INHOMOGENEOUS PARTICLE DENSITY DISTRIBUTION IN A CURRENT-CARRYING MESOSCOPIC CONDUCTOR

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ABSTRACT

Landauer's residual resistivity dipole picture is studied in a system with multiple coherent scatterings. The particle density distribution within a mesoscopic conductor under nonequilibrium conditions is calculated and shown to have both short and long-range fluctuations which, in a charged system, significantly modify the internal electrical field.

There are two key ingredients in Landauer's theory of quantum transport [1], of which the first, that transport should be viewed as a wave transmission process, has been generally accepted and become a cornerstone of mesoscopic physics. The second part of the Landauer theory recognizes the inhomogeneity of the internal electrical field in a disordered, current-carrying conductor. Landauer's original argument goes as follows. Consider a conductor carrying a constant (and fixed) current. If we move one of the scatterers by a small distance, the conductance and therefore the voltage will change. Contrary to what one might expect from the usual picture of a linearly slant potential (but consistent with one's intuition), the corresponding change in voltage is generally not spread out uniformly across the entire sample, but rather is localized in the neighborhood of the scatterer. The internal electrical field in a current-carrying conductor is therefore highly nonuniform even in a nominally homogeneous conductor and depends sensitively on the scattering configuration. Such an inhomogeneity is important in electromigration [2], nonlinear transport [3,4,5] and ac transport [3], among other things.

The internal field and its effect on carrier dynamics in semiconducting devices are, of course, the bread and butter of solid state electronics. Much less is known about the quantum inhomogeneity in conductors. We have completed a numerical and analytical study of this Landauer inhomogeneity, focusing in particular on the mesoscopic aspects of the problem. This paper summarizes our major conclusions, outlines the numerical approach used, and presents the numerical results.

The quantity of interest here is the electron density; the electrostatic potential can be related to the density using, *e.g.,* Thomas-Fermi approximation. We consider a mesoscopic conductor connected to two reservoirs with well-defined chemical potentials μ_1 and μ_2, with $\delta\mu \equiv \mu_1 - \mu_2 \geq 0$. The existence of such reservoirs is a key assumption in the modern treatment of quantum transport in mesoscopic systems. If $\Delta\mu = 0$, the current is zero, the particle density can in principle be calculated (using, *e.g.*, density functional theory) and is generally nonuniform. Consider now the *change* in particle density when a nonzero $\Delta\mu$ is applied on the system:

$$\delta n(x) = \int_{\mu_2}^{\mu_1} dE \sum_{\alpha} |\Psi_\alpha(x)|^2 \delta(E - E_\alpha), \tag{1}$$

where $\Psi_\alpha(x)$ is the scattering wave function incident from the left (μ_1) side and is given by the Lippmann–Schwinger equation,

$$\Psi_\alpha = \Phi_\alpha + G^+(E_\alpha)V\Phi_\alpha. \tag{2}$$

Here $G^+(E_\alpha) = [E_\alpha - H + i0^+]^{-1}$ is the Green's function, V is the scattering potential, and Φ characterizes the incoming state. Therefore δn is given by

$$\delta n(x) = \int_{\mu_2}^{\mu_1} \frac{dE}{2\pi i} < x|\Delta G(E)|x >, \tag{3}$$

where $\Delta G \equiv G^- - G^+$. For a particular realization of the impurity configuration, Eq. (3) has to be calculated numerically. We use the recursive Green's functions method proposed by Lee and Fisher [6] to evaluate (3) for a 2D tight–binding model,

$$H = V_x \sum_{j,k} a^+_{j+1,k}a_{j,k} + H.c. + V_y \sum_{j,k} a^+_{j,k+1}a_{j,k} + H.c. + \sum_{j,k} E_{j,k}a^+_{j,k}a_{j,k}, \tag{4}$$

where j and k label the sites in the x and y directions and $E_{j,k}$ is a random site energy. If one denotes the Green's function for the last column of a system in which all sites $j > j_o$ are removed by $G^L(j_o) \equiv G^L_{k,k'}(j_o, j_o)$ (and similarly for the first column Green's function $G^R(j_o)$ for a system in which all sites $j < j_o$ are deleted), the Green's function for a particular column $G(j) \equiv G_{k,k'}(j,j)$ can be calculated as an $N_t \times N_t$ dimensional matrix

$$G(j)^{-1} = G^o(j)^{-1} - V_x^2 G^R(j+1) - V_x^2 G^L(j-1), \tag{5}$$

where N_t is the number of lateral sites of the sample and $G^o(j_o)$ is the Green's function for the isolated j'th column. $G^L(j_0)$ satisfies the recursion relation

$$G^L(j_o)^{-1} = G^o(j_o)^{-1} - V_x^2 G^L(j_o - 1); \tag{6}$$

similarly $G^R(j_0)$ satisfies

$$G^R(j_o)^{-1} = G^o(j_o)^{-1} - V_x^2 G^R(j_o + 1). \tag{7}$$

We first compute the Green's function for the semi-infinite perfect lattice (representing the left lead). Using this as the seed, all the left Green's functions can be computed recursively using Eq. (6). Similarly we generate the right Green's functions G^R. The true Green's function is then obtained from Eq. (5). We use hard wall boundary conditions in the direction perpendicular to the overall current. This formalism can be easily generalized to three dimensional systems or to systems with multiple leads.

Fig. 1 shows a typical example of the potential fluctuation in a 50 x 50 system (a) along a line x = const (penpendicular to the current) and as a function of the bias, and (b) along a line y = const and as a function of the bias. Notice that (1) the potential exhibits rapid spatial variations, due to the short mean free path (on the order of a few lattice constants) and the overlapping Friedel oscillations (see below), (2) the equipotential lines are not necessarily normal to the direction of the overall current, and (3) at a given point in the sample, the local voltage does not necessarily increase monotonically with the external voltage.

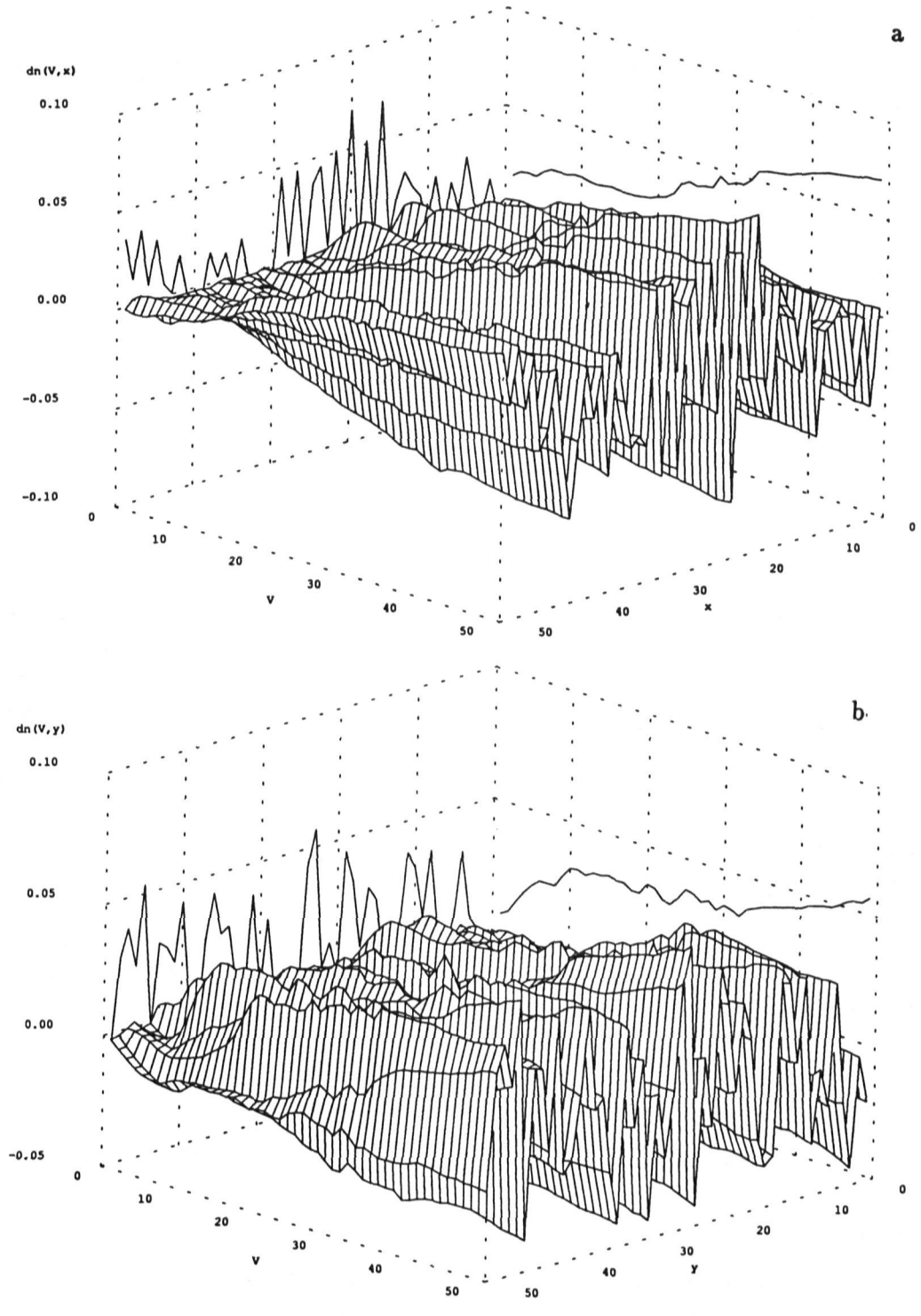

Figure 1: The potential fluctuation dn in a 50×50 system as a function of the external voltage V (in unit of 1/40 the bandwidth) and the position. (a) along a line ($x = 25$) perpendicular to the direction of the average current, and (b) along a line ($y = 20$) parallel to the current.

To gain further insight into the field fluctuations, we calculate diagrammatically the irreducible density–density correlation function in a current carrying system,

$$\begin{aligned} F(x,y;\mu_1,\mu_2) &\equiv < \delta n(x)\delta n(y) > - < \delta n(x) >< \delta n(y) > \\ &= -\int_{\mu_2}^{\mu_1} \frac{dE_1 dE_2}{4\pi^2} [< x|\Delta G(E_1)|x >< y|\Delta G(E_2)|y >]_{\rm av}, \end{aligned} \tag{8}$$

Within the Thomas-Fermi approximation, the local potential fluctuation is given by

$$\begin{aligned} < (\delta\phi)^2 > - < \delta\phi >^2 &= \frac{1}{(eN)^2} F(x,x;\mu_1,\mu_2) \\ &= \begin{cases} \frac{3}{\pi}(k_F\ell)^{-2}V^2, & eV << 1/\tau; \\ 3(k_F\ell)^{-2}(e\tau)^{-1}V, & eV > 1/\tau. \end{cases} \end{aligned} \tag{9}$$

Here N is the density of states at the Fermi level, k_F the Fermi wavevector, ℓ the elastic mean free path, τ the mean free time, and V the voltage applied on the system. The spatial correlation of the potential fluctuations can be similarly calculated. Details of these calculations will be presented elsewhere.

We find that the potential fluctuations consist of two parts. First, there is the Landauer "residual resistivity dipole" [1] term which is modulated by a certain kind of Friedel oscillation [7]; this term has a short correlation length on the order of the elastic mean free path. The second component is a multiple scattering contribution; its correlation decays only algebraically over long distance scales. In the small voltage limit, the *local* rms fluctuations is down from the voltage by a factor of order $(k_F\ell)^{-1}$. This is expected from Landauer's original derivation which shows that the fluctuation is proportional to the scattering cross section of the scatterer. It is also interesting to observe that while $(\delta\phi)^2$ grows like $(\Delta\mu)^2$ for small $\Delta\mu$, for large $\Delta\mu$ it is proportional to $\Delta\mu$: the local potential undergoes a random walk as the overall voltage is increased. Taking into consideration the spatial correlation discussed above, this reveals an extremely complicated potential landscape in a current-carrying, nominally uniform conductor.

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1. R. Landauer, IBM J. Res. Dev. **1**, 223 (1957); Z. Phys. B **21**, 247 (1975); IBM J. Res. Dev. **32**, 306 (1988).
2. R. S. Sorbello and C. S. Chu, IBM J. Res. Dev. **32**, 58 (1988), and references therein.
3. R. Landauer, Z. Phys. B **68**, 217 (1987).
4. H.-S. Tang and Y. Fu, Phys. Rev. Lett. **67**, 485 (1991).
5. P. N. G. de Vegvar, AT&T Bell Laboratories preprint (1992).
6. P. A. Lee and D. S. Fisher, Phys. Rev. Lett. **47**, 882 (1981); A. D. Stone, Phys. Rev. Lett. **54**, 2692 (1985).
7. W. Zwerger, L. Bönig, and K. Schönhammer, Phys. Rev. B **41**, 6434 (1991).