PHYSICAL REVIEW B VOLUME 52, NUMBER 15 15 OCTOBER 1995-I

Electron transport in the presence of random impurities: Transition from ballistic to diffusive regimes

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(Received 6 June 1995)

A transport theory is developed for multibarrier mesoscopic devices that contain a random configuration of short-range impurity potentials. The theory is based on the self-consistent second Born approximation within the Keldysh formulation. The self-energy of the system is estimated to describe the average two-terminal resistance of an ensemble of nearly identical systems. The theory describes the transition from the ballistic to the diffusive regime of operation as a function of a disorder parameter characterizing the density as well as the strength of the impurities. It is shown that as the strengths of the elastic tunnel barriers are increased, the transition from ballistic to diffusion regime occurs at larger values of the disorder parameter.

I. INTRODUCTION

Investigations into the role of elastic barriers on the transport properties of mesoscopic devices have been an active area of research for many years. References 1–6 are a few examples that include the effects of scattering from known tunnel barriers on the transport of electrons in mesoscopic devices. These theories have been reasonably successful in describing electron transport in devices using a sample-specific Hamiltonian.

In this paper, we deal with the transport properties of devices that in addition to known tunnel barriers contain a random configuration of impurities. We restrict our model to devices with large lateral cross sections. The current flow is considered to be one dimensional (1D). The primary objective is to determine the effects of the random impurities on the average electrical characteristics of nearly identical multibarrier systems. The effects of such scattering are generally included in transport models via a phenomenological constant imaginary potential[5] or a constant mean free path.[7] The imaginary potential or the mean free path is related to a constant phase-breaking or relaxation time. We intend to show that such an approach may have limited validity only for devices without any potential barriers. In the transport model presented in this paper, the phase-breaking time is not a constant, rather it is a function of both the space and the energy.

We note that while a large variety of the devices have finite cross sections, much of the attention has been focused on *strictly* one-dimensional systems.[2–5,8] This was also pointed out by Fertig, He, and Das Sarma[9] who investigated the effects of elastic impurity scattering in double-barrier quantum well (DBQW) structures. The authors used a microscopic perturbation theory based on Green's functions with an energy-independent self-energy and a tight-binding model. An obvious consequence of neglecting multidimensionality of DBQW's is that one must ignore the scattering processes that allow the transverse momentum to change.[9]

Our transport model is based on the nonequilibrium Green's function technique (the Keldysh formalism).[10–12] The Keldysh formalism has been proven to be quite successful in describing mesoscopic devices in the presence of disorder and inelastic scatterings.[13–17] There are some advantages of the Keldysh technique over other methods; unlike the Kubo formalism, the Keldysh approach can describe the nonlinear response of mesoscopic devices under large bias and at nonzero temperatures. Moreover, the Green's functions in the position coordinates allows determination of the spatially varying local quantities of interest, such as the local density of states. This is particularly important for our model, as will be shown later.

Suhrke, Wilke, and Keiper[16] have used the Keldysh technique to develop a transport model for quasi-1D quantum wires. Their model considers inhomogeneity only in the transverse directions due to the lateral confinements. This makes their model inapplicable to some multibarrier devices in which the inhomogeneity is in the direction of the current flow. Recently, Davidovich and Gornsztejn[17] used the Keldysh formalism to analyze the effects of an impurity layer of known configuration in the barriers of a 3D DBQW device on resonant tunneling.

Previously, we used the Keldysh formalism in developing a generalized transport theory for devices that contain random impurities.[18] The model describes the average transport properties of an ensemble of similarly prepared 3D multibarrier structures containing random potentials. The model does not assume any particular form either for the impurity potentials or for the device geometry and it is valid for arbitrary voltages and temperatures, if one ignores other forms of scattering. A drawback of the theory is that it requires the knowledge of full green's functions, which needs to be computed using a nonlocal form of the self-energy.

The primary purpose of this paper is to obtain transport equation for the multibarrier devices described earlier. To simulate these devices, we consider inhomogeneity in the direction of the current flow; however, we assume that the system is translationally invariant in the lateral plane. In the model, the tunneling barriers are in-

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cluded in the Hamiltonian. The effects of the randomly distributed short-ranged impurities (represented by δ-function potentials in space) on the expected transport properties will be included via the self-energy. The self-energy, resulting from the ensemble averaging process, leads to irreversible damping (or phase breaking) of the electron wave.[19] We derive an expression for the phase-breaking scattering rate that is shown to be proportional to the local density of states. It is recognized that the use of terms such as phase breaking, associated with elastic scattering, may surprise some readers. However, the *impurity-averaged* perturbation theory with an elastic interaction in conjunction with coupling to reservoirs does lead to phase breaking within the self-consistent Born approximation. In fact, in the linear regime of operation, Hershfield has shown the equivalence of the scattering formulation (the Landauer formula) with dephasing and the self-consistent Born approximation.[20]

Although the transport properties of mesoscopic systems are well studied in both the ballistic and the diffusive regimes, there has been relatively less research on the transition behavior. Recently de Jong[7] calculated the average resistance of an ensemble of similarly prepared wires from the ballistic up to the diffusive regime using a semiclassical approach. Our transport model is used to study the average resistance of the devices with large lateral widths in the ballistic regime ($L_\phi \gg L$) as well as the transition from the ballistic into the diffusive regime ($L_\phi < L$), where L_ϕ is an effective phase-breaking length and L is the length of the device.

In Sec. II, we derive a position and energy-dependent electron phase-breaking time for arbitrary device structures. Sections III and IV contain derivations to our transport equations applicable to arbitrary and multibarrier device structures, respectively. Section V includes some numerical results. The conclusions are summarized in Sec. VI.

II. SELF-ENERGY AND THE PHASE-BREAKING TIME

We consider devices with a random distribution of impurities of concentration n_0 and assume that the impurity potential is uncorrelated and is very short ranged so that for an impurity at location R, the potential $U(\mathbf{r})$ is

$$U(\mathbf{r}) = V_0 \delta^3(\mathbf{r} - R) \; . \tag{2.1}$$

It is obvious that the presence of random impurities leads to fluctuations of the transport quantities from one sample to another. In small devices, such fluctuations can be significant; for a review of the effects of localization and fluctuations on the device properties, see Ref. 21. However, our interest is in the behavior of a class of devices rather than in that of a particular sample. Thus, the averaging over the ensemble of the impurities needs to be performed[22] to obtain an estimate of the expected values of the transport coefficients. However, it is known that in 1D systems, where *all* states are localized, the issue of averaging is very subtle.[23,24] On the other hand, the situation is quite different in higher dimensions particularly for low impurity densities. The corrections due to weak localization in multidimensions have been shown to be much smaller than other relevant contributions.[9,22] In 3D devices, the linearized form of the nonequilibrium Green's function techniquê (particle-particle correlation) is expected to give identical results as that of the Kubo formalism (current-current correlation) (Ref. 13) within the scope of the second Born approximation. Moreover, the resulting impurity-averaged quantities follow the envelopes that contain the fluctuations.

We average over the ensemble of the impurities described by Eq. (2.1). Using the second Bron approximation and neglecting all diagrams with intersecting interaction lines, the self-energy can be written as[16,19]

$$\Sigma(\mathbf{r}_1,\mathbf{r}_2;t_1,t_2) = n_o V_0^2 G(\mathbf{r}_1,\mathbf{r}_2;t_1,t_2)\delta^3(\mathbf{r}_1-\mathbf{r}_2) \; . \tag{2.2}$$

The general form of the Dyson equation in the Keldysh formalism[11,12] is given by Mahan[13]

$$\overline{G}(X_1,X_2) = \overline{G_0}(X_1,X_2) + \int dX_3 dX_4 \overline{G_0}(X_1,X_3)\overline{\Sigma}(X_3,X_4) \times \overline{G}(X_4,X_2) \; , \tag{2.3}$$

where $X = \mathbf{r}, t$, and $\overline{\Sigma}$ and $\overline{G}$ are (2×2) matrices given as

$$\overline{G} = \begin{bmatrix} G_t & -G^< \\ G^> & -G_{\overline{t}} \end{bmatrix} , \quad \overline{\Sigma} = \begin{bmatrix} \Sigma_t & -\Sigma^< \\ \Sigma^> & -\Sigma_{\overline{t}} \end{bmatrix} .$$

Thus, using Eq. (2.2), the off-diagonal elements of the $\overline{\Sigma}$ matrix[13] are given as

$$\Sigma^\alpha(\mathbf{r}_1,\mathbf{r}_2;t_1,t_2) = n_o V_0^2 G^\alpha(\mathbf{r}_1,\mathbf{r}_2;t_1,t_2)\delta^3(\mathbf{r}_1-\mathbf{r}_2) \; , \tag{2.4}$$

where $\alpha = >$ or $<$. Equation (2.3) is a (2×2) matrix equation involving four different Green's functions from which we obtain the retarded Green's function G^R defined by the relation

$$G^R(X_1,X_2) = \theta(t_1-t_2)[G^>(X_1,X_2) - G^<(X_1,X_2)] \; , \tag{2.5}$$

because much of the transport properties of the system can be obtained from the information about the G^R. The details of the derivations for the retarded Green's function are shown in the Appendix. Using Eqs. (A7), (A8), and (A3) of the Appendix, finally we obtain,

$$\left[E - H_{\text{mod}}(\mathbf{r}_1) + \frac{i\hbar}{2}\left[\frac{1}{\tau_\phi(\mathbf{r}_1;E)}\right]\right] G^R(\mathbf{r}_1,\mathbf{r}_2;E) = \delta^3(\mathbf{r}_1-\mathbf{r}_2) \; , \tag{2.6}$$

where $H_{\text{mod}}(\mathbf{r}_1) = H(\mathbf{r}_1) + \sigma(\mathbf{r}_1;E)$. σ comes from the real part of the self-energy and is defined in the Appendix. The term τ_ϕ represents the electron phase-breaking time due to impurities and is given by

$$\frac{1}{\tau_\phi(\mathbf{r};E)} = \frac{2\pi n_0}{\hbar} V_0^2 N_0(\mathbf{r};E) \; . \tag{2.7}$$

Here $N_0(\mathbf{r};E) = -(1/\pi)\text{Im}[G^R(\mathbf{r},\mathbf{r};E)]$ represents the spatially varying local 3D density of states (DOS). Interestingly, the expression for τ_ϕ given by Eq. (2.7) agrees with the expectation that for elastic phase-breaking scattering, the inverse phase-breaking time (i.e, the

scattering rate) is proportional to the density of states.[25] At zero temperature and for homogeneous systems, it reduces to the well-known expression $1/\tau_\phi = (2\pi n_o/\hbar)V_0^2 N_0(E_F)$ for the electron phase-breaking scattering time,[19] where the DOS is a constant in spatial coordinates evaluated at the Fermi energy level.

III. TRANSPORT EQUATION FOR ARBITRARY STRUCTURES

An equation for the current density for arbitrary multiterminal structures can be derived using the "less-than" Green's function $G^<(\mathbf{r}_1,\mathbf{r}_2;E)$ contained in the off-diagonal element of the (2×2) matrix equation.[14] Thus, using Eqs. (A1) and (A3), one obtains

$$G^<(\mathbf{r}_1,\mathbf{r}_2;E) = \int d\mathbf{r}' d\mathbf{r}'' G^R(\mathbf{r}_1,\mathbf{r}';E)\Sigma^<(\mathbf{r}',\mathbf{r}'';E) \times G^A(\mathbf{r}'',\mathbf{r}_2;E) \; . \tag{3.1}$$

Now, upon substituting Eq. (2.4) in Eq. (3.1), and using the relationships $G^A(\mathbf{r}_1,\mathbf{r}_2;E) = G^{R*}(\mathbf{r}_2,\mathbf{r}_1;E)$ and $n(\mathbf{r};E) = -(1/2\pi)iG^<(\mathbf{r},\mathbf{r};E)$, we obtain an expression for the electron density:

$$n(\mathbf{r};E) = n_0 V_0^2 \int d\mathbf{r}' |G^R(\mathbf{r},\mathbf{r}';E)|^2 n(\mathbf{r}';E) \; . \tag{3.2}$$

Although the integral equation for the electron density has been derived assuming a local form of self-energy, it may be mentioned that a similar integral relationship also holds for the generalized electron distribution function $n(\mathbf{r}_1,\mathbf{r}_2;E) = -(1/2\pi)iG^<(\mathbf{r}_1,\mathbf{r}_2;E)$ when the self-energy functions assume a nonlocal form.[18] The self-energies become nonlocal when the impurity potential is not considered to be a δ function in space.

When voltages are applied at the contacts of a multiterminal device, the current in the ith terminal is given by the equation

$$I_i = \int dE \int \mathbf{J}(\mathbf{r};E)\cdot d\mathbf{S}_i \; , \tag{3.3}$$

where

$$\mathbf{J}(\mathbf{r};E) = \frac{-e\hbar}{4\pi m^*}(\nabla - \nabla')G^<(\mathbf{r},\mathbf{r}';E)|_{\mathbf{r}=\mathbf{r}'} \; . \tag{3.4}$$

Using Eqs. (3.1) and (3.2) in Eq. (3.4),

$$\mathbf{J}(\mathbf{r};E) = \frac{e}{m^*} n_o V_0^2 \int d\mathbf{r}' |G^R(\mathbf{r},\mathbf{r}';E)|^2 \times [\hbar \nabla \theta(\mathbf{r},\mathbf{r}';E)] n(\mathbf{r}';E) \; , \tag{3.5}$$

where $G^R(\mathbf{r},\mathbf{r}';E) = |G^R(\mathbf{r},\mathbf{r}';E)| \exp[i\theta(\mathbf{r},\mathbf{r}';E)]$.

IV. TRANSPORT EQUATION FOR MULTIBARRIER MESOSCOPIC SYSTEMS

The device structure considered in this paper can be schematically represented by Fig. 1. The device has three regions. Regions I and III are made of the same material that need not be ideal. Region II of our device contains all the barriers and the wells. We assume that the devices are translationally invariant in the lateral plane (the y-z plane). The Hamiltonian can be decomposed into the lateral and the longitudinal components. Then,

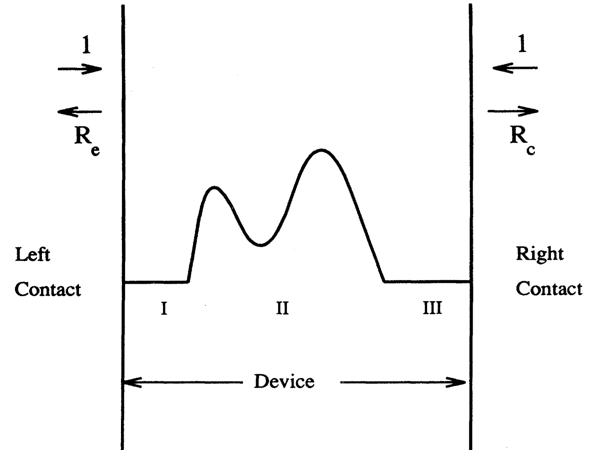

FIG. 1. The schematic diagram of our device. R_e (R_c) represents the coherent reflection coefficient evaluated at the boundary between the left (right) contact and the device containing random impurities.

$H(\mathbf{r}) = H(x) + H(\rho)$, where $\rho = (y,z)$ and $H(\rho) = (\hbar^2/2m^*)\nabla_\rho^2$. If a quantity g is a function of two coordinate variables $\mathbf{r}_1$ and $\mathbf{r}_2$, is can be expressed as $g(\mathbf{r}_1,\mathbf{r}_2;E) = g(x_1,x_2,\rho_1-\rho_2;E)$. One can Fourier transform it with respect to the relative transverse coordinates as shown below:

$$g(\mathbf{r}_1,\mathbf{r}_2;E) = \frac{1}{(2\pi)^2}\int d\mathbf{k}_\parallel g(x_1,x_2,\mathbf{k}_\parallel;E) e^{i\mathbf{k}_\parallel\cdot(\rho_1-\rho_2)} \; . \tag{4.1}$$

Moreover, if a quantity is a function of a single coordinate variable $\mathbf{r}$, it becomes a function of x only, so that $\tau_\phi(\mathbf{r};E) \to \tau_\phi(x:E)$, $n(\mathbf{r};E) \to n(x;E)$, $\mathbf{J}(\mathbf{r};E) \to \mathbf{J}(x;E)$, etc. Thus, writing $G^R(\mathbf{r}_1,\mathbf{r}_2;E)$ in a form given by Eq. (4.1), and operating on it by the $H(\rho)$, Eq. (2.6) can be written as

$$\left[E - \frac{\hbar^2 \mathbf{k}_\parallel^2}{2m^*} - H_{\text{mod}}(x_1) + i\frac{\hbar}{2\tau_\phi(x_1;E)}\right] G^R(x_1,x_2,\mathbf{k}_\parallel;E) = \delta(x_1-x_2) \; . \tag{4.2}$$

Here $G^R(x_1,x_2,\mathbf{k}_\parallel;E)$ is the one-dimensional Green's function that depends both on the total energy as well as the transverse wave-vector $\mathbf{k}_\parallel$. In related work, Lake and Datta[25] tried to decompose the Green's function for a similar structure. However, their 1D equation does not contain the term $\hbar^2\mathbf{k}_\parallel^2/2m^*$ because of an algebraic error. Neglect of this term will introduce serious mistakes in the results.

Using the properties of the transverse invariance and the definition of τ_ϕ as given by Eq. (2.7), the current density is expressed as a sum of the 1D transverse mode current densities:

$$\mathbf{J}(x;E) = \frac{1}{(2\pi)^2}\int d\mathbf{k}_\parallel \mathbf{J}(x,\mathbf{k}_\parallel;E) \; , \tag{4.3}$$

where

$$\mathbf{J}(x,\mathbf{k}_\parallel;E)=\frac{e}{m^*}n_o V_0^2\int dx'|G^R(x,x',\mathbf{k}_\parallel;E)|^2 \times\left[\hbar\frac{\partial}{\partial x}\theta(x,x',\mathbf{k}_\parallel;E)\right]n(x';E). \tag{4.4}$$

Since elastic phase-breaking processes due to impurities do not change electron energy, current continuity is maintained at each energy separately. In other words, $(\partial/\partial x)\mathbf{J}(x;E)=0$. Equation (4.4) can now be solved for each transverse mode along with the appropriate boundary conditions for the injected currents described by

$$\mathbf{J}^+(0,\mathbf{k}_\parallel;E)=\frac{e}{\pi\hbar}[1-R_e(\mathbf{k}_\parallel;E)]f_0(E,\mu_L)\ , \tag{4.5}$$

$$\mathbf{J}^-(L,\mathbf{k}_\parallel;E)=-\frac{e}{\pi\hbar}[1-R_c(\mathbf{k}_\parallel;E)]f_0(E,\mu_R)\ . \tag{4.6}$$

Here, we assume that the contacts are in thermal equilibrium characterized by single chemical potentials μ_L and μ_R for the left and the right contacts, respectively. The distribution functions f_0 in the contacts is approximately the Fermi-Dirac distribution. The coherent reflection coefficient $R_e(R_c)$ is evaluated at the left (right) boundary between the contact and device.[26] Consequently, the term like $[1-R_e(\mathbf{k}_\parallel;E)]$ does not represent the transmission probability across the full length of the device; it merely estimates the fraction of the electrons that are injected across the contact-device interface. Although contacts are usually treated as ideal thermal reservoirs that absorb and thermalize all incident electrons before reinjecting into the device, such a description is often not valid.[27] In case of nonideal contacts, the conductance properties of the device, measured between the contacts, may be significantly modified by the nature of the contacts.[28] Following Oakeshott,[29] we will model the contacts as imperfect ones, which are represented by strongly disordered regions characterized by a constant phase-breaking time.

In steady state, the current [Eq. (4.3)] is independent of position and the total current $\mathbf{J}_T$ is obtained by integrating Eq. (4.3) over energy E. Noting that the applied voltage is given by $eV_a=(\mu_L-\mu_R)$, the conductance is determined from the relation $G=\mathbf{J}_T/V_a$. The expression for the conductance can be recast into the familiar general form

$$G=\frac{e^2}{\pi\hbar}\int dE\left[-\frac{\partial f_0(E)}{\partial E}\right]T_{\text{eff}}(E)\ . \tag{4.7}$$

Here $T_{\text{eff}}(E)$ is the effective transmission coefficient summed over all the transverse modes at energy E. It is given by the equation

$$T_{\text{eff}}(E)=\frac{1}{(2\pi)^4}\int d\mathbf{k}_\parallel d\mathbf{k}'_\parallel[1-R_e(\mathbf{k}_\parallel;E)] \times\mathcal{T}_{L\to R}(\mathbf{k}'_\parallel,\mathbf{k}_\parallel;E)\ . \tag{4.8}$$

$\mathcal{T}_{L\to R}(\mathbf{k}'_\parallel,\mathbf{k}_\parallel;E)$ is the fraction of the injected electrons from the left reservoir with transverse wave-vector $\mathbf{k}_\parallel$ that leaves the device from the right with wave-vector $\mathbf{k}'_\parallel$. We have verified that for small biases. $\mathcal{T}_{L\to R}(\mathbf{k}'_\parallel,\mathbf{k}_\parallel;E)$ are independent of the current flow through the device.

V. RESULTS AND DISCUSSION

In this section, we present results of the self-consistent solutions to Eqs. (2.6) and (2.7). The numerical technique used in the calculations are similar to that discussed in the appendix of Ref. 15. Results presented in this paper are for zero temperature and small bias voltages. Applications of our model to the nonlinear regimes and/or at finite temperatures will be presented elsewhere. In this paper, the strength and the density of impurities is quantified by a single dimensionless parameter $\beta=3.24\times10^{66}n_o V_0^2$, where n_o and V_0 are in Système International units.[16] Using this definition, we rewrite Eq. (2.7) as $\tau_\phi=5.33\times10^{31}/\beta N_0$ sec. The contacts, modeled as strongly disordered regions, have a constant τ_ϕ of 10^{-13} sec.

In Fig. 2, we present theoretical plots of the phase-breaking time τ_ϕ as a function of position x for a DBQW device. The widths of the well and the barrier regions are 50 Å and 30 Å, respectively; the barrier height is 0.3 eV. The lowest resonant energy E_0 for this well is approximately 0.08 eV. To generate these plots, we have used two values of Fermi level E_F and $\beta=0.1$. The boundary conditions are applied at the contacts that are located 1000 Å from the barriers. Notice that for a given E_F, the phase-breaking time in multibarrier devices varies by more than an order in magnitude. This is because of the energy and spatial variation of the 3D density of states (see inset) for such structures. Thus, it is our opinion that in transport models for disordered multibarrier device structures, the use of phenomenological constant phase breaking or relaxation time or constant mean free paths may only be reasonable only for homogeneous devices.

Figure 3 shows plots of the theoretical two-probe con-

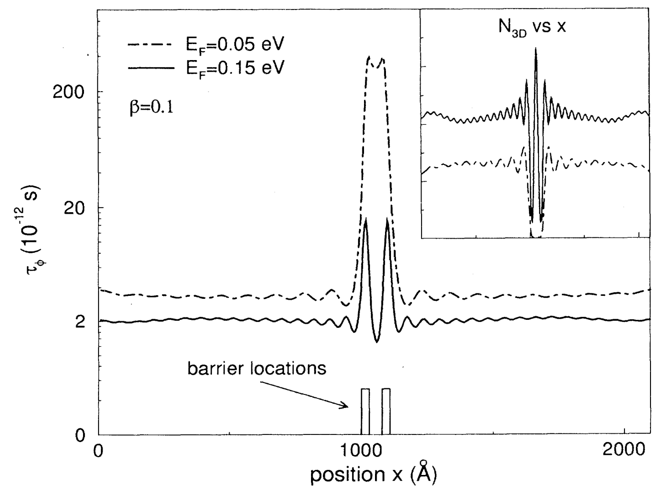

FIG. 2. τ_ϕ vs x for DBQW device for two different values of E_F. The inset shows the 3D density of states as a function of x.

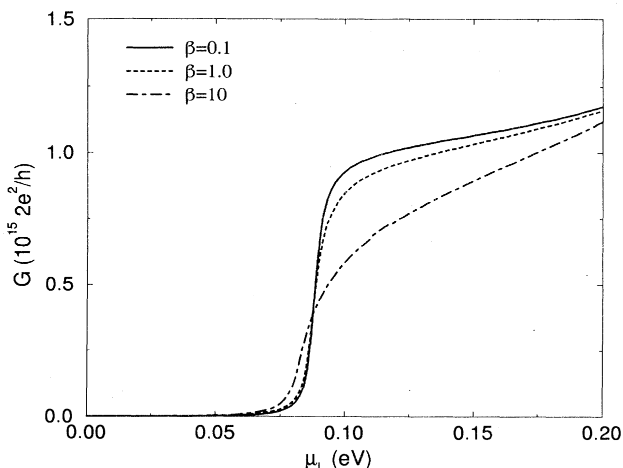

FIG. 3. Two-probe conductance G as function of the reservoir chemical potential μ_L for three different values of the disorder β for the DBQW device.

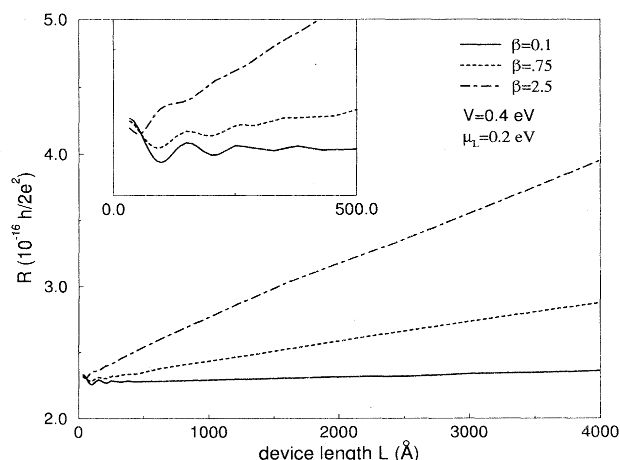

FIG. 5. Resistance R vs length L for a single barrier device of barrier height $V=0.4$ eV for three different values of β.

ductance (per unit area) as a function of the chemical potential μ_L in the left contact of the aforementioned DBQW structure. The plots are for three values of β. As expected,[9] the conductance makes a sharp jump at $\mu_L = E_0$. However, the transition width increases with increasing disorder and the conductance does not saturate beyond $\mu_L = E_0$. We think that the saturation characteristic seen in Fertig, He, and Das Sarma's conductance curve[9] stems from the fact that their coupling coefficients between the well and the reservoirs are energy independent.

Let us now consider a different device (of length L) that contains a single 20-Å barrier of height V at its center. In Fig. 4, we show the average two-probe resistance per unit area $R = 1/G$ as a function of the disorder parameter β and $L = 2250$ Å. As indicated in the figure, the plots correspond to three values of the barrier height V. Note that the shapes of the plots are almost identical. As expected, the resistance is larger for larger barrier heights. Each of

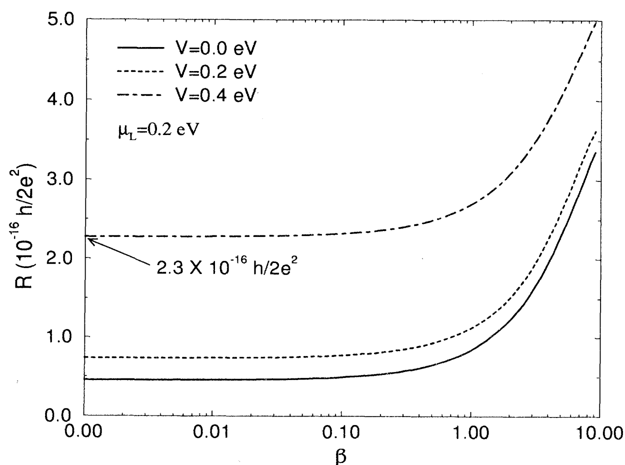

FIG. 4. Resistance R vs disorder β for a single barrier device for three different values of the barrier height V.

the curves is virtually flat for small values of β and it increases significantly only when β exceeds a certain critical value (β_c). Note that while we have used values of β up to ten, such values may violate the assumption of low impurity density.

Figure 5 shows plots of the two-probe resistance versus the length L. The barrier height V is 0.4 eV. Note that the plots contain oscillations for small L due to the interference effects. The interferences are due to multiple reflections between the barrier and the contacts. The reflection of an electron incident on the imperfect contact takes place because of the "impedance mismatch" between the two regions. Since the region I and III in the device contain phase-breaking processing, reflected wave functions from the barrier lose their phase coherence as they propagate towards the contacts. Consequently, as L increases, these interference effects decrease and the curves gradually become linear with slopes that depend on β. This transition occurs at smaller values of L if the disorder parameter is larger. Plots for a homogeneous device ($V=0$, not shown) do not contain such oscillations because in the absence of the barrier, the interference effects due to the multiple reflections from the device-contact interfaces are very weak.

Figures 4 and 5 clearly show a gradual transition from the ballistic to diffusive regimes of operation as functions of the device length and the disorder parameter β. Extrapolating the straight line asymptotes of the plots to $L=0$ (in Fig. 5), we obtain approximately $(1/G_0') = 2.3 \times 10^{-16}$ (in units of $h/2e^2$). This value is the same as that in the plot in Fig. 4 for the $V=0.4$-eV barrier case for $\beta=0$. To interpret the numerical results, we use the following approach. It is known that the expression for the two-probe conductance of a 1D chain[30,31] is given as

$$G = \frac{e^2}{\pi\hbar}\left[1+\frac{L}{2L_\phi}\right]^{-1} .$$

For homogeneous mesoscopic devices, the coherent reflection coefficient $R_e \simeq 0$. Thus, using Eqs. (4.7) and

(4.8), one can derive an expression for the two-probe conductance as

$$G(E_F)=G_0(E_F)\left[1+\frac{L}{2L_\phi(E_F)}\right]^{-1}, \tag{5.1}$$

where $G_0(E_F)=m^*E_F/2\pi\hbar^2(e^2/\pi\hbar)$ represent the number of the transverse channels per unit area at energy E_F times the conductance of a single channel $e^2/\pi\hbar$. The term $L_\phi(E_F)=\tau_\phi(E_F)v_{\rm av}(E_F)$ is the phase-breaking length, where $v_{\rm av}$ is the velocity of the electron averaged over all the transverse modes. Since for a homogeneous system τ_ϕ is a constant (for a given β), the phase-breaking length is also constant. Thus, the above expression naturally separates the ballistic transport regime from diffusive transport regime simply by the value of the ratio L/L_ϕ.

The situation is quite different when the device contains a barrier. In this case, the reflections from the barrier contribute to the resistance. However, due to the phase-breaking scatterings from the random impurities, the effects of the reflected electrons are localized only in the immediate neighborhood of the barrier.[31] If the length of the device is less than the extent of the interference region, the conductance shows oscillations and cannot be expressed in the form of Eq. (5.1). However, for large L, one can derive an expression similar to Eq. (5.1) (see Eq. (26) of Ref. 31) with $G_0(E_F)$ replaced by $G_0'(L,E_F)$. $G_0'(L,E_F)$ contains the contribution of the potential barrier to the resistance and is smaller than $G_0(E_F)$ for $V=0$. $G_0'(L,E_F)$ gradually becomes independent of L for large L because the interference effects are localized only near the barrier.

For nonhomogeneous systems, the estimation of L_ϕ is not trivial since it require spatial averaging and averaging over all the transverse modes. We have, therefore, taken a simpler approach that uses the numerically calculated resistance and Eq. (5.1). We define an effective phase-breaking length as

$$L_\phi=\frac{L}{2}\frac{G}{G_0'-G}.$$

Figure 6 shows the plot of L_ϕ/L versus β for devices with $L=2250$ Å. From Figs. 4 and 6, one finds that whenever L_ϕ becomes comparable to L, R begins to increase significantly as a function of β. We can also define that the transition from the ballistic to the diffusive regime occurs at a critical value of β_c when $L_\phi/L=0.5$ (or simply when $R=2R_0$). Using these definitions, we observe in Fig. 7 that the transition is influenced by the strength of the barrier potential. If the barrier height increases, such a transition occurs at a larger value of the critical disorder parameter β_c. This can be explained by noting that the presence of a barrier lowers the density of state in the immediate vicinity of the barrier. A smaller density of states in turn reduces the scattering probability of electrons with random impurities and to observe a transition from the ballistic to diffusion regime, the disorder parameter must be increased.

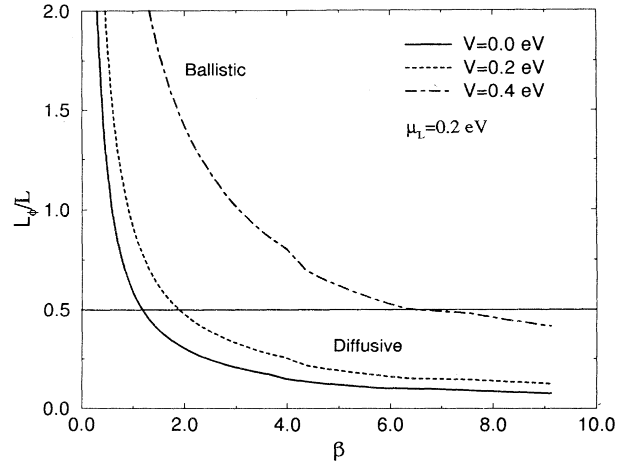

FIG. 6. L_ϕ/L vs disorder β for the devices used in the calculation of Fig. 4. The horizontal line represents the condition $2L_\phi=L$.

VI. CONCLUSION

In this paper we present a transport model that deals with the problem of estimating the expected value of conductance of mesoscopic devices containing random impurities and a known configuration of potential barriers. Our model uses the second Born approximation within the nonequilibrium Green's function approach. Using the process of ensemble averaging, we have derived an expression for the phase-breaking time for carriers. The expression for the phase-breaking time is used to describe electron transport in 3D multibarrier devices. Our calculated results show that the phase-breaking time in multibarrier devices is a function of both the disorder strength and the local density of states. Its value can vary within the devices by orders of magnitude.

We have investigated the transition of the device

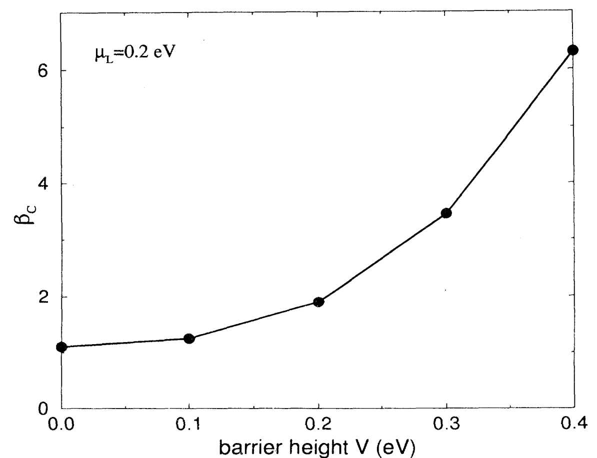

FIG. 7. The plot of β_c vs the barrier height V in single barrier devices. β_c is the value of the critical disorder when transition from the ballistic transport to the diffusive transport takes place.

operation from the ballistic to the diffusive regime. A simple model based on our numerical calculations is developed to study this behavior in devices containing a tunnel barrier. It is observed that the transition depends not only on the disorder, but also on the strength of the potential barrier structure.

ACKNOWLEDGMENT

The authors would like to express their sincere thanks to Professor G. D. Mahan for his comments and suggestions.

APPENDIX: EQUATION FOR THE GREEN'S FUNCTION

The derivation for the scattering time shown in this appendix is similar to that used in Ref. 14. Operating on Eq. (2.3) with $[i\hbar(\partial/\partial t_1)-H(\mathbf{r}_1)]$ and using the fact that for the noninteracting Green's function one has

$$\left[i\hbar\frac{\partial}{\partial t_1}-H(\mathbf{r}_1)\right]\overline{G}_0(X_1,X_2)=\delta^4(X_1-X_2)I\ ,$$

we obtain

$$\left[i\hbar\frac{\partial}{\partial t_1}-H(\mathbf{r}_1)\right]\overline{G}(X_1,X_2)=\delta^4(X_1-X_2)I+\int dX_3\overline{\Sigma}(X_1,X_3)\times\overline{G}(X_3,X_2)\ . \quad \text{(A1)}$$

From Eq. (A1), one obtains the following equation for the retarded Green's function G^R [Eq. (2.5)]:

$$\left[i\hbar\frac{\partial}{\partial t_1}-H(\mathbf{r}_1)\right]G^R(X_1,X_2)-\int dX_3\Sigma^R(X_1,X_3)G^R(X_3,X_2)=\delta^4(X_1-X_2)\ . \quad \text{(A2)}$$

Fourier transforming Eq. (A2) with respect to the relative time coordinate t_1-t_2 under the steady-state condition, one obtains

$$[E-H(\mathbf{r}_1)]G^R(\mathbf{r}_1,\mathbf{r}_2;E)-\int d\mathbf{r}_3\Sigma^R(\mathbf{r}_1,\mathbf{r}_3;E)G^R(\mathbf{r}_3,\mathbf{r}_2;E)=\delta^3(\mathbf{r}_1-\mathbf{r}_2)\ . \quad \text{(A3)}$$

The expression for the retarded self-energy term, given as

$$\Sigma^R(\mathbf{r}_1,\mathbf{r}_2;t_1-t_2)=\theta(t_1-t_2)[\Sigma^>(\mathbf{r}_1,\mathbf{r}_2;t_1-t_2)-\Sigma^<(\mathbf{r}_1,\mathbf{r}_2;t_1-t_2)]\ , \quad \text{(A4)}$$

is also Fourier transformed with respect to t_1-t_2 to obtain

$$\Sigma^R(\mathbf{r}_1,\mathbf{r}_2;E)=i\int\frac{dE'}{2\pi}\frac{\Sigma^>(\mathbf{r}_1,\mathbf{r}_2;E')-\Sigma^<(\mathbf{r}_1,\mathbf{r}_2;E')}{E-E'+i\epsilon}=n_oV_0^2\delta^3(\mathbf{r}_1-\mathbf{r}_2)\times\int\frac{dE'}{2\pi}\frac{iG^>(\mathbf{r}_1,\mathbf{r}_1;E')-iG^<(\mathbf{r}_1,\mathbf{r}_1;E')}{E-E'+i\epsilon}\ . \quad \text{(A5)}$$

Using relations for the hole density $p(\mathbf{r};E)=(1/2\pi)iG^>(\mathbf{r},\mathbf{r};E)$, the electron density $n(\mathbf{r};E)=-(1/2\pi)iG^<(\mathbf{r},\mathbf{r};E)$, and the density of states $N_0(\mathbf{r};E)=p(\mathbf{r};E)+n(\mathbf{r};E)$, one can rewrite Eq. (A5) as the following:

$$\Sigma^R(\mathbf{r}_1,\mathbf{r}_2;E)=n_oV_0^2\delta^3(\mathbf{r}_1-\mathbf{r}_2)\int\frac{dE'}{2\pi}\frac{2\pi N_0(\mathbf{r}_1;E')}{E-E'+i\epsilon}\ . \quad \text{(A6)}$$

The real and imaginary parts of $\Sigma^R(\mathbf{r}_1,\mathbf{r}_2;E)$ from Eq. (A6) are, therefore, given by

$$\mathrm{Re}[\Sigma^R(\mathbf{r}_1,\mathbf{r}_2;E)]=\sigma(\mathbf{r}_1;E)\delta^3(\mathbf{r}_1-\mathbf{r}_2)=n_oV_0^2\delta^3(\mathbf{r}_1-\mathbf{r}_2)P\int dE'\frac{N_0(\mathbf{r}_1;E')}{E-E'} \quad \text{(A7)}$$

and

$$-\mathrm{Im}[\Sigma^R(\mathbf{r}_1,\mathbf{r}_2;E)]=\frac{\hbar\delta^3(\mathbf{r}_1-\mathbf{r}_2)}{2\tau_\phi(\mathbf{r}_1;E)}=n_oV_0^2\delta^3(\mathbf{r}_1-\mathbf{r}_2)\frac{2\pi N_0(\mathbf{r}_1;E)}{2}\ . \quad \text{(A8)}$$

Equations (A7) and (A8) are then substituted into Eq. (A3) to obtain Eq. (2.6).

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