multiple-barrier structures. Our formulation is based on the quantum kinetic approach as opposed to the single-particle approach; therefore, the model inherently accounts for the exclusion principle and incorporates phase randomizing and/or inelastic collisions. Also in this paper, we propose a physically meaningful decomposition of the density of states for left- and right-moving electrons. The total and the decomposed densities of states are then used to define chemical potentials that may be measured by the symmetric and asymmetric voltage probes. The present approach eliminates some unphysical features reported in earlier work and enables us to propose an alternative, but equivalent, expression to the well-known Tsu-Esaki equation for the tunneling current. In our transport equations, the usual transmission coefficients are not needed; instead, we introduce the concept of a state-current density that may be used to describe the current through tunneling barrier structures. Moreover, we use this concept of the state-current density to comment on the coherent and the sequential tunneling mechanisms for double-barrier structures.

I. INTRODUCTION

With the advent of molecular beam epitaxial and metalorganic chemical vapor deposition techniques, many materials and device structures have been proposed and fabricated during the last decade. Some of these devices have shown excellent characteristics and have encouraged further exploration.[1-3] Many theoretical models are also being developed to explain the physical principles that govern the operation of such devices.[4-26] Because of the smaller sizes of these structures, the transport mechanism is dictated by quantum-mechanical interference. Therefore quantum-effect devices require a description of electronic transport that is substantially different from that of semiclassical transport mechanisms used for conventional devices.[4,5,10-22] In this description of electronic properties of quantum devices, there are several quantities which are of interest to researchers, such as the transmission coefficient and[4-6,20] the density of states (DOS).[6-8] These basic quantities have many different applications; the transmission and the reflection coefficients are central to the Büttiker-Landauer description[6] of the conductances of a system at $T \approx 0$ K and the electronic DOS is required in a description of the transition probabilities[10-13] and in the interpretation of optical properties of many material.[8]

Calculations of DOS for periodic and random materials are common in the literature. Though most of the techniques are fairly well known, these calculations are better suited to application to bulk materials (e.g., the coherent-potential approximation) or for the very dilute concentration of noninteracting impurity atoms (e.g., perturbation techniques).[9] For modern nanofabricated devices neither of the above techniques is useful. The interference effects due to successive elastic scatterers govern the operation of these devices. Unlike alloys, the positions and the strengths of the scatterers in these structures are not random. Therefore the usual method of statistical averaging[9] is not applicable and one must solve for the DOS using the complete sample-specific Hamiltonian.

The second important feature of quantum-effect devices is that these systems are "open."[27] Therefore the effects of the boundary conditions on the device performance are critical and the DOS in these devices will depend on the precise description of boundary conditions. Some of the models reported in the literature require that the wave functions go to zero or be periodic at the boundaries.[8-13] These boundary conditions may not be physical in the sense that quantum-effect devices are small and are coupled to contacts that act as electron reservoirs. It has been recognized that deep within the reservoirs the electrons lose their phase memory completely due to inelastic collision events. Therefore these electrons must be described by quasinormal modes characterized by complex eigenenergies.[27] The normalization of the corresponding eigenfunctions, needed in the calculation of the DOS, is not trivial at all.

Sometimes the calculation of the DOS may be needed in the presence of an applied bias.[8] One notes that external bias destroys the periodic boundary condition assumed for the bulk and is responsible for current in the device. Hence any proposal for the calculation of the DOS should account for the asymmetry of the structure and also provide a theoretical framework for the description of the electron transport. For example, such calculations are needed in the description of the sequential transport mechanism across double-barrier structures (DBS).[10-13] Any convincing argument for or against this theory must, therefore, calculate the DOS in a biased structure.

A general formalism that calculates the DOS should also be able to prescribe a method that can decompose the DOS, in a physically meaningful way, between the energy states for the positive- and negative-flowing electrons and holes. This is needed because if asymmetric voltage probes[25] are used to couple to the positive- and negative-flowing electronic current streams, the formalism must predict the correct chemical potentials. Furthermore, a complete procedure must also specify the calculation of the phase-sensitive DOS.[25] The DOS, calculated in the presence of elastic scatterers, should approach the phase-insensitive DOS as the phase-randomizing scattering rate is increased.

In this paper, we present a method for the calculation of the local DOS for nanofabricated quantum-effect devices. We have modeled these devices as open systems using the steady-state quantum transport theory proposed by Datta and co-workers.[15–18] Also, we show that there are two reasons for the unphysical behavior of the separate chemical potentials, defined by them,[15] for the left- and right-moving electrons. First, in order to define separate chemical potentials one needs to be able to correctly decompose the electrons into two groups, left- and right-moving electrons. We have earlier reported such a procedure.[19] Second, one must also be able to obtain separate DOS's for left-moving and right-moving electron and holes. In this paper, we therefore propose a physically meaningful framework for the decomposition of the total DOS into states for the positive- and negative-flowing electrons. We then show that separate chemical potentials can indeed by defined with the help of our decomposition procedure. It is important to mention that the above procedures are not in violation of the uncertainty principle[15] because the retarded Green's functions are estimated using the effective mass equation within the envelope function approximation. Therefore the local density of electrons and the DOS are inherently defined as an average over a unit cell of the periodic lattice.

In Sec. II we develop a formalism for the calculation of the DOS based on the quantum kinetic equation. A simple formula is derived for the total density of states that does not require the specification of a complete set of orthonormal wave functions.[15] Therefore the calculation of the DOS has been simplified enormously. Moreover, we include the effects of phase-breaking and inelastic processes that tend to wash out the interference effects due to elastic potential barriers. In Sec. III we present our procedure for the decomposition of the total DOS. We show that, contrary to the common assumption, the DOS does not split into halves.[15] Based on the definition of the decomposed DOS, we suggest an alternative, physically meaningful description of tunneling current through elastic barriers. Section IV contains derivations of expressions for the chemical potentials in the one-dimensional (1D) structures under applied bias. We include a discussion on the use of asymmetric probes for the measurement of chemical potentials in Sec. V. In Sec. VI we discuss the implications of the concept of the state-current densities and the quantum kinetic formulation on the existing tunneling theories for the DBS. Sections VII and VIII include some numerical results and the conclusions, respectively.

II. CALCULATION OF THE DENSITY OF STATES: THE MODEL

In this section we present a formulation for the determination of the DOS in a region of elastic scatterers connected to electron reservoirs. We include the effect of phonon scattering following the model by Datta.[15–18] He used a form of Hamiltonian that assumes that the inelastic collisions are caused by a distribution of independent oscillators. Each oscillator interacts with the electrons through a δ potential in the space. This assumption reduced the electron self-energy to a δ function in space. The Keldysh formulation[21] was employed to rigorously justify the use of imaginary optical potentials. Datta also derived a kinetic equation for steady-state quantum transport using only the diagonal elements of the correlation function $G^{<}(r,r;E)$. We shall extend and modify Datta's formulation for 1D structures to propose two differential equations that govern the evolution of the DOS for the positive- and the negative-moving electrons as a function of x.

Details of our description of electronic transport have been reported earlier.[19] For the sake of continuity, we will define only the relevant quantities. The key idea of our formulation is the following. We describe the electronic states using composite propagating waves, traveling with spatially varying group velocities, rather than just plane waves with wave numbers $\pm k(x)$.[6] In our model the transport of electrons in a quantum system is completely and uniquely described by two group velocities $v_g^+(x,E_x)$ and $v_g^-(x,E_x)$ for the positive- and negative-flowing electrons, respectively.[14,19,22–24] In fact all the relevant transport coefficients, e.g., the scattering rates and the forward and backward scattering probabilities, can be expressed in terms of these quantities. The transport electrons may encounter inelastic collisions at random points in space. However, regardless of the location of their last scattering, electrons with the same energy and traveling in the same direction have the same local group velocity. This simple yet important fact is central to our transport model.

In many widely studied quantum structures, the elastic barriers are present only in the direction of current flow. Therefore we can easily decompose the DOS into two DOS's: one for the longitudinal direction and the other for the lateral direction. For such quantum structures with wide lateral widths, e.g., the single- or multiple-barrier structures, the DOS as a function of total electron energy E can be easily calculated by carrying out the convolution integral in energy between the 1D DOS and the lateral DOS. We will therefore ignore the lateral DOS in our formulation and concentrate only on the 1D DOS for the longitudinal component of the energy E_x. The expression for the 1D DOS (for both spins) is given as

$$N(x,E_x)=-\frac{2}{\pi}\operatorname{Im}G^R(x,x,E_x)\ . \tag{1}$$

Here $G^R(x,x,E_x)$ is the solution of the Schrödinger equation modified by the presence of the optical (local) potential:[16,17]

$$\left[E_x - H_0(x) + \frac{i\hbar}{2\tau_\phi(x,E_x)}\right] G^R(x,x_1,E_x) = \delta(x - x_1) \; . \tag{2}$$

The Hamiltonian $H_0(x)$ contains the potential energy term that is determined by the band discontinuity and the self-consistent Hartree potential, and $\tau_\phi(x,E_x)$ is the phase-breaking time. The function $G^R(x,x_1,E_x)$ therefore contains all the interference effects due to elastic barriers located in a dissipative environment.

Although the direct calculation of the retarded Green's function is often difficult, we use a straightforward technique to compute the diagonal elements of the Green's function.[19] In the following we will briefly describe our method. Using Eq. (1) the DOS is given by[19]

$$N(x,E_x) = \mathrm{Im}\left[\frac{i8/\hbar\pi}{Z^+(x,E_x) - Z^-(x,E_x)}\right] , \tag{3}$$

where $Z^+(x,E_x) = Z(x^+,x,E_x)$ and $Z^-(x,E_x) = Z(x^-,x,E_x)$ and the function $Z(x,x_1,E_x)$ is defined as

$$Z(x,x_1,E_x) = \left[\frac{2\hbar}{im^*}\frac{\partial G^R(x,x_1,E_x)/\partial x}{G^R(x,x_1,E_x)}\right] \tag{4}$$

and is calculated using the known values of the logarithmic derivative in the asymptotic regions inside the electron reservoirs connected to the structure. One of the key results in this formulation is for the function $Z(x,x_1,E_x)$;[19]

$$\tfrac{1}{2}\mathrm{Re}[Z(x,x_1,E_x)] = \begin{cases} v_g^+(x,E_x), & x > x_1 \quad (5) \\ v_g^-(x,E_x), & x < x_1 . \quad (6) \end{cases}$$

The terms $v_g^+(x,E_x)$ and $v_g^-(x,E_x)$ are the local group velocities of the right-moving and the left-moving electrons, respectively. It can be shown that $v_g^+(x,E_x) > 0$ and $v_g^-(x,E_x) < 0$. It is interesting to note that the density of states does not require any specification of the basis functions and altogether avoids such calculations.

III. DECOMPOSITION OF THE DOS

While the density of states is a very well-known quantity, it is not obvious that these do not always split into halves for the right- and the left-moving electrons, respectively.[15] This is particularly true especially in the presence of elastic barriers. In the past, an attempt to decompose the DOS into two parts in the momentum space using the Wigner formalism has resulted in a negative DOS, which is physically inconsistent.[15] In the following we present a rigorous derivation that leads to a simple scheme for such a decomposition. Interestingly, we accomplish this in real space. The decomposition of the DOS has several important consequences. We will discuss these later in this paper. Note that in the determination of the total DOS we have used Eq. (1). In this case we use another equivalent definition of the DOS (for a single spin), which is intuitively more appealing than the former:[15–17]

$$N(x,E_x) = \frac{\hbar}{2\pi}\int_{-\infty}^{\infty} dx_1 \frac{|G^R(x,x_1,E_x)|^2}{\tau_\phi(x_1,E_x)} \; . \tag{7}$$

While both of these expressions for the 1D DOS can be derived from the theory of quantum kinetic equations, Eq. (7) has a very simple physical interpretation.[17] If electrons and holes are injected by inelastic scattering at a steady rate at the point x_1, they will propagate in both directions and establish a local electron and hole density proportional to $|G^R(x,x_1,E)|^2$. The total contribution at any x from all x_1's determines the local DOS. Now let us consider any point x in space. If the electrons and holes are injected at any x_1 on the *left* of x, then a fraction of those electrons and holes that propagate in the positive directions will contribute to the local DOS. Note that both the electrons and the holes travel with the same positive group velocity $v_g^+(x,E_x)$ (Ref. 19) and, therefore, they contribute to the DOS for the right-moving electron. A similar argument can be used to show that the DOS contributed by all points on the *right* of x will be for the left-moving electrons and holes. Thus we can now decompose the DOS into the right- and the left-moving DOS's, $N^+(x,E_x)$ and $N^-(x,E_x)$, respectively, in the following fashion:

$$N^+(x,E_x) = \frac{\hbar}{2\pi}\int_{-\infty}^{x} dx_1 \frac{|G^R(x,x_1,E)|^2}{\tau_\phi(x_1,E_x)} \tag{8}$$

and

$$N^-(x,E_x) = \frac{\hbar}{2\pi}\int_{x}^{\infty} dx_1 \frac{|G^R(x,x_1,E)|^2}{\tau_\phi(x_1,E_x)} \; . \tag{9}$$

Note that Eqs. (7)–(9) depend on $\tau_\phi(x,E_x)$ which is a function of the electron and the hole densities, $n(x,E_x)$ and $p(x,E_x)$, respectively. However, since $n(x,E_x)$ and $p(x,E_x)$ themselves depend on the DOS, one would need an iterative procedure. This means, in a biased structure the estimation of the DOS then becomes an integral part of a self-consistent procedure for the calculation of the current flow through the structure. Therefore the DOS in a quantum system is inherently related to the transport of particles, i.e., the electrons and the holes. The changes in the DOS, therefore, reflect the influences of the elastic barriers and phase-breaking processes on the transport of these particles via $G^R(x,x_1,E_x)$.

Now, in order to evaluate $N^{\pm}(x,E_x)$, let us define two quantities:

$$J_N^+(x,E_x) = N^+(x,E_x)v_g^+(x,E_x) \; , \tag{10}$$

$$J_N^-(x,E_x) = N^-(x,E_x)v_g^-(x,E_x) \; . \tag{11}$$

The terms $J_N^{\pm}(x,E_x)$ may be called the *state-current density* since they are products of the DOS's and their respective group velocities. Using Eqs. (8)–(11) and following a derivation similar to that described in Ref. 19, we find $J_N^{\pm}(x,E_x)$ satisfies the following differential equations:

$$\frac{dJ_N^+(x,E_x)}{dx} = -\alpha^+(x,E_x)J_N^+(x,E_x) + r^+(x,E_x)\frac{N(x,E_x)}{\tau_\phi} \tag{12}$$

and

$$\frac{dJ_N^-(x,E_x)}{dx} = -\alpha(x,E_x)J_N^-(x,E_x) + r^-(x,E_x)\frac{N(x,E_x)}{\tau_\phi}\ , \tag{13}$$

where

$$r^\pm(x,E_x) = \frac{|v_g^\pm(x,E_x)|}{v_g^+(x,E_x) - v_g^-(x,E_x)}$$

and

$$\alpha^\pm(x,E_x) = \frac{1}{\tau_\phi v_g^\pm(x,E_x)}\ .$$

We could in principle solve for the two equations subject to appropriate boundary conditions. However, we use a trick which makes the direct solution unnecessary. If we add Eqs. (12) and (13), it can be easily seen that

$$\frac{dJ_N}{dx} = \frac{dJ_N^+(x,E_x)}{dx} + \frac{dJ_N^-(x,E_x)}{dx} = 0\ .$$

This means that the function $J_N(x,E_x)$ is a constant in space. However, the value of this constant turns out to be zero, because deep within the reservoir, where all the effects of the interferences have been washed out, $N^+(x,E_x) = N^-(x,E_x) = N/2$ and $v_g^+(x,E_x) = \hbar k/m^*$ and $v_g^-(x,E_x) = -\hbar k/m^*$. Therefore individual contributions from the J_N^+ and J_N^- cancel. We arrive at the following two equations for $N^\pm(x,E_x)$:

$$N^+(x,E_x) + N^-(x,E_x) = N(x,E_x)\ , \tag{14}$$

$$N^+(x,E_x)v_g^+(x,E_x) + N^-(x,E_x)v_g^-(x,E_x) = 0\ . \tag{15}$$

The solutions are

$$N^+(x,E_x) = r^-(x,E_x)N(x,E_x) \tag{16}$$

and

$$N^-(x,E_x) = r^+(x,E_x)N(x,E_x)\ . \tag{17}$$

The above result is amazingly simple and is somewhat unexpected. Note that both of the DOS's are positive definite and therefore are physically consistent. Equations (16) and (17) predict that the decomposition of the DOS is again dictated by the group velocities. The physical interpretation of Eq. (15) is that the net state-current density at any x must be zero even under bias while a constant steady-state current is flowing through the device.

An important consequence of the decomposition of the DOS is that we can now propose an alternative point of view for the theory of tunneling without involving the transmission coefficients. Let us consider a quantum device that contains tunneling barriers. We neglect the inelastic collisions only in the barrier region; the contacts (electron reservoirs) always contain phase-breaking and/or inelastic collision processes. The neglect of inelastic processes is nonessential and is invoked only for simplicity. The Tsu-Esaki tunnel current, flowing from left to right, for such a coherent system is given by[20]

$$J_{L\to R} = e\int dE_x T(E_x)v(E_x)N(E_x)F(E_x)\ , \tag{18}$$

where $T(E_x)$ is the transmission coefficient calculated on the right of the boundary between the left reservoir and the device, $v(E_x) = \hbar k(E_x)/m^*$ is the forward velocity of electrons, $N(E_x) = [2\pi\hbar v(E_x)]^{-1}$ is the usual 1D density of states (for a single spin) for positively traveling electrons, and $F(E_x)$ is the Fermi-Dirac electron distribution function.[12] In the Tsu-Esaki model, electrons are characterized by a velocity $\hbar k/m^*$. Upon scattering from an elastic barrier a part of the electrons are considered to be reflected. The reflected electrons travel with a velocity $-\hbar k/m^*$. On the other hand, the expression for the tunneling current in our formalism is

$$J_{L\to R} = e\int dE_x J_N^+(E_x)F(E_x)\ . \tag{19}$$

The above expression is evaluated at the same position as indicated earlier. Notice that the right-moving state-current density $J_N^+(E_x)$ enters in this definition in a very meaningful fashion. The term represents the maximum current-carrying capacity of the energy states at E_x. Multiplication by $eF(E_x)$ therefore gives the probable electronic current density at energy E_x. Thus, in our model, the elastic barrier essentially changes the maximum current-carrying capacity of the states in the neighboring regions by modifying both the group velocities and the DOS. In the absence of inelastic collisions $[\tau_\phi(x,E_x) = \infty]$, $J_N^+(x,E_x)$ is constant throughout the structure [see Eq. (12)], and the right-moving electrons starting from the left reservoir always travel in the same direction. Note that, while this picture is quite different from that of Tsu and Esaki, both of these equations give the same numerical results.

IV. CALCULATION OF CHEMICAL POTENTIALS

In this section, we present expressions for the chemical potentials[25] in a purely 1D structure at vanishingly low temperatures. We mention that in 1D structures, the Fermi-Dirac electron distribution function $F(E_x)$ in Eq. (19) is replaced by the Fermi-Dirac probability function $f(E_x)$ characterized by a chemical potential μ^+ for the right-moving electrons.[28] Similarly the left-moving electron density is determined by a different chemical potential μ^-. Here we remove the assumption invoked in Sec. III. We now consider a structure that contains inelastic or phase-randomizing scatterers everywhere. In this case, electrons moving with a particular group velocity may be scattered and a fraction of the scattered electrons may reverse their direction of travel. Let us now connect two direction-insensitive voltage probes at positions $x = x_1$ and x_2. In the following discussion, the subscripts 1 and 2 on μ's refer to these two probe locations. We assume here that the reservoirs are located at large distances from the probes compared to the phase-breaking length. An external applied voltage between the electron reservoirs creates a chemical potential difference, $\mu_1-\mu_2$, between these two points. The current is carried by electrons with energies almost equal to $(\mu_1+\mu_2)/2$ and, therefore, we can omit the energy dependence from our expressions. Under biased condition, the three chemical potentials $\mu(x)$, $\mu^+(x)$, and $\mu^-(x)$ will be functions of x. At the probe locations the three chemical potentials are related by the inequalities: $\mu_1^+>\mu_1>\mu_1^-$ and $\mu_2^+>\mu_2>\mu_2^-$, respectively. Using equations from Refs. 19 and 28, the net injected right-moving current at $x=x_1$, using Eq. (19), is given as $eN^+(x_1)v_g^+(x_1)(\mu_1^+-\mu_2^-)$. The current densities $J^{\pm}(x,E_x)$ for the right- and the left-moving electrons, respectively, are then calculated using the procedure presented earlier.[19]

The variations in the chemical potentials are given by[19]

$$\mu(x)-\mu_2^-=\frac{n(x)}{N(x)}(\mu_1^+-\mu_2^-) \ . \tag{20}$$

Similarly, using the definition of the decomposed DOS we can now define the chemical potentials for the right- and the left-moving electrons, respectively, as

$$\mu^+(x)-\mu_2^-=\frac{n^+(x)}{N^+(x)}(\mu_1^+-\mu_2^-) \ , \tag{21}$$

$$\mu^-(x)-\mu_2^-=\frac{n^-(x)}{N^-(x)}(\mu_1^+-\mu_2^-) \ , \tag{22}$$

where $n^+(x)+n^-(x)=n(x)$ is the total electron density, $N^+(x)+N^-(x)=N(x)$, and $n^{\pm}(x)=J^{\pm}(x)/ev_g^{\pm}(x)$. It can easily be verified that the three chemical potentials defined above are related by the following equation: $\mu(x)=\mu^+(x)r^-+\mu^-(x)r^+$.

Using Eq. (20) at $x=x_1$ and x_2 we can show that

$$\mu_1^+=\frac{\mu_1\eta_1+\mu_2\eta_2}{\eta_1+\eta_2} \ , \tag{23}$$

$$\mu_2^-=\frac{\mu_1\kappa_1+\mu_2\kappa_2}{\kappa_1+\kappa_2} \ , \tag{24}$$

where $\kappa_1=-\xi(x_2)$, $\kappa_2=\xi(x_1)$, $\eta_1=1+\kappa_1$ and $\eta_2=\kappa_2-1$ and $\xi(x)=n(x)/N(x)$. Moreover, using Eqs. (20)–(24), we also express the chemical potential $\mu(x)$ as functions of μ_1 and μ_2 as

$$\mu(x)=\frac{\mu_1\lambda_1(x)+\mu_2\lambda_2(x)}{\lambda_1+\lambda_2} \ , \tag{25}$$

where $\lambda_1(x)=\xi(x)-\xi(x_2)$, $\lambda_2(x)=\xi(x_1)-\xi(x)$. Similar expressions can be derived for $\mu^{\pm}(x)$ by *only* replacing $\xi(x)$ by $\xi^{\pm}(x)=n^{\pm}(x)/N^{\pm}(x)$. Note that Eqs. (23)–(25) have the same denominator equal to $\xi(x_1)-\xi(x_2)$, and the functions that multiply μ_1 and μ_2 always add up to unity. We mention that all the quantities calculated above are phase sensitive. The phase information is retained both in the number of electrons $n(x)$ and the DOS $N(x)$. In order to compute the phase-averaged quantities, in all the above expressions we replace $\xi(x)$ and $\xi^{\pm}(x)$ by $\langle\xi(x)\rangle$ and $\langle\xi^{\pm}(x)\rangle$, respectively. The average can be taken over an integral number of wavelengths.

V. MEASUREMENTS OF THE CHEMICAL POTENTIALS BY ASYMMETRIC PROBES

In this section we comment on the use of the asymmetric voltage probes proposed by Büttiker.[25] Such probes, in our formulation, couple asymmetrically with the two streams flowing with individual group velocities. In other words, the probes allow different fractions of the current streams to equilibrate and in doing so break the left-right symmetry of the direction-independent probe. We mention that our probe and that of Büttiker are not formally the same because Büttiker's asymmetric probes couple either the k or the $-k$ plane-wave states in the extreme cases. On the other hand, our probes couple the positive and negative group velocity states in the extreme cases. However, by using appropriate mapping functions all the potentials measured by our asymmetric probes may be translated to Büttiker's measurement and vice versa. Now if we define θ as the coupling parameter,[25] then the chemical potential measured by our asymmetric probe is

$$\mu_\theta(x)=\frac{\mu_1\sigma_1+\mu_2\sigma_2}{\sigma_1+\sigma_2} \ , \tag{26}$$

where

$$\sigma_1=\lambda_1^+(x)r^-(x)\sin\theta+\lambda_1^-(x)r^+(x)\cos\theta \ ,$$

$$\sigma_2=\lambda_2^-(x)r^+(x)\sin\theta+\lambda_2^+(x)r^-(x)\cos\theta \ .$$

This equation reduces in various limits to the extreme cases described in Sec. IV. For example, $\mu_{\pi/4}(x)=\mu(x)$, $\mu_0(x)=\mu^+(x)$, and $\mu_{\pi/2}(x)=\mu^-(x)$. For all intermediate values of θ the probe will continuously couple both streams from one extreme to the other.

VI. RESONANT VERSUS SEQUENTIAL TUNNELING

The concept of the state-current density and the quantum kinetic formulation can be used to combine the two transport models (the resonant or coherent[4,20] and the sequential or incoherent tunneling[10–13]) into a single comprehensive model for tunneling barrier devices. The DOS plays a crucial role in the transport processes of carriers across each barrier in the sequential theory for DBS. In the present formulation, *coherent* particles in a dissipative environment are responsible for the formation of the local DOS. In view of these statements, it is therefore necessary to discuss the similarities and differences between the present quantum kinetic approach and the existing models for the sequential tunneling theory.[10–13]

Note that in the quantum kinetic approach, the particles (electrons and holes) that contribute to the DOS remain coherent and they carry the phase memory of their respective paths since their most recent scattering. In fact there is no requirement that the particles that contribute to the local DOS must be scattered into the same states by inelastic processes. It is possible that a fraction of the electrons may actually be inelastically scattered after they have reached the present location. However, these particles that suffered collisions and those which did not propagate again and also contribute to the DOS at other locations at different energies. In other words, particles are *transported coherently*, in a dissipative environment, from one local DOS to another and at the same time they themselves are *responsible for the formation of the local DOS.* The effect of inelastic dissipation processes is essentially to modify the number of such coherent particles.

The sequential tunneling process has been defined as "a two-step process in which electrons first tunnel from the emitter electrode into the *quasibound state* in the QW (quantum well), and then from the well into the collecting electrode."[11] Such a statement is not incompatible with the quantum transport model because the quasibound *current-carrying* states are essentially the result of such a sequential transport mechanism. To model sequential tunneling process, Weil and Vinter[12] employed a space-averaged DOS in the well which has the following form:

$$\rho_w(E)=\frac{\Gamma_e/\pi}{(E-E_r)^2+\Gamma_e^2}\ ,$$

where Γ_e is the elastic broadening due to the finite lifetime of carriers in the well, E and E_r are electron energy and the resonant energy, respectively. Weil and Vinter calculated the "sequential" current using a transition Hamiltonian between the emitter and the well states and showed that the current equals the coherent current calculated using the Tsu-Esaki model. This result showed that their model is only an alternate description of the same coherent tunneling process.[14,26]

On the other hand, the expression of Gupta and Ridley for the "sequential" current [see Eq. (11), Ref. 13] replaces Γ_e in the Weil-Vinter current equation by $\Gamma_e+\Gamma_i$, where Γ_i is due to inelastic scattering. Since the total current was modeled as a weighted sum of the coherent and incoherent currents, the authors calculated the coherent current separately using a Tsu-Esaki-type equation [see Eq. (10), Ref. 13]. In our opinion, the modified Weil-Vinter current expression[13] describes the transport of both the coherent and incoherent electrons. This is because the DOS in the well, used by Gupta and Ridley, applies to both types of electrons. Therefore contrary to their interpretation, we think that the sequential current J_s^{13} is actually the total current and it is unnecessary to compute a weighted sum to obtain the total current. This argument is easy to understand in the light of quantum kinetic approach in which one can describe the total tunneling current, without the aid of a transmission coefficient, solely by the state-current densities associated with the electronic DOS.

We think that the greatest challenge for existing theory for the sequential tunneling lies in the correct estimation of the DOS within the well. Such a calculation can become more difficult, if not impossible, if inelastic processes are considered. We agree with Büttiker[26] that unless phase-breaking inelastic processes are explicitly included in the well, one cannot *a priori* assume that the injected electrons have encountered phase-breaking collisions as they propagate sequentially across each barrier. The inelastic processes modify the transport mechanisms of coherent particles that follow different quantum-mechanical paths and thereby affect the local DOS. Since the local DOS, on the other hand, influences the scattering rates $1/\tau_\phi(x,E_x)$,[15–18] of the inelastic phase-breaking processes, one must calculate the DOS in a self-consistent fashion.

In the literature, the term "coherent tunneling" has been used only to describe electrons that tunnel through both of the barriers without undergoing any phase-breaking scattering.[4–20] However, note that every electron remains coherent between two scattering events. In this sense, the real difference between a "coherent" and an "incoherent" electron is their path lengths between two successive phase-breaking collisions. We have shown[29] that even a purely coherent tunneling model for the DBS, generally given by Eq. (18), should not ignore the fact that the emitter and the collector contacts are always dissipative. Therefore the coherent models must also include some form of "limited coherence length"[27] in the calculation of $T(E_x)$. It is our opinion that, in a dissipating environment that contains arbitrary elastic tunneling barriers, the two existing models of transport for the DBS has been accounted for in the quantum kinetic formulation. Interestingly, quantum kinetic transport theory[19,29] does not require separate equations for the coherent and incoherent electrons to estimate their contributions to the total current.

VII. RESULTS AND DISCUSSION

In this section we apply our formalism to calculate the DOS and the chemical potentials for some representative quantum structures. In all of the calculations we have chosen constant values for τ_ϕ. The effective masses for the electrons in the well (barriers) are $0.067m_0$ ($0.096m_0$), where m_0 is the free-electron mass. The barrier heights

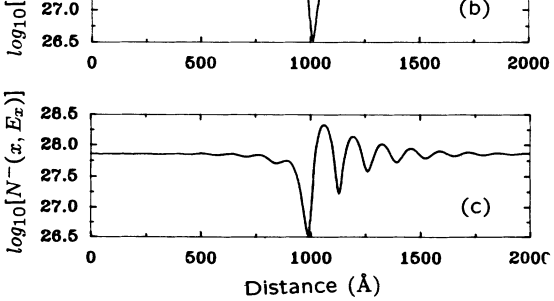

FIG. 1. Theoretical 1D DOS for a single barrier as a function of position x for $E_x=0.033$ eV. (a), (b), and (c) are for $N(x,E_x)$, $N^+(x,E_x)$, and $N^-(x,E_x)$, respectively. The value for $\tau_\phi=1.\times10^{-13}$ s.

in all of the calculations have been kept at 0.275 eV.

In Fig. 1 we present the calculated density of states for a single-barrier structure. The plot shows the DOS as a function of position, in Å, for an electron energy of 0.033 eV. The barrier height and the width are 0.275 eV and 30 Å, respectively. Figures 1(a), 1(b), and 1(c) are for the total, the right-moving, and the left-moving DOS, respectively. As can be seen from Fig. 1(a), the DOS has a minimum at the center of the barrier. If one moves away from the center toward the left or right, the DOS increases rapidly and oscillates. The amplitude of the oscillation decreases and the DOS eventually approaches the value of $\approx 1.44\times 10^{28}$ states/J m which corresponds to the unperturbed DOS in the absence of the barrier. Again the decrease in the amplitude of the oscillations is the result of inelastic scattering processes. Figures 1(b) and 1(c), on the other hand, show an interesting feature that only the local DOS for electrons approaching the barrier shows rapid oscillations. However, as the electrons pass through the barrier, the corresponding local DOS becomes much smoother. The total DOS shown in Fig. 1(a) is the sum of the other two shown in Figs. 1(b) and 1(c), as expected.

Figure 2 shows a simplified energy-band diagram of a double-barrier structure under biased conditions. We have chosen the well and the barrier widths to be 50 Å each. Positions a, b, and c in this figure are locations in the left spacer region, in the first barrier, and in the quantum well, respectively. All of our calculations for the DOS correspond to these three points on the device. For simplicity we ignore all the space charge effects. We assume that the applied bias creates a uniform electric field. While the division of the applied voltage is not accurate, the schematic diagram does resemble a DB structure under bias.[28]

As discussed earlier, the calculation of the DOS in structures under bias must be done within the self-consistent procedure of the current-voltage (I-V) characteristics. The reason that such a calculation is needed is the following. The phase-breaking time $\tau_\phi(x,E_x)$ is a function of the electron and the hole densities, $n(x,E_x)$ and $p(x,E_x)$,[16] respectively. Since

$$p(x,E_x)=N(x,E_x)-n(x,E_x)\ ,$$

one needs to know the DOS's to calculate the values of $\tau_\phi(x,E_x)$. Although our formulation inherently contains carrier transport, in the following calculations for DBS, we did not include the self-consistent current-voltage (I-V) calculation.[19] Instead, the value of τ_ϕ has been taken as a parameter only to demonstrate our procedure. Therefore the results presented below should be regarded as approximate, since these represent only the first-order calculations in a self-consistent iterated procedure.

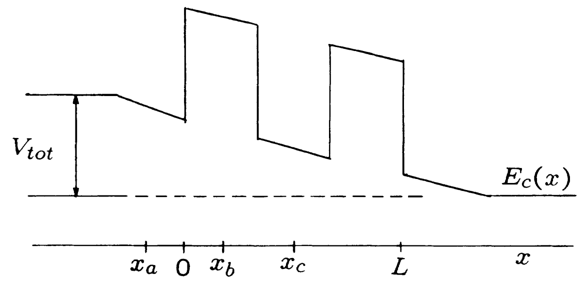

FIG. 2. Schematic plot for the potential energy diagram for a double-barrier structure.

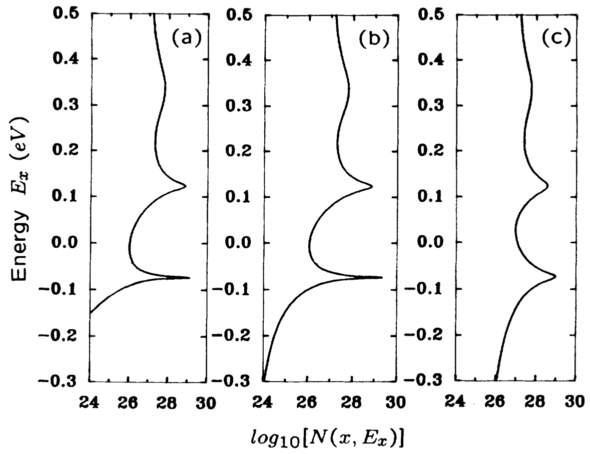

FIG. 3. Theoretical 1D DOS for a biased double-barrier structure as a function of longitudinal energy E_x with τ_ϕ as a parameter. The plot is for the center of the well and the bias voltage is 0.3 V. (a), (b), and (c) correspond to $\tau_\phi=\infty$, 1.0×10^{-11}, and 1.0×10^{-13} s, respectively.

In Figs. 3(a), 3(b), and 3(c), we plot the DOS versus the electron energy in the well (position c, Fig. 2) for $\tau_\phi=\infty$, 10^{-11}, and 10^{-13} s, respectively. The total bias voltage on the structure is 0.3 V. Here, we have chosen the flat part of the conduction band on the left as the reference; therefore the applied bias lowers the center of the band to -0.15 eV. Notice that while the DOS falls very sharply around -0.15 eV for $\tau_\phi=\infty$, for other values of τ_ϕ it seems that the DOS is nonzero below the conduction-

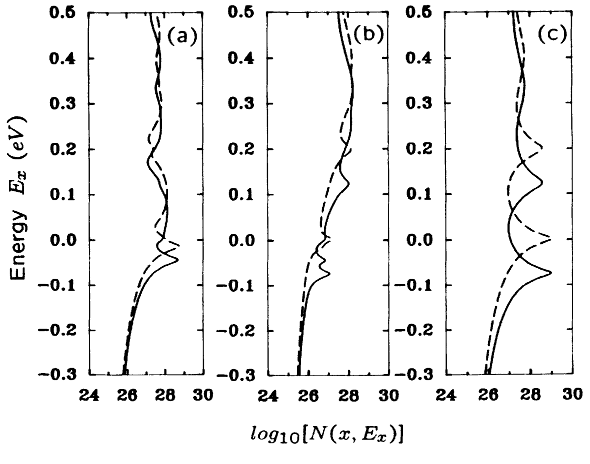

FIG. 4. Theoretical 1D DOS $N(x,E_x)$ as a function of E_x. (a), (b), and (c) correspond to plots at positions x_a, x_b, and x_c (see Fig. 3) in a biased double-barrier structure, respectively. Here, $\tau_\phi=1.0\times 10^{-13}$ s. The dashed and the solid curves correspond to the applied biases of 0.2 and 0.3 V, respectively.

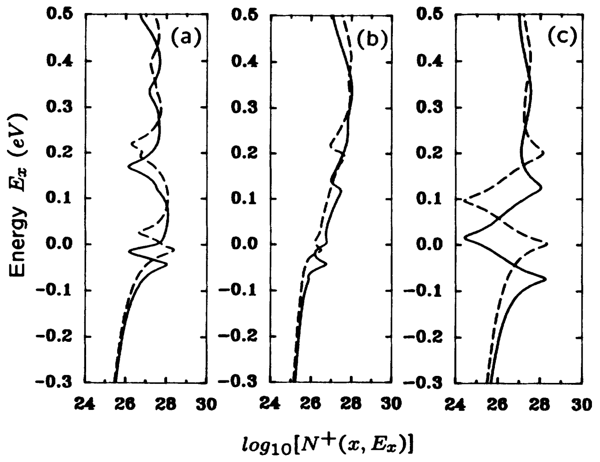

FIG. 5. Theoretical 1D DOS $N^+(x,E_x)$ as a function of E_x. (a), (b), and (c) correspond to plots at positions x_a, x_b, and x_c (see Fig. 3) in a biased double-barrier structure, respectively. Here, $\tau_\phi = 1.0\times10^{-13}$ s. The dashed and the solid curves correspond to the applied biases of 0.2 and 0.3 V, respectively.

band edge. We mention again that the results are not wrong because these represent the shape of the DOS function only at the end of the first iteration. In the following iterations, if carried out, the value of $\tau_\phi(x,E_x)$ for these energy ranges would become progressively larger. Larger values of $\tau_\phi(x,E_x)$ will eventually decrease the DOS below the conduction band. Note that within the well there are two peaks in the DOS that correspond to the resonant energies of the system. However, these three figures clearly show the dependence of the DOS on τ_ϕ, especially that the resonant peaks broaden as the scattering rate is increased.

We have also investigated the effects of applied bias on the shape and the location of the DOS at the three locations mentioned earlier. In Figs. 4, 5, and 6, we plot $N(x_i,E_x)$, $N^+(x_i,E_x)$, and $N^-(x_i,E_x)$ versus E_x, respectively, here for $i=a,b,c$ in (a), (b), and (c), respectively. Figures 4(a), 4(b), and 4(c) show some very interesting features. For example, for a bias voltage of 0.2 V, the peaks in the three regions almost coincide around 0.0 eV. However, as the bias voltage is increased to 0.3 V, the locations of these peaks in energy are separated. Furthermore, notice that within the barrier [Fig. 4(b)], there are two peaks located at energies around −0.40 and −0.75 eV. These peaks coincide with the peaks at −0.4 eV in Fig. 4(a) and at −0.75 eV in Fig. 4(b), respectively. Interestingly, by comparing this figure with Figs. 5(b) and 6(b), one finds that these peaks also coincide with peaks in $N^+(x_b,E_x)$ and $N^-(x_b,E_x)$, respectively.

In Fig. 7 we present $N(x,E_x)$, $N^+(x,E_x)$, and $N^-(x,E_x)$ as a function of position in a DBS under a bias of 0.3 V. We chose an energy of 0.033 eV which does not coincide with any of the resonant energies in the well. This calculation was carried out for $\tau_\phi = 1.0\times10^{-13}$ s. Note that at the off-resonant energy, the average magnitude of the DOS is more than an order of magnitude smaller than the peaks in the density outside the structure. The spatial separations in the peaks in the DOS become smaller as one moves to the right because the kinetic energy of electrons increases with a simultaneous decrease in the de Broglie wavelengths.

Figures 8 and 9 show plots of the chemical potentials for the total, the right-moving, and the left-moving electrons in a 1D quantum wire with a single potential barrier. In these plots the values of τ_ϕ are 10^{-12} and 10^{-13} s, respectively. The total chemical potentials show the Friedel-like oscillations[25] that disappear with increased scattering. The envelopes on the top and the bottom represent the chemical potentials for the positive- and the negative-flowing electrons. In order to generate these plots, we have calculated the total current and the

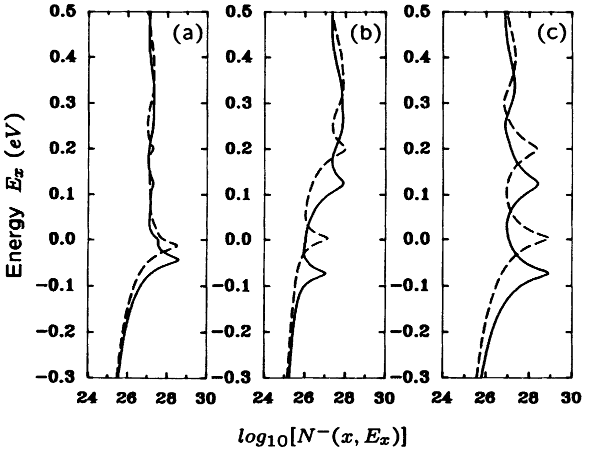

FIG. 6. Theoretical 1D DOS $N^-(x,E_x)$ as a function of E_x. (a), (b), and (c) correspond to plots at positions x_a, x_b, and x_c (see Fig. 3) in a biased double-barrier structure, respectively. Here, $\tau_\phi = 1.0\times10^{-13}$ s. The dashed and the solid curves correspond to the applied biases of 0.2 and 0.3 V, respectively.

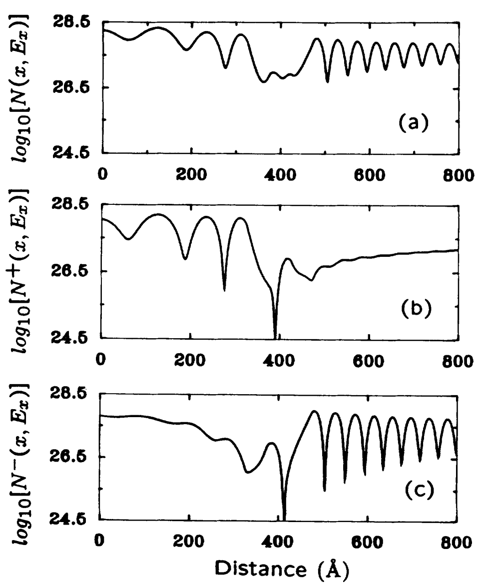

FIG. 7. Theoretical 1D DOS for a double barrier as a function of position x for $E_x = 0.033$ eV. (a), (b), and (c) are for $N(x,E_x)$, $N^+(x,E_x)$, and $N^-(x,E_x)$, respectively. $\tau_\phi = 1.0\times10^{-13}$ s.

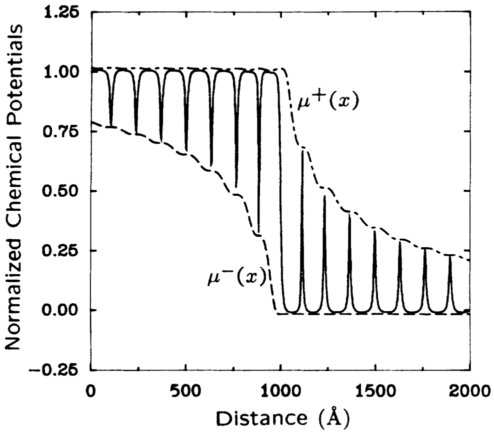

FIG. 8. Plots of the chemical potential $\mu(x)$ (solid curve) as a function of position for $\tau_\phi = 1.0\times10^{-12}$ s. The plot has been normalized to $\mu_1-\mu_2$. The upper and the lower envelopes correspond to $\mu^+(x)$ and $\mu^-(x)$, respectively.

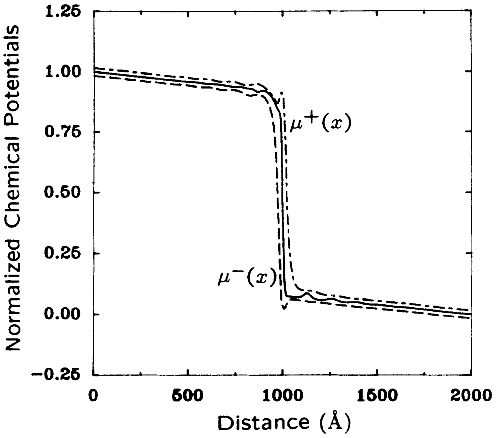

FIG. 9. Plots of the chemical potential $\mu(x)$ (solid curve) as a function of position for $\tau_\phi = 1.0\times10^{-13}$ s. The plot has been normalized to $\mu_1-\mu_2$. The upper and the lower envelopes correspond to $\mu^+(x)$ and $\mu^-(x)$, respectively.

decomposed currents $J^{\pm}(x,E_x)$ in this structure using the transport equation developed in Ref. 19. Note that unlike in earlier work,[15] these chemical potentials do not show any unphysical behavior.

VIII. CONCLUSIONS

This paper deals with the DOS in quantum structures. We present some numerical results to confirm the validity of the formulation proposed in this paper. This is one of a series of papers demonstrating that in order to get physically meaningful and internally consistent results for electron transport, the group velocity states may be more convenient than the usual k states.[14,19,28] The main contributions of our paper are listed below.

(1) We have presented a new formulation, using logarithmic derivatives of the retarded Green's function, for the calculation of the DOS for quantum structures. Our method is based on the quantum kinetic formulation and includes the effects of the phase-randomizing and/or the inelastic processes on the DOS.

(2) We develop a procedure by which the DOS can be split between states for the right-moving and the left-moving electrons. This enables us to write an alternative expression of the Tsu-Esaki equation for the tunneling current through an elastic barrier. Our current expression is based on the state-current densities $J_N^{\pm}(x,E_x)$. In the description of the carrier transport, the state-current densities $J_N^{\pm}(x,E_x)$ are more useful than merely the density of states. We have proved a property for the state-current density that while the $J_N^{\pm}(x,E_x)$ may be altered due to the presence of elastic barriers and phase-breaking processes, the net local state-current density $J_N(x,E_x)$ is always zero.

(3) We show that the proposed decomposition of the DOS and the electron densities for each of the current streams[19] may be used to estimate physically consistent chemical potential in 1D structures.

(4) In our opinion, the present usage of the terms sequential and coherent tunneling found in the literature is too restricting. The present formulation may resolve the ongoing debate and may provide a single comprehensive electron-transport theory for many quantum structures.

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