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QUANTUM KINETIC ANALYSIS OF MESOSCOPIC SYSTEMS: LINEAR RESPONSE

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Numerical results are presented for R_{xx} and R_{xy} in a rectangular Hall geometry from B = 0 − 10T. At low fields we find the usual semiclassical results while at high fields both Shubnikov-de Haas oscillations and the quantum Hall effect are evident. Electrochemical potential profiles and current flow patterns are also discussed. The analysis is based on a linear response equation derived earlier from the Keldysh formalism. This equation assumes low temperatures and point-like phase-breaking scatterers. We also discuss how this equation is generalized to high temperatures and extended scatterers.

1. Introduction

Quantum kinetic equations provide a general approach for incorporating phase-breaking processes into transport problems. Two different formulations have been used (see discussions in Refs. 1 and 2). The first is the density matrix approach based on the Liouville equation[3–6]. The second approach was developed independently by Keldysh[7] and by Kadanoff and Baym[8]. In homogeneous systems[9–10] it is customary to make the so called 'gradient expansion' which is inapplicable to mesoscopic devices with rapid spatial variations in the potential. However, the basic formalism is quite general and has been applied to tunneling devices[11], to current fluctuations in mesoscopic devices[12], to resonant tunneling diodes[13–14] and to single electron charging effects[15]. It is the purpose of this paper to describe our work in applying this formalism to *linear steady-state* electronic transport in mesoscopic systems.

2. The Method

Earlier we have derived[16] the following linear response equation starting from the Keldysh formalism:

$$I(\mathbf{r}) = \frac{e}{h}\int d\mathbf{r}'\, T_0(\mathbf{r},\mathbf{r}')\left[\mu(\mathbf{r})-\mu(\mathbf{r}')\right] \qquad (1)$$

where

$$T_0(\mathbf{r},\mathbf{r}') = \left.\frac{\hbar^2\,|G^R(\mathbf{r},\mathbf{r}',E_F)|^2}{\tau_\phi(\mathbf{r},E_F)\tau_\phi(\mathbf{r}',E_F)}\right|_{\text{at equilibrium}} \qquad (2)$$

The retarded Green function is obtained from a Schrödinger-like equation including a self-energy potential.

$$\left[E - H_0(\mathbf{r}) - \sigma(\mathbf{r},E) + \frac{i\hbar}{2\tau_\phi(\mathbf{r},E)}\right] G^R(\mathbf{r},\mathbf{r}',E) = \delta(\mathbf{r}-\mathbf{r}') \qquad (3)$$

The numerical analysis proceeds as follows. We first compute $G^R(\mathbf{r},\mathbf{r}',E)$ on a lattice using the tight-binding formalism. The contacts are treated as open boundaries extending to infinity. Electron-electron interactions are neglected altogether. We also neglect the real part of the self-energy $\sigma(\mathbf{r},E)$ and assume that the imaginary part $\hbar\tau_\phi^{-1}(\mathbf{r};E)$ is proportional to the local density of states $N_0(\mathbf{r},E) = -\mathrm{Im}\,G^R(\mathbf{r},\mathbf{r},E)/\pi$. This is true for elastic point-like scatterers. The computation of $G^R(\mathbf{r},\mathbf{r},E)$ from Eq. (4) has to be carried out iteratively so that a self-consistent value of τ_ϕ is obtained. Once $G^R(\mathbf{r},\mathbf{r}',E)$ and $\tau_\phi(\mathbf{r},E)$ have been obtained we can compute the kernel $T_0(\mathbf{r},\mathbf{r}')$ and proceed to solve the integral equation (1). First we compute $\mu(\mathbf{r})$ everywhere within the device (where $I(\mathbf{r})=0$), assuming the boundary conditions $\mu(\mathbf{r})=\mu_i$ in contact 'i'. Next we compute the external current $I(\mathbf{r})$ within the contact regions and integrate it over each contact to obtain the corresponding terminal current. The detailed current density $\delta\mathbf{J}(\mathbf{r})$ within the structure (due to electrons near the Fermi energy) can also be computed once $\mu(\mathbf{r})$ has been obtained throughout the device.

$$\delta\mathbf{J}(\mathbf{r}) = \frac{\hbar^2}{2\pi m^*}\int d\mathbf{r}'\,\frac{\mu(\mathbf{r}')-E_F}{\tau_\phi(\mathbf{r}';E_F)}\,\mathrm{Im}\left[G^R(\mathbf{r},\mathbf{r}',E_F)^*\,\nabla G^R(\mathbf{r},\mathbf{r}';E_F)\right] - \frac{e\hbar}{2\pi m^*}\mathbf{A}(\mathbf{r})\int d\mathbf{r}'\,\frac{\mu(\mathbf{r}')-E_F}{\tau_\phi(\mathbf{r}';E_F)}\left|G^R(\mathbf{r},\mathbf{r}';E_F)\right|^2 \qquad (4)$$

Further details can be found in Refs. 16-19.

3. Numerical Example

We now present some numerical results for the electrochemical potential profile and current flow pattern in a

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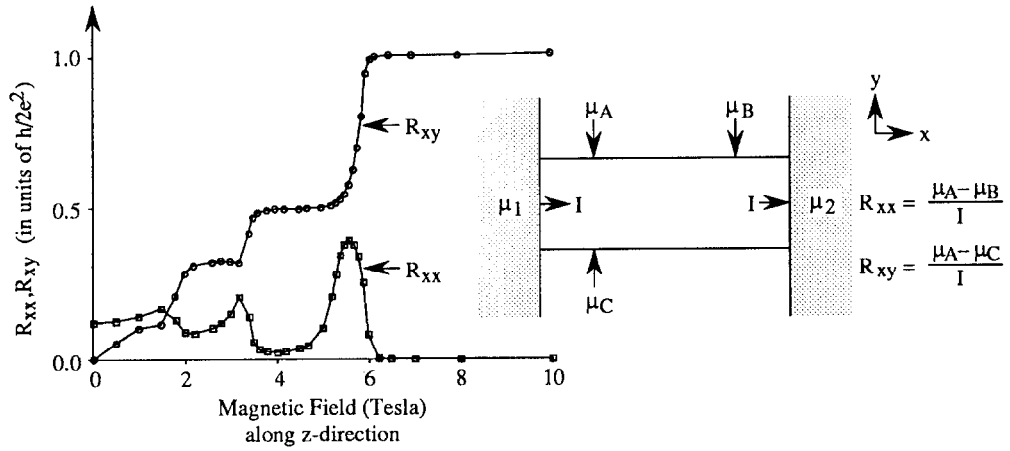

Fig. 1. Calculated R_{xx} and R_{xy} vs. B for a rectangular Hall bar geometry shown in inset (after Ref. 19).

rectangular Hall bar (~3500Å × 750Å) obtained by solving Eqs. (1-4). Fig. 1 shows the structure simulated. From the longitudinal and transverse drops in the electrochemical potential across the bar we compute R_{xx} and R_{xy} as a function of the magnetic field B (actual probes are not included in order to avoid any probe-related artifacts). At low magnetic fields we obtain the usual semiclassical results, namely, a constant R_{xx} and a linearly increasing R_{xy}. There is no weak localization or conductance fluctuations since we do not include any coherent scatterers – the resistance arises solely from phase-breaking scatterers. At high fields when the cyclotron radius gets comparable to the width of the Hall bar (~750Å) we obtain Shubnikov-deHaas oscillations in R_{xx} due to the formation of Landau levels. At the same time we see the quantum Hall effect with plateaus in R_{xy}.

Next we look at two values of the magnetic field: B = 5.6T corresponding to a peak in R_{xx}, and B = 10T corresponding to a valley in R_{xx}. The potential distribution $\mu(x,y)$, the current distribution $\mathbf{J}(x,y)$ and the local density of states $N_0(E,y)$ are shown in Fig. 2. At B = 5.6T the density of states at the Fermi energy is evenly spread out across the Hall bar while at B = 10T the density of states is peaked near the edges and nearly zero in-between. Consequently, at B = 10T, the current flows near one edge with no coupling to the other edge and the electrochemical potential drops abruptly in the middle. But, at B = 5.6T, the current flow is spread out across the width and the potential drop occurs near the edges. This agrees with the edge state description of the quantum Hall effect that has received much attention lately[20]. We are not aware of any other direct computations of the electrochemical potential in the quantum Hall regime though it is believed that the electrochemical potential profile plays an important role in the accuracy of the quantization of R_{xy}. We have also calculated the electrostatic potential profile and find it to be in good agreement with earlier results.

The above approach thus provides a tractable approach to incorporating phase-breaking processes into quantum transport in the linear response regime. Devices with up to 1000 nodes can be analyzed in less than an hour on a Sun-4 workstation.

4. Generalization of Eq. (1)

Eq. (1) has two main limitations:

(1) Phase-breaking processes are assumed to be caused by point scatterers. Consequently we cannot introduce phase relaxation without simultaneously introducing momentum relaxation. This is an important limitation because at low temperatures the phase breaking time τ_ϕ and the momentum relaxation time τ_m are generally unequal.

(2) Different energies are assumed to be in equilibrium with each other. A recent derivation from linear response theory[2i] does not make this assumption, but zero temperature and elastic scattering are assumed. We thus cannot use Eq. (1) at high temperatures.

An obvious question to ask is whether Eq. (1) can be generalized to remove these assumptions. Recently we have derived a generalized linear response equation free from these restrictions[22–24]. Here we will just state the results. When we linearize the kinetic equation without making any assumptions regarding energy equilibration we obtain the following equation (assuming point phase-breaking scatterers):

$$I(\mathbf{r},E) = \frac{e}{h}\int d\mathbf{r}' \int dE'\, T(\mathbf{r},E;\mathbf{r}',E') \left[\mu(\mathbf{r},E) - \mu(\mathbf{r}',E')\right] \quad (5)$$

where the 'potential' $\mu(\mathbf{r},E)$ is *defined* by

$$\frac{n(\mathbf{r},E)}{N_0(\mathbf{r},E)} = f(\mathbf{r},E) = \frac{1}{e^{(E-e\mu(\mathbf{r},E))/k_BT}+1} \quad (6)$$

$n(\mathbf{r},E)$ being the electron density per unit energy and $N_0(\mathbf{r},E)$, the local density of states. Note that any function $f(\mathbf{r},E)$ lying between 0 and 1 can be written in the form shown in Eq. (6) so that this involves no loss of generality. If $f(\mathbf{r},E)$ is a Fermi-Dirac function then $\mu(\mathbf{r},E)$ is independent of energy (E) and Eq. (5) reduces to our earlier result, Eq. (1).

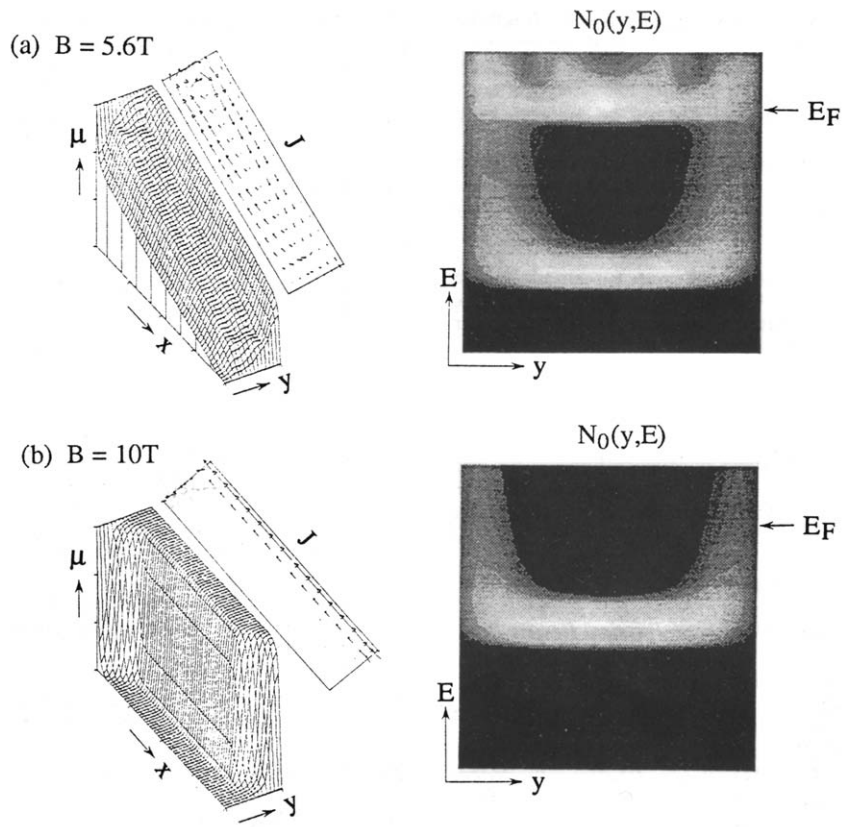

Fig. 2 Electrochemical potential (μ), current density (J) and local density of states (N_0) at (a) B = 5.6T and (b) B = 10T. The density of states $N_0(E,y)$ is plotted using a gray-scale - a lighter shade corresponds to a higher value. The Fermi energy E_F is indicated with an arrow.

An important insight due to Büttiker[25] is the equivalence of floating probes and phase-breaking scatterers. From this perspective, one could view Eq. (1) as the Büttiker formula[26] applied to a structure with a continuous distribution of probes corresponding to a continuous distribution of phase-breaking scatters[27]. Eq. (5) shows that in general one needs a conceptual probe connected at each point **r** to every energy E. We recover Eq. (1) if the probes at different energies E (at the same point **r**) all float to the same potential $\mu(\mathbf{r})$. This could happen if there is a lot of inelastic scattering which effectively 'short' together probes as different energies. However, even if there are no inelastic processes, $\mu(\mathbf{r},E)$ can be nearly independent of energy over the energy range (k_BT) where transport takes place. This is true if $k_BT < \Gamma_C$ where Γ_C is the range of energies over which the transmission characteristics are nearly constant. Low temperature mesoscopic experiments possibly belong to this category so that we can use Eq. (1) rather than Eq. (5). However, as we go to smaller structures, it is likely that more and more interesting quantum effects will arise in the transport regime with $k_BT > \Gamma_C$. In this regime transport will occur largely through coherent and incoherent hopping between localized states with differing energies. To describe transport accurately in this regime it will be necessary to include the energy coordinate explicitly as in Eq. (5).

When we allow for extended scatterers, Eq. (5) is modified to[23,24]

$$I(\rho,E) = \frac{e}{h}\int d\rho \int dE\, T(\rho,E;\rho',E')\left[\mu(\rho,E)-\mu(\rho',E')\right] \quad (7)$$

where ρ represents *a pair of points* ($\mathbf{r}_1,\mathbf{r}_2$). The 'potential' $\mu(\rho,E)$ is defined as in Eq. (6) in terms of the ratio $f(\rho,E)$ of the correlation function $-iG^<(\rho,E)$ to the spectral density $A_0(\rho,E)$. Thus, Büttiker's probe model for phase-breaking scatterers in its original form is accurate if we have both (1) point scatterers and (2) equilibration among energy channels. But with suitable extension the basic physical picture can be aplied more generally with a voltage probe connected to each point ($\mathbf{r}_1,\mathbf{r}_2,E$) in 'phase' space. This is an interesting result that follows rigorously from the quantum kinetic formalism and would be difficult

to foresee on purely phenomenological grounds. It will be noted that it is only for point-scatterers that the transmission from one 'probe' to another is real and can be interpreted as a probability function. With extended scatterers the function is complex and cannot be viewed as a transmission probability.

Finally, we would like to mention that each of these equations (1), (5) and (7) can be shown to obey the reciprocity relation[26] thus proving its general validity all the way from phase-coherent to incoherent transport[22-24].

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