Interacting One-Dimensional Electrons
Driven by Two-Dimensional Reservoir Electrons

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Abstract

We derive an effective 1D theory from the Hamiltonian of the 3D system which consists of a mesoscopic conductor and reservoirs. We assume that the many-body interaction have the same magnitude in the conductor as that in the reservoirs, in contrast to the previous theories which made the ad hoc assumption that the many-body interaction were absent in the reservoirs. We show the following: (i) The effective potentials of impurities and two-body interaction for the 1D modes become weaker as $x$ goes away from the conductor. (ii) On the other hand, the interaction between the 1D and the reservoir modes is important in the reservoir regions, where the reservoir modes excite and attenuate the 1D modes through the interaction. (iii) As a result, the current $\hat{I}_1$ of the 1D modes is not conserved, whereas the total current $\hat{I}$ is of course conserved. (iv) For any steady state the total current $\langle I \rangle$, its equilibrium fluctuation $\langle \delta I^2 \rangle^{eq}$ at low frequency, and non-equilibrium fluctuation $\langle \delta I^2 \rangle^{noneq}$ at low frequency, of the original system are independent of $x$, whereas $\langle \delta I^2 \rangle^{eq}$ and $\langle \delta I^2 \rangle^{noneq}$ at higher frequencies may depend on $x$. (v) Utilizing this property, we can evaluate $\langle I \rangle$, $\langle \delta I^2 \rangle^{eq}$, and $\langle \delta I^2 \rangle^{noneq}$ at low frequency from those of the 1D current $\hat{I}_1$. (vi) In general, the transmittance $T$ in the Landauer formula should be evaluated from a single-body Hamiltonian which includes a Hartree potential created by the density deformation which is caused by the external bias.

Key words: mesoscopic system, one-dimensional system, reservoir
1. Identification of the single-body part of the 3D Hamiltonian

We consider a system which consists of a mesoscopic conductor and reservoirs (Fig. 1), in which electrons are interacting each other according to the three-dimensional (3D) Hamiltonian (in the Heisenberg picture),

\[ \hat{H} = \hat{H}_0^0 + \hat{V}_0 \]

\[ = \int d^3r \hat{H}_0^0(r, t) + \frac{1}{2} \int d^3r \int d^3r' \hat{V}_0(r, r', t), \]  

\[ \hat{H}_0^0(r, t) = \hat{\psi}^\dagger(r, t) \left[ -\frac{\hbar^2}{2m} \nabla^2 + u_c(r) + u_i(r) + e\phi_{ext}(r) \right] \hat{\psi}(r, t), \]  

\[ \hat{V}_0(r, r', t) = \hat{\rho}(r, t)v(r - r')\hat{\rho}(r', t), \]  

where \( \hat{\psi}(r, t) \) is the 3D electron field, \( u_c \) the confining potential, \( u_i \) the potential of impurities and/or defects, \( \phi_{ext} \) the external electrostatic potential, and \( v(r - r') \equiv e^2/|r - r'| \) denotes the Coulomb potential between the local charge density \( \hat{\rho}(r, t) \equiv \hat{\psi}^\dagger(r, t)\hat{\psi}(r, t) - \rho_{BG}(r) \). Here, \( e\hat{\psi}^\dagger(r, t)\hat{\psi}(r, t) \) is the charge density of the electrons and \(-e\rho_{BG}\) is that of the background charges which are assumed to be fixed. Note that we cannot simply add to \( \hat{H} \) the position-dependent “chemical potential term” like \(-\int d^3r \mu(r)\hat{\psi}^\dagger(r, t)\hat{\psi}(r, t)\), because it does not commute with \( \hat{H} \).

We are interested in a steady state, which may be either equilibrium or non-equilibrium. Its density operator is denoted by \( \hat{\xi} \), which is to be determined self-consistently. The average charge density of this state is \( \text{Tr} \left[ \hat{\xi} e\hat{\rho}(r, t) \right] \equiv e\rho_{av}(r) \), which is a function of the bias voltage. Although \( \rho_{av}(r) \) vanishes at \( r \to \infty \), it is finite and \( r \) dependent in finite regions of space, because mesoscopic systems (conductor plus reservoirs) are spatially inhomogeneous. The finite \( \rho_{av} \) induces a long-range effect, which does not vanish by the screening, through the Coulomb interaction. To construct a meaningful 1D theory, in which the interaction of a “1D field” (Eq. (17)) with a “reservoir field” (Eq. (16)) is not strong, we must remove the long-range effect from the interaction Hamiltonian. This can be accomplished by rewriting Eqs. (1)-(4) as

\[ \hat{H} = \hat{H}_0^0 + \hat{V} + V_{av} \]

\[ = \int d^3r \hat{H}_0^0(r, t) + \frac{1}{2} \int d^3r \int d^3r' \left[ \hat{V}(r, r', t) + V_{av}(r, r') \right], \]

\[ \hat{H}_0^0(r, t) = \hat{\psi}^\dagger(r, t) \left[ -\frac{\hbar^2}{2m} \nabla^2 + u_c(r) + u_i(r) + e\phi_{av}(r) \right] \hat{\psi}(r, t), \]

\[ \hat{V}(r, r', t) = \delta\hat{\rho}(r, t)v(r - r')\delta\hat{\rho}(r', t), \]

\[ V_{av}(r, r') = -\rho_{av}(r)v(r - r')\rho_{av}(r'). \]

Here, \( \delta\hat{\rho}(r, t) \equiv \hat{\rho}(r, t) - \rho_{av}(r) \) denotes the charge fluctuation around \( \rho_{av} \), and \( \phi_{av}(r) \) is the average electrostatic potential;

\[ e\phi_{av}(r) \equiv \int d^3r' v(r - r')\rho_{av}(r') + e\phi_{ext}(r). \]

The advantage of rewriting \( \hat{H} \) in the form of Eqs. (5)-(10) is that effects of \( \hat{V} \) is much weaker than those of the original interaction \( \hat{V}_0 \). In particular, \( \hat{V} \) does not cause the long-range effect because it is already included in \( \hat{H}_0^0 \). It is therefore much better to start with
these equations, taking $\hat{H}^0$ (rather than $\hat{H}_0$) as the single-body part. For example, we can derive the Landauer formula by neglecting $\hat{V}$ in Eq. (4):

$$G = (2e^2/h)T[\phi_{av}].$$

(11)

Here, the transmittance $T[\phi_{av}]$ is calculated from $\hat{H}^0$, Eq. (4), which includes the self-consistent potential $\phi_{av}$. On the other hand, if we neglected $V_0$ in Eq. (1), we would obtain $G = (2e^2/h)T[\phi_{av} = 0]$. This is different from Eq. (11) when the bias voltage is finite. Since actual measurements on mesoscopic conductors and on the quantum Hall effect are often performed under a non-negligible bias, one should use Eq. (11) for these experiments.

2. Decomposition of the electron field

Using the above form of the Hamiltonian, we now decompose the electron field into two parts. We are interested in the case where the variation of $W(x)$ of Fig.1 is slow, i.e., $W(x) \simeq W(x + \lambda_F)$, where $\lambda_F$ is a length of the order of the Fermi wavelength. Otherwise, undesirable reflections would occur at the boundary regions between the conductor and reservoirs, and experimental results for such samples would not be very interesting. We do not want reflections either in the conductor except for reflections by impurities and/or defects. If the bias voltage is not too high, these conditions can be stated as the assumption that the $x$ dependence of $u^\epsilon(r) + e\phi_{av}(r) \equiv u(r)$ is weak, i.e., $u(x, y, z) \simeq u(x + \lambda_F, y, z)$.

We assume that only the lowest subband (see Eq. (14) below) is occupied by electrons.

Under these assumptions we can find approximate solutions of the single-body Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + u(r)\right] \varphi(r) = \varepsilon \varphi(r),$$

(12)

for $\varepsilon$ not far from the Fermi energy, in the following form:

$$\varphi_k(r) \simeq \frac{1}{\sqrt{\mathcal{L}}} \exp \left[i \int_0^x K_k(x)dx \right] \varphi^\perp(y, z; x),$$

(13)

where $\mathcal{L}$ is the normalization length in the $x$ direction, and $\varphi^\perp(y, z; x)$ is the normalized eigenfunction belonging to the lowest eigenvalue $u^\perp(x)$ of the following eigenvalue equation (in which $x$ is regarded as a parameter):

$$\left[-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + u(r)\right] \varphi^\perp(y, z; x) = u^\perp(x) \varphi^\perp(y, z; x).$$

(14)

The $x$-dependent wavenumber $K_k(x)$ is defined by $\varepsilon_k = h^2 K_k(x)^2/2m + u^\perp(x)$, where $\varepsilon_k$ denotes the eigenenergy of the state $\varphi_k(r)$. The $\varepsilon_k$ can be expressed as $\varepsilon_k = h^2 k^2/2m + \varepsilon^\perp$, where $k \equiv K_k(0)$ and $\varepsilon^\perp \equiv u^\perp(0)$ are the wavenumber and the lowest subband energy, respectively, at the center of the conductor. We call $\varphi_k$’s “conductor modes”. There are other solutions to Eq. (14), which are denoted by $\varphi_\nu$. They include states whose $\varepsilon$ is far from the Fermi energy, states belonging to higher subbands, and states which decay exponentially in the conductor. We call these solutions “reservoir modes.” The $r$ dependence of the electron field $\hat{\psi}(r, t)$ can be expanded in terms of $\varphi_k$’s and $\varphi_\nu$’s. We can thus decompose the electron field into two parts as $\hat{\psi}(r, t) = \psi_C(r, t) + \psi_R(r, t)$, where
\[ \hat{\psi}_C(\mathbf{r}, t) \equiv \sum_k \varphi_k(\mathbf{r}) \int d^3r' \varphi_k^*(\mathbf{r}') \hat{\psi}(\mathbf{r}', t) \equiv \sum_k \varphi_k(\mathbf{r}) \hat{c}_k(t), \]  
\[ \hat{\psi}_R(\mathbf{r}, t) \equiv \sum_\nu \varphi_\nu(\mathbf{r}) \int d^3r' \varphi_\nu^*(\mathbf{r}') \hat{\psi}(\mathbf{r}', t) \equiv \sum_\nu \varphi_\nu(\mathbf{r}) \hat{d}_\nu(t). \]  

We call \( \hat{\psi}_R \) the “reservoir field.”

We now construct a 1D field \( \hat{\psi}_1(x, t) \) from the 3D field \( \hat{\psi}_C(\mathbf{r}, t) \) as

\[ \hat{\psi}_1(x, t) \equiv \int \int dydz \varphi^+(y, z; x) \hat{\psi}_C(\mathbf{r}, t) \simeq \sum_k \frac{1}{\sqrt{E}} \exp \left[ i \int_0^L K_k(x) dx \right] \hat{c}_k(t). \]

This 1D field has the same contents as \( \hat{\psi}_C \), because the inverse transformation can be accomplished as \( \hat{\psi}_C(\mathbf{r}, t) = \varphi^+(y, z; x) \hat{\psi}_1(x, t) \). In terms of \( \hat{\psi}_1 \) and \( \hat{\psi}_R \), the Hamiltonian can be recast as

\[ \hat{H} = \hat{H}_0^C + \hat{V}_C + \hat{V}_{CR} + \hat{H}_0^R + \hat{V}_R + \hat{V}_{av} \]  

Here, \( \hat{H}_0^C (\hat{H}_0^R) \) denotes the single-body part of the 1D (reservoir) field, \( \hat{V}_C (\hat{V}_R) \) is its mutual interaction, and \( \hat{V}_{CR} \) denotes the interaction between the 1D and reservoir fields. In particular, \( \hat{H}_0^C = \int dx \hat{H}_0^C(x, t) \) and \( \hat{V}_C = \frac{1}{2} \int dx \int dx' \hat{V}_C(x, x', t) \), where,

\[ \hat{H}_0^C(x, t) \simeq \hat{\psi}_1^\dagger(x, t) \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + u_1^+(x) + u_1^1(x) \right] \hat{\psi}_1(x, t), \]

\[ \hat{V}_C(x, x', t) = \delta \hat{\rho}_1(x, t)v_1(x, x')\delta \hat{\rho}_1(x', t). \]

Here, \( \delta \hat{\rho}_1(x, t) \equiv \hat{\psi}_1^\dagger(x, t)\hat{\psi}_1(x, t) - \langle \hat{\psi}_1^\dagger(x, t)\hat{\psi}_1(x, t) \rangle \) is the density fluctuation of the 1D field, and

\[ u_1^1(x) \equiv \int \int dydz |\varphi^+(y, z; x)|^2 u^i(\mathbf{r}), \]

\[ v_1(x, x') \equiv \int \int dydz \int \int dy'dz'|\varphi^+(y, z; x)|^2 v(\mathbf{r} - \mathbf{r}') |\varphi^+(y', z'; x')|^2. \]

The 3D impurity potential \( u^i(\mathbf{r}) \) is spatially averaged, with the weight \( |\varphi^+|^2 \), to give the effective 1D impurity potential \( u_1^1(x) \). In the conductor region, \( u_1^1(x) \) has the same order of magnitude as \( u^i(\mathbf{r}) \). In the reservoir regions, on the other hand, \( u_1^1(x) \) becomes smaller because \( \varphi^+ \) extends over the width \( W(x) \) in the \( y \) direction, and \( u_1^1(x) \) is the averaged value of the random variable \( u^i(\mathbf{r}) \) over this wide area. As \( x \to \pm \infty \), in particular, \( u_1^1(x) \to 0 \) if \( W(x) \to \infty \).

We can say the same for the two-body interaction potential \( v_1(x, x') \). In the conductor region, the major effect of the integrals over \( y, z, y', z' \) of Eq. (22) is simply to smear out the singularity of \( v(\mathbf{r} - \mathbf{r}') \) at \( \mathbf{r} = \mathbf{r}' \) by averaging over the conductor width. In the reservoir regions, on the other hand, the interaction becomes extremely weak as we show now. When \( x \) or \( x' \) is in a reservoir region(s), \( v_1(x, x') \) is screened by the reservoir modes through \( \hat{V}_{CR} \). It is therefore better to rewrite \( \hat{V}_C + \hat{V}_{CR} \) in Eq. (18) as \( \hat{V}_{C}^{sc} + \hat{V}_{CR}^{sc} \), where \( \hat{V}_{C}^{sc} \) is the screened, short-range interaction and \( \hat{V}_{CR}^{sc} \equiv \hat{V}_{CR} + \hat{V}_C - \hat{V}_{C}^{sc} \). For large \( |x - x'| \) it is clear that \( \hat{V}_{C}^{sc} \) becomes vanishingly weak as \( |x - x'| \) is increased. For \( x \sim x' \), on the other hand, the weakness of \( \hat{V}_{C}^{sc} \) is never trivial because the screening is ineffective at a short distance. To
investigate this case, we consider the behavior of the original, long-range potential \( v_1(x, x') \). It is easy to show that \( v_1(x, x') \propto 1/W(x) \) as \( x \sim x' \to \pm \infty \). Hence \( v_1 \to 0 \) if \( W(x) \to \infty \). Since the interaction potential of \( V_C^{sc} \) decays more quickly than \( v_1 \), it also approaches zero, more quickly, as \( x \sim x' \to \pm \infty \).

We have thus shown that the potentials of both the impurities and two-body interaction for the 1D field vanish as \( x \) and/or \( x' \) go away from the conductor. (It should be stressed that \( W(x) \to \infty \) is necessary for this property; otherwise, the impurity potential and the short range part of the interaction would remain finite in all regions.) This may partly justify the 1D models [2] in which a 1D field is assumed to become free as \( x, x' \to \pm \infty \). However, note that \( V_C^{SR} \) will cause additional effects on the 1D field: the reserver modes excite, attenuate, and renormalize the 1D field [1].

3. Calculation of the total current from the 1D current

We now turn to observables. What is measured in most experiments is the current \( \hat{I} \) which is given by \( \hat{I}(x, t) \equiv \int \int dy dz \hat{J}_x(r, t) \), where \( \hat{J}_x \) denotes the x component of the current density. From the continuity equation for \( \hat{J} \) and \( \hat{\rho} \), we have

\[
\frac{\partial}{\partial x} \hat{I}(x, t) + \frac{\partial}{\partial t} \hat{\Lambda}(x, t) = 0,
\]

where \( \hat{\Lambda} \) is the 1D density of electrical charge; \( \hat{\Lambda}(x, t) \equiv \int \int dz e\hat{\rho}(r, t) \). For a steady state, either equilibrium or non-equilibrium, Eq. (23) yields

\[
\frac{\partial}{\partial x} \langle \hat{I}(x, t) \rangle = -\frac{\partial}{\partial t} \langle \hat{\Lambda}(x, t) \rangle = 0.
\]

That is, the average current \( \langle \hat{I}(x, t) \rangle \) is independent of \( x \).

Note, however, that this is not the case for the current fluctuations. For example, consider the symmetrized correlation function of \( \delta \hat{I}(x, t) \equiv \hat{I}(x, t) - \langle \hat{I}(x, t) \rangle \),

\[
C_{II}(x, t - t') \equiv \langle \delta \hat{I}(x, t) \delta \hat{I}(x, t') + \delta \hat{I}(x, t') \delta \hat{I}(x, t) \rangle/2,
\]

which may be taken as a definition of the current fluctuation. Equation (23) and the time-translational invariance yield

\[
\frac{\partial}{\partial x} C_{II}(x, t) = \frac{\partial}{\partial t} \left[ C_{IA}(x, t) + C_{AI}(x, -t) - C_{IA}(x, -t) - C_{AI}(x, t) \right],
\]

where we have introduced the (non-symmetrized) density-current correlation, \( C_{IA}(x, t - t') \equiv \langle \delta \hat{I}(x, t) \hat{\Lambda}(x, t') \rangle \) and \( C_{AI}(x, t - t') \equiv \langle \hat{\Lambda}(x, t) \delta \hat{I}(x, t') \rangle \). It is seen that the current fluctuation generally depends on the position \( x \).

However, we can show that the low-frequency component of its spectral intensity, \( \langle \delta I^2 \rangle_\omega \equiv \int e^{i\omega t} C_{II}(x, t) dt \), is independent of \( x \). To show this, we note that any real systems which possess the thermodynamic stability must have the “mixing property”; namely, any correlation functions decay as \( |t - t'| \to \infty \). This property might be lost if one took an oversimplified model, such as integrable models, for \( \tilde{H} \). However, our \( \tilde{H} \) contains both the conductor and reservoir modes as well as their interactions. It is quite reasonable to assume that such a complicated 3D model has the mixing property. Therefore, \( C_{II}(t) \) vanishes as \( t \) exceeds a “correlation time” \( \tau_c \). Then, for \( \omega \ll 1/\tau_C \) we find from Eq. (23)

\[
\frac{\partial}{\partial x} \langle \delta I^2 \rangle_\omega \simeq \frac{\partial}{\partial x} \langle \delta I^2 \rangle_{\omega=0} = 2 \left[ C_{IA}(x, \infty) + C_{AI}(x, -\infty) - C_{IA}(x, -\infty) - C_{AI}(x, \infty) \right].
\]
The right-hand side vanishes because of the mixing property. We have thus obtained the theorem: For a steady state, the average current is independent of $x$, and the low-frequency ($\omega \ll 1/\tau_c$) component of the spectral intensity of current fluctuation is also independent of $x$, whereas higher-frequency components may depend on $x$. This theorem is quite general: It applies to any steady states, either equilibrium or nonequilibrium, of real systems and of any theoretical models which are realistic enough so that they have the mixing property.

The theorem is very useful for our effective 1D theory. Let us define the current of the 1D field by

$$I_1(x,t) \equiv \frac{e}{2m} \left[ \hat{\psi}_1^*(x,t) \left\{ \frac{\hbar}{i} \frac{\partial}{\partial x} \hat{\psi}_1(x,t) \right\} + \text{h.c.} \right].$$  (27)

Note that this 1D current is not conserved because of the interaction $\hat{V}_{CR}$, which transforms the 1D current into the reservoir current and vice versa. At first sight, this might seem to cause difficulties. Fortunately, however, the above theorem guarantees that we can evaluate $\langle I \rangle$ and $\langle \delta I^2 \rangle_{\omega \ll 0}$ at arbitrary $x$. If we take $x = 0$ (the center of the conductor), $\hat{I}(x,t) \simeq I_1(x,t)$ because the reservoir field does not contribute there. Therefore, we can evaluate $\langle I \rangle$ and $\langle \delta I^2 \rangle_{\omega \ll 0}$ by evaluating $\langle I_1 \rangle$ and $\langle \delta I_1^2 \rangle_{\omega \ll 0}$ at $x = 0$. This may partly justify the Landauer-like approach [3], in which one evaluates the DC conductance and nonequilibrium current fluctuation by evaluating $\langle I_1 \rangle$ and $\langle \delta I_1^2 \rangle_{\omega \ll 0}$ using an effective 1D model.

We have thus shown that it is sufficient to evaluate the 1D current $\hat{I}_1$. Therefore, we can project out the reservoir degrees of freedom, which should behave as the usual two- or three-dimensional electrons because the reservoirs are large, in the standard manner [4]. By doing so, we can derive either the generalized Langevin equation [4] for $\hat{I}_1$, or the Liouville equation for the reduced density operator [4], $\hat{\zeta}_C \equiv \text{Tr}_R[\hat{\zeta}]$, where the trace is taken over the Hilbert space of the reservoir field. The original 3D model of the conductor plus reservoirs has thus been reduced to the 1D model. Detailed discussions and applications to various problems will be described elsewhere [1].

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References

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Figure caption

Fig.1 The mesoscopic conductor and reservoirs.
Fig. 1 A. Shimizu and T. Miyadera