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Steady-state quantum kinetic equation

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Starting from the Dyson equation in the Keldysh formulation, we derive a kinetic equation for steady-state quantum transport under the simplifying assumption that the inelastic scattering is caused by uncorrelated point scatterers, such as impurities with internal degrees of freedom. This assumption allows us to write a transport equation that involves only the electron density and not the spatial correlations of the wave function. Assuming local thermodynamic equilibrium we then simplify the transport equation to a form which resembles the Landauer-Büttiker formula extended to include a continuous distribution of probes.

Since 1985, experiments on mesoscopic structures have revealed a wealth of new quantum effects such as the Aharonov-Bohm effect, conductance fluctuations, nonlocal effects, and the quantized conductance of point contacts. Much of the current theoretical work on mesoscopic structures is based on the Landauer formula as modified by Büttiker for multiprobe structures,[1,2]

$$I_i = \frac{e^2}{h}\sum_j (T_{ij}\mu_j - T_{ji}\mu_i) = \frac{e^2}{h}\sum_j T_{ij}(\mu_j - \mu_i)\,, \quad (1)$$

where we note that $\sum_j (T_{ij} - T_{ji}) = 0$. Equation (1) reduces the problem of computing the conductance of a device to that of computing its scattering matrix. It is usually assumed that there is no phase-breaking scattering process within the device; all such processes occur in the contacts. The scattering matrix for the device can then be computed from the time-independent Schrödinger equation $H_0\Psi = E\Psi$, where

$$H_0 = [(\mathbf{p} - e\mathbf{A})^2/2m^* + eV]\,; \quad (2)$$

$\mathbf{A}(\mathbf{r})$ and $V(\mathbf{r})$ are the vector and scalar potentials. This approach has been quite successful in explaining qualitatively many of the recent experimental observations in mesoscopic systems.[3] However, in order to make quantitative comparisons, it is necessary to include the phase-breaking processes that are inevitably present in any device. Phase-breaking processes are those that involve a change in the state of the scatterer and thus cannot simply be included in the Schrödinger equation by choosing a time-varying scattering potential $V(\mathbf{r},t)$. To include irreversible dissipative processes within the device one has to include the reservoir explicitly and trace over the states of the reservoir. Diagrammatic techniques based on the Kubo formalism do include phase-breaking processes, but these techniques are more suited to computing ensemble-averaged rather than sample-specific properties.[4]

Quantum kinetic equations[5] provide a powerful approach to including dissipative processes in quantum transport theory for both linear and nonlinear response.[6] Here the semiclassical distribution function $f(\mathbf{r},\mathbf{k},t)$ is replaced by the Wigner distribution function $W(\mathbf{r},\mathbf{k},E,t)$, which is obtained from the Green's function $G^<(\mathbf{r}_1,\mathbf{r}_2;t_1,t_2) = i\langle\psi^\dagger(\mathbf{r}_2,t_2)\psi(\mathbf{r}_1,t_1)\rangle/\hbar$ by transforming to center-of-mass and relative coordinates, and then Fourier transforming with respect to the relative coordinate: $\mathbf{r}_1 - \mathbf{r}_2 \to \mathbf{k}$, $t_1 - t_2 \to E$. An equation of motion for the Green's function (and hence the Wigner distribution function) is derived starting from the Dyson equation in the Keldysh formulation:[5]

$$[i\hbar\,\partial/\partial t_1 - H_0(\mathbf{r}_1)]\mathbf{G}(X_1,X_2) = \delta^4(X_1 - X_2)I + \int dX_3\,\Sigma(X_1,X_3)\mathbf{G}(X_3,X_2)\,, \quad (3)$$

where X stands for $(\mathbf{r},t)$ and I is the (2×2) identity matrix. $\mathbf{G}$ is a (2×2) matrix

$$\begin{bmatrix} G^T & -G^< \\ G^> & -G^{\bar{T}} \end{bmatrix}$$

whose elements are defined by

$$G^<(X_1,X_2) = \frac{i}{\hbar}\langle\psi^\dagger(X_2)\psi(X_1)\rangle\,, \quad (4a)$$

$$G^>(X_1,X_2) = -\frac{i}{\hbar}\langle\psi(X_1)\psi^\dagger(X_2)\rangle\,, \quad (4b)$$

$$G^T(X_1,X_2) = \Theta(t_1 - t_2)G^>(X_1,X_2) + \Theta(t_2 - t_1)G^<(X_1,X_2)\,, \quad (5a)$$

$$G^{\bar{T}}(X_1,X_2) = \Theta(t_1 - t_2)G^<(X_1,X_2) + \Theta(t_2 - t_1)G^>(X_1,X_2)\,. \quad (5b)$$

The angular brackets $\langle\cdots\rangle$ denote an average over the available states of the system, that is, a trace over the reservoir states. The self-energy function Σ is also a (2×2) matrix of the same form as $\mathbf{G}$. It is convenient to define two additional functions as follows:

$$G^R(X_1,X_2) = \Theta(t_1 - t_2)[G^>(X_1,X_2) - G^<(X_1,X_2)]\,, \quad (6a)$$

$$G^A(X_1,X_2) = \Theta(t_2 - t_1)[G^<(X_1,X_2) - G^>(X_1,X_2)]\,. \quad (6b)$$

The retarded and the advanced self-energy functions Σ^R and Σ^A are also defined similarly.

In this paper we will derive a simple quantum kinetic equation starting from Eq. (3) that can be used to describe steady-state transport; similar results were derived by us earlier using a heuristic one-electron picture.[7] Usually in quantum transport theory we encounter the independent variables $(\mathbf{r}_1,\mathbf{r}_2;t_1,t_2)$ or equivalently $(\mathbf{r};\mathbf{k};E;t)$, as we just discussed. Because we restrict ourselves to steady-state transport, the time variable $t=(t_1+t_2)/2$ is averaged over. This leaves us with functions of the form $G(\mathbf{r}_1,\mathbf{r}_2;E)$ or $G(\mathbf{r},\mathbf{k};E)$. A further simplification is achieved by assuming a special form for the inelastic scattering. We arrive at a transport equation that only involves the diagonal elements $G(\mathbf{r},\mathbf{r};E)$ of the Green's functions. Spatial correlations of the field represented by the off-diagonal elements $G(\mathbf{r}_1,\mathbf{r}_2;E)$, $\mathbf{r}_1\neq\mathbf{r}_2$ do not appear in this equation. In order to achieve this simplification, we assume that inelastic scattering is caused by a distribution of independent oscillators, each of which interacts with the electrons through a *δ potential*. Multiphonon processes are neglected in evaluating the self-energy function, just as one does in deriving Fermi's "golden rule;" however, the elastic processes are treated exactly. With these assumptions, the self-energy is a δ function in space leading to a simple transport equation. This model closely approximates a laboratory sample with impurities having internal degrees of freedom. For other types of inelastic scattering the model may not be accurate; however, we believe that it should still be possible to describe much of the essential physics of dissipation in quantum transport.

The simplification described above is important for two reasons. First, the number of independent variables is reduced from $(\mathbf{r}_1,\mathbf{r}_2;E)$ [or equivalently, $(\mathbf{r};\mathbf{k};E)$] to $(\mathbf{r};E)$. Second, the diagonal elements have simple physical interpretations; for example, the electron density per unit energy $n(\mathbf{r};E)$ is identified with

$$n(\mathbf{r};E)=-iG^{<}(\mathbf{r},\mathbf{r};E)/2\pi\,, \tag{7a}$$

while the hole density (in the same band) per unit energy $p(\mathbf{r};E)$ is identified with

$$p(\mathbf{r};E)=+iG^{>}(\mathbf{r},\mathbf{r};E)/2\pi\,. \tag{7b}$$

The transport equation can thus be understood in simply physical terms, and involves only positive quantities. This may make numerical solutions less sensitive to grid size.

Our model is closely related to the Landauer picture. Since the inelastic scattering process is purely local, it can be viewed as an exit into a reservoir followed by reinjection into the main structure.[8] From this point of view it would seem that distributed inelastic scattering processes can be simulated by connecting a continuous distribution of reservoirs throughout a structure. Indeed, when we simplify our transport equation assuming *local thermodynamic equilibrium* we obtain what looks like Eq. (1) generalized to include a continuous distribution of probes. A direct generalization of Eq. (1), however, would appear to be a phenomenological approach to simulating inelastic scattering. This paper provides the rigorous justification for such an approach, by deriving the transport equation starting from a model Hamiltonian.

The model. We consider any arbitrary structure in which the propagation of electrons is described by the one-electron effective-mass Hamiltonian, H_0 [Eq. (2)]. The vector and scalar potentials $\mathbf{A}(\mathbf{r})$ and $V(\mathbf{r})$ include the Hartree potential obtained from a self-consistent solution with the Poisson equation, as well as externally imposed potentials, and all sources of *elastic* scattering such as impurities, defects, boundaries, etc. For the inelastic scattering we assume a reservoir of independent oscillators labeled by the index m:

$$H_p=\sum_m \hbar\omega_m(a_m^\dagger a_m+\tfrac{1}{2})\,. \tag{8}$$

We assume that each oscillator interacts with the electrons through a δ potential, so that the interaction Hamiltonian H' can be written as

$$H'=\sum_m U\,\delta(\mathbf{r}-\mathbf{r}_m)(a_m^\dagger+a_m)\,. \tag{9}$$

The strength of inelastic scattering can be adjusted through the density of scatterers per unit volume per unit energy, described by some function $J_0(\mathbf{r};\hbar\omega)$. The summation over m is eventually replaced by an integral.

$$\sum_m \rightarrow \int d\mathbf{r}\int d(\hbar\omega)J_0(\mathbf{r};\hbar\omega)\,. \tag{10}$$

Self-energy function. In calculating the self-energy we restrict ourselves to one-phonon processes as one does in deriving Fermi's "golden rule." For one-phonon processes the self-energy function can be shown to be a δ function, assuming that the reservoir of oscillators is in a state of thermodynamic equilibrium:

$$\Sigma^{>}(\mathbf{r}_1,\mathbf{r}_2;E)=-\frac{i\hbar}{\tau^{>}(\mathbf{r}_1;E)}\delta(\mathbf{r}_1-\mathbf{r}_2)\,, \tag{11a}$$

$$\Sigma^{<}(\mathbf{r}_1,\mathbf{r}_2;E)=\frac{i\hbar}{\tau^{<}(\mathbf{r}_1;E)}\delta(\mathbf{r}_1-\mathbf{r}_2)\,, \tag{11b}$$

where

$$\frac{1}{\tau^{>}(\mathbf{r};E)}=\frac{2\pi}{\hbar}\int dE'\,F(\mathbf{r};E'-E)p(\mathbf{r};E')\,, \tag{12a}$$

$$\frac{1}{\tau^{<}(\mathbf{r};E)}=\frac{2\pi}{\hbar}\int dE'\,F(\mathbf{r};E-E')n(\mathbf{r};E')\,, \tag{12b}$$

$$F(\mathbf{r};\epsilon)=U^2J_0(\mathbf{r};|\epsilon|)\times\begin{cases}N(\epsilon), & \epsilon>0,\\ N(|\epsilon|)+1, & \epsilon<0,\end{cases} \tag{13}$$

$$N(\hbar\omega)=(e^{\hbar\omega/k_BT}-1)^{-1}\,. \tag{14}$$

Physically $1/\tau^{>}(\mathbf{r};E)$ is the rate at which electrons are scattered out of energy E at the point $\mathbf{r}$ assuming that it is initially full. Similarly $1/\tau^{<}(\mathbf{r};E)$ is the rate at which holes are scattered out of energy E at the point $\mathbf{r}$ assuming that it is initially empty. The retarded self-energy function is given by

$$\mathrm{Im}\Sigma^{R}(\mathbf{r}_1,\mathbf{r}_2;E)=\frac{-\hbar}{2\tau^{R}(\mathbf{r}_1;E)}\delta(\mathbf{r}_1-\mathbf{r}_2)\,, \tag{15a}$$

$$\mathrm{Re}\Sigma^{R}(\mathbf{r}_1,\mathbf{r}_2;E)=\sigma^{R}(\mathbf{r}_1;E)\delta(\mathbf{r}_1-\mathbf{r}_2)\,, \tag{15b}$$

where

$$\frac{1}{\tau^{R}(\mathbf{r};E)}=\frac{1}{\tau^{>}(\mathbf{r};E)}+\frac{1}{\tau^{<}(\mathbf{r};E)}\,, \tag{16}$$

and

$$\sigma^{R}(\mathbf{r};E)=\frac{\hbar}{2\pi}\mathrm{P}\int\frac{dE'}{(E-E')\tau^{R}(\mathbf{r};E')}\,. \tag{17}$$

P represents the principal value of the integral.

Transport equation. To derive the transport equation we start from Eq. (3) and consider only the component involving $G^<$ on the left, which can be rewritten as

$$\left[i\hbar\frac{\partial}{\partial t_1}-H_0(\mathbf{r}_1)\right]G^<(X_1,X_2)-\int dX_3\Sigma^R(X_1,X_3)G^<(X_3,X_2)=\int dX_3\Sigma^<(X_1,X_3)G^A(X_3,X_2)\,. \tag{18}$$

Fourier transforming with respect to t_1-t_2 and using Eqs. (15a), (15b), and (11b),

$$\left[E-H_0(\mathbf{r}_1)-\sigma^R(\mathbf{r}_1;E)+\frac{i\hbar}{2\tau^R(\mathbf{r}_1;E)}\right]G^<(\mathbf{r}_1,\mathbf{r}_2;E)=i\hbar\frac{G^A(\mathbf{r}_1,\mathbf{r}_2;E)}{\tau^<(\mathbf{r}_1;E)}\,. \tag{19}$$

It can also be shown from Eq. (3) that

$$\left[E-H_0(\mathbf{r}_1)-\sigma^R(\mathbf{r}_1;E)+\frac{i\hbar}{2\tau^R(\mathbf{r}_1;E)}\right]G^R(\mathbf{r}_1,\mathbf{r}_2;E)=\delta^3(\mathbf{r}_1-\mathbf{r}_2)\,. \tag{20}$$

Using Eq. (20) we can write the solution to Eq. (19) as

$$G^<(\mathbf{r}_1,\mathbf{r}_2;E)=i\hbar\int d\mathbf{r}_3\frac{G^R(\mathbf{r}_1,\mathbf{r}_3;E)G^A(\mathbf{r}_3,\mathbf{r}_2;E)}{\tau^<(\mathbf{r}_3;E)}\,. \tag{21}$$

We now set $\mathbf{r}_1=\mathbf{r}_2\equiv\mathbf{r}$; using Eq. (7a) and noting that $G^A(\mathbf{r}_1,\mathbf{r}_2;E)=[G^R(\mathbf{r}_2,\mathbf{r}_1;E)]^*$,

$$n(\mathbf{r};E)=\frac{\hbar}{2\pi}\int d\mathbf{r}'\frac{|G^R(\mathbf{r},\mathbf{r}';E)|^2}{\tau^<(\mathbf{r}';E)}\,. \tag{22}$$

By considering the component of the matrix equation, Eq. (3), corresponding to $G^>$ instead of $G^<$, we obtain

$$p(\mathbf{r};E)=\frac{\hbar}{2\pi}\int d\mathbf{r}'\frac{|G^R(\mathbf{r},\mathbf{r}';E)|^2}{\tau^>(\mathbf{r}';E)}\,. \tag{23}$$

Adding Eqs. (22) and (23) and using Eq. (16), we obtain an important relationship.

$$N_0(\mathbf{r};E)=\frac{\hbar}{2\pi}\int d\mathbf{r}'\frac{|G^R(\mathbf{r},\mathbf{r}';E)|^2}{\tau^R(\mathbf{r}';E)}\,, \tag{24}$$

where $N_0(\mathbf{r};E)=n(\mathbf{r};E)+p(\mathbf{r};E)$ is the electronic density of states. Equation (24) represents an identity that can also be derived directly from Eq. (20).

External current. So far we have not considered any external sources. We will now modify Eqs. (22) and (23), somewhat heuristically to include the external current which is assumed to be injected or extracted incoherently. First, we note that since the self-energy is a δ function [Eqs. (11a) and (11b)], the rate at which electrons are inelastically scattered out is given by $n(\mathbf{r};E)/\tau^>(\mathbf{r};E)$, while the rate at which holes are inelastically scattered out is given by $p(\mathbf{r};E)/\tau^<(r;E)$. Equations (22) and (23) can be rewritten in terms of the inelastic scattering rates as

$$\frac{en(\mathbf{r};E)}{\tau^>(\mathbf{r};E)}=I_n(\mathbf{r};E)+\frac{e\hbar}{2\pi}\int d\mathbf{r}'\frac{|G^R(\mathbf{r},\mathbf{r}';E)|^2}{\tau^<(\mathbf{r}';E)\tau^>(\mathbf{r};E)}\,, \tag{25a}$$

$$\frac{ep(\mathbf{r};E)}{\tau^<(\mathbf{r};E)}=I_p(\mathbf{r};E)+\frac{e\hbar}{2\pi}\int d\mathbf{r}'\frac{|G^R(\mathbf{r},\mathbf{r}';E)|^2}{\tau^<(\mathbf{r};E)\tau^>(\mathbf{r}';E)}\,. \tag{25b}$$

We have added the terms $I_n(\mathbf{r};E)$ and $I_p(\mathbf{r};E)$ to account for the external source; these are related to the externally injected current per unit volume per unit energy $I(\mathbf{r};E)$ by $I(\mathbf{r};E)=I_p(\mathbf{r};E)-I_n(\mathbf{r};E)$. To determine I_n and I_p individually we multiply Eq. (25a) by $\tau^>(\mathbf{r};E)$ and Eq. (25b) by $\tau^<(r;E)$, add them, and compare with Eq. (24). This yields

$$en(\mathbf{r};E)=-I(\mathbf{r};E)\tau^R(\mathbf{r};E)+\frac{e\hbar}{2\pi}\int d\mathbf{r}'\frac{|G^R(\mathbf{r},\mathbf{r}';E)|^2}{\tau^<(\mathbf{r}';E)}\,, \tag{26a}$$

$$ep(\mathbf{r};E)=I(\mathbf{r};E)\tau^R(\mathbf{r};E)+\frac{e\hbar}{2\pi}\int d\mathbf{r}'\frac{|G^R(\mathbf{r},\mathbf{r}';E)|^2}{\tau^>(\mathbf{r}';E)}\,. \tag{26b}$$

Substituting for $\tau^<(\mathbf{r}';E)$ from Eq. (12b) and $\tau^>(\mathbf{r}';E)$ from Eq. (12a), we obtain the desired transport equation.

$$n(\mathbf{r};E)=-I(\mathbf{r};E)\tau^R(\mathbf{r};E)/e+\int d\mathbf{r}'\int dE'K_n(\mathbf{r},\mathbf{r}',E,E')n(\mathbf{r}';E')\,, \tag{27a}$$

$$p(\mathbf{r};E)=I(\mathbf{r};E)\tau^R(\mathbf{r};E)/e+\int d\mathbf{r}'\int dE'K_p(\mathbf{r},\mathbf{r}';E,E')p(\mathbf{r}';E')\,, \tag{27b}$$

where the kernels are given by

$$K_n(\mathbf{r},\mathbf{r}';E,E')=|G^R(\mathbf{r},\mathbf{r}';E)|^2F(\mathbf{r}';E-E')\,, \tag{28a}$$

$$K_p(\mathbf{r},\mathbf{r}';E,E')=|G^R(\mathbf{r},\mathbf{r}';E)|^2F(\mathbf{r}';E'-E)\,. \tag{28b}$$

Either Eq. (27a) or (27b) may be solved to obtain the carrier density per unit energy.

Local thermodynamic equilibrium. We will now simplify the transport equation, assuming that the distribution of electrons at any point can be characterized by a local electrochemical potential:

$$n(\mathbf{r};E)=N_0(\mathbf{r};E)f(\mathbf{r};E)=\frac{N_0(\mathbf{r};E)}{\exp\{[E-e\mu(\mathbf{r})]/k_BT\}+1}\,, \tag{29}$$

where $\mu(\mathbf{r})$ is the local electrochemical potential. With this assumption, it can be shown that

$$\frac{n(\mathbf{r};E)}{\tau^>(\mathbf{r};E)}=\frac{p(\mathbf{r};E)}{\tau^<(\mathbf{r};E)}\,, \tag{30}$$

$$\tau^R(\mathbf{r};E)=\tau^<(\mathbf{r};E)f(\mathbf{r};E)=\tau^>(\mathbf{r};E)[1-f(\mathbf{r};E)]\,. \tag{31}$$

Note that Eqs. (30) and (31) are only valid under conditions of local thermodynamic equilibrium. As Eq. (30) shows, the rate at which electrons are scattered out inelastically at any point is then exactly balanced by the rate at which holes are scattered out. This local balance is not expected to hold, in general, when the system is driven far from equilibrium.

Subtracting Eq. (25b) from Eq. (25a), using Eqs. (30) and (31), and noting that $I = I_p - I_n$, we obtain

$$I(\mathbf{r};E) = \frac{e}{h}\int d\mathbf{r}'\,T(\mathbf{r},\mathbf{r}';E)[f(\mathbf{r}';E) - f(\mathbf{r};E)]\,, \qquad (32)$$

where

$$T(\mathbf{r},\mathbf{r}';E) = \frac{\hbar^2 |G^R(\mathbf{r},\mathbf{r}';E)|^2}{\tau^R(\mathbf{r};E)\,\tau^R(\mathbf{r}';E)}\,. \qquad (33)$$

It is evident that if $\mu(\mathbf{r})$ is equal to a constant μ_0 everywhere, the corresponding distribution function satisfies Eq. (32) with the external current $I(\mathbf{r};E)$ set equal to zero. We now expand $f(\mathbf{r};E)$ in a Taylor series about $\mu = \mu_0$ and integrate over E to obtain

$$I(\mathbf{r}) = \frac{e^2}{h}\int d\mathbf{r}'\,T_0(\mathbf{r},\mathbf{r}')[\mu(\mathbf{r}') - \mu(\mathbf{r})]\,, \qquad (34)$$

where

$$T_0(\mathbf{r},\mathbf{r}') = \int dE\left(-\frac{\partial f_0}{\partial E}\right) T(\mathbf{r},\mathbf{r}';E)\,. \qquad (35)$$

$I(\mathbf{r})$ is the total external current integrated over all energies. Equation (34) looks like Eq. (1) generalized to a continuous distribution of probes. This is not surprising since the inelastic scatterers in our model act like independent reservoirs in the Landauer model. It can be shown that the coefficients $T_0(\mathbf{r},\mathbf{r}')$ have the same properties as the coefficients T_{ij},[1] namely, $T_0(\mathbf{r},\mathbf{r}')\,|_H = T_0(\mathbf{r}',\mathbf{r})\,|_{-H}$ and $\int d\mathbf{r}'\,[T_0(\mathbf{r}',\mathbf{r}) - T_0(\mathbf{r},\mathbf{r}')] = 0$.

To summarize, we have presented a simple steady-state quantum transport equation that involves only the electron density per unit energy $n(\mathbf{r};E)$ and not the spatial correlations of the wave function. Under conditions of local thermodynamic equilibrium, the electron density $n(\mathbf{r};E)$ can be written in terms of a local chemical potential $\mu(\mathbf{r})$ and the transport equation reduces to a form that resembles Eq. (1) for a structure having a continuous distribution of probes. We believe that the simplicity of this transport equation will make it feasible to obtain numerical solutions for specific microstructures self-consistently with the Poisson equation, and thereby quantitatively answer some of the fundamental questions of quantum transport.[2] Also, by comparing the predictions of our model with experiment, it should be possible to identify new phenomena arising from correlations between inelastic scatterers.

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