A local approach for global partial density of states

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To apply the scattering approach for the problem of AC transport through coherent quantum conductors, various partial density of states must be evaluated. If the global partial density of states (GPDOS) is calculated externally using the energy derivatives of the scattering matrix, the results are not precise unless the conductor has a large scattering volume. We propose a local formula for GPDOS which is suitable for any finite scattering volume. We apply this formula to compute the emittance of a two-dimensional quantum wire under the multi-mode and finite temperature condition.

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The dynamic conductance of a quantum coherent mesoscopic system under a time dependent external field is the subject of recent interests [1, 2, 3, 4, 5, 6]. In contrast to dc-transport in the linear regime, where the internal potential distribution inside a sample does not appear explicitly, the AC-response depends sensitively on the internal potential distribution. This internal potential is due to the charge distribution generated by the applied external AC-field at the leads and it has to be determined self-consistently [1]. A particular useful approach to investigate AC transport properties of coherent quantum conductors, is to study the AC-response of the system to an external perturbation which prescribes the potentials in the reservoirs only [1, 1]. The external potentials effectively determine the chemical potential of the reservoirs and the potential distribution in the conductor must be considered a part of the response which is to be calculated self-consistently. In this approach, Büttiker and his coworkers [1, 8] have formulated a current conserving formalism for the low frequency admittance of mesoscopic conductors.

In the theory of Büttiker, Prêtre and Thomas [1], it is necessary to consider the Coulomb interactions between the many charges inside the sample, in order to preserve the current conservation. For a multi-probe conductor the low frequency admittance is found to have the form [8, 9]

\[ G_{\alpha\beta}(\omega) = G_{\alpha\beta}(0) - i\omega E_{\alpha\beta} + O(\omega^2), \]

where \( G_{\alpha\beta}(0) \) is the dc-conductance, \( E_{\alpha\beta} \) is the emittance [8], and \( \alpha \) (or \( \beta \)) labels the probe. The emittance \( E_{\alpha\beta} \) describes the current response at probe \( \alpha \) due to a variation of the electro-chemical potential at probe \( \beta \) to leading order with respect to frequency \( \omega \). It can be written as [8]

\[ E_{\alpha\beta} = \frac{dN_{\alpha\beta}}{dE} - D_{\alpha\beta}, \tag{1} \]

where the term \( dN_{\alpha\beta}/dE \) is the global partial density of states (GPDOS) [11, 12] which is related to the scattering matrix. It describes the density of states of carriers injected in probe \( \beta \) reaching probe \( \alpha \) and is due to the response to the external perturbation. The term \( D_{\alpha\beta} \) is due to the Coulomb interaction of electrons inside the sample and is the response to the internal potential. \( D_{\alpha\beta} \) can be computed from the local density of states [1, 8] which is related to the electron dwell times through the relation \( \sum_{\alpha} D_{\alpha\beta} = \tau_{d\beta}/h \) where \( \tau_{d\beta} \) is the dwell time for particles coming from the probe \( \beta \). Electric current conservation, namely \( \sum_{\alpha} G_{\alpha\beta}(\omega) = 0 \), means that \( \sum_{\alpha} E_{\alpha\beta} = 0 \) or equivalently [1, 11]

\[ \frac{dN_\beta}{dE} \equiv \sum_{\alpha} \frac{dN_{\alpha\beta}}{dE} = \sum_{\alpha} D_{\alpha\beta} \tag{2} \]
where \( dN_\beta/dE \) is the DOS for electron coming from the probe \( \beta \). Clearly the current conservation is established since one realizes that \( \sum_\alpha dN_{\alpha\beta}/dE \) is the physical quantity called injectance which is identical to \( \sum_\alpha D_{\alpha\beta} \).

The physical meaning and the important role played by the various partial density of states (PDOS) is the subjects of extensive discussions. While in one-dimensional (1D) systems the PDOS can be evaluated analytically via the help of scattering Green’s function, in 2D one is usually forced to use numerical methods due to the complexity of the problem, except for very special and exactly solvable cases. In the AC transport formalism outlined above, the GPDOS can be expressed approximately in terms of the energy derivative of the scattering matrix elements:

\[
\frac{dN_{\alpha\beta}}{dE} = \frac{1}{4\pi i} \int dE \left( -\frac{df}{dE} \right) Tr \left[ s_{\alpha\beta}^{\dagger} \frac{ds_{\alpha\beta}}{dE} - \frac{ds_{\alpha\beta}^{\dagger}}{dE} s_{\alpha\beta} \right]. \tag{3}
\]

In Eq. (3) \( f(E) \) is Fermi distribution function and \( s_{\alpha\beta} \) is the scattering matrix of dimensions \( M_\alpha \times M_\beta \) where \( M_\alpha \) is the number of quantum channels supported by the lead \( \alpha \). Because for a given system one may be able to obtain the scattering matrix, Eq. (3) thus provides a practical means of computing the GPDOS.

Using explicit 2D examples, it has been numerically demonstrated in Ref. and analytically shown in Ref. that the DOS \( dN_\beta/dE \) computed from Eq. (3) is only accurate up to correction terms which are exponentially decaying functions of the scattering volume away from thresholds of successive transport channels. At the thresholds, the correction terms diverge. Hence precise current conservation can not be obtained from the explicit calculations until the correction terms are added. A more serious problem is that we only know how to correct the DOS since we can compare the left and right hand sides of Eq. (4), but we don’t know how to distribute the correction terms among the PDOS of Eq. (3). The whole issue comes about since the external response in the theoretical formalism is really formulated with a time dependent perturbation at minus or plus infinity which are asymptotically far from the scattering region, while for every practical calculation one wants to consider what happens in some finite scattering volume.

The purpose of the present work is to formulate a procedure which allows a precise determination of the GPDOS \( dN_{\alpha\beta}/dE \) for any finite scattering volume. We have used a general approach similar to that employed by Christen and Büttiker in computing the non-linear transport coefficients by eliminating the GPDOS. This is possible if we assume that electric current conservation
is satisfied. In doing so all the required quantities for the emittance become local, thus can be calculated precisely using the new formula (see below) within a finite scattering volume. We have applied this formula to compute the emittance of a T-shaped quantum wire under the multi-mode and finite temperature condition.

To proceed we recall from our previous investigations\cite{6,14} of 2D quantum conductors, that the discrepancy between the DOS as computed externally or internally is related to the mode mixing of the 2D scattering. In 2D situations complicated mode mixing takes place. This mode mixing generates evanescent modes which can not propagate in the leads. For a scattering volume with a finite linear size $L$, the evanescent modes may “leak” out of the volume. However when we calculate the GPDOS from the scattering matrix using Eq. (3), these “leaked” evanescent modes are not explicitly included, leading to a slightly inaccurate calculation. On the other hand, when we compute the local density of states \textit{internally} (see below) using the scattering wavefunctions, all the modes, including the evanescent modes, are included. Indeed, as emphasized by Büttiker\cite{8}, the AC transport formalism guarantees electric current conservation when the scattering volume is large enough to ensure that there is no electric field lines penetrating the surface of the volume. This condition is certainly violated due to the “leaked” evanescent modes when the volume is small. Since evanescent modes do not contribute to electric current (but does to the DOS), it seems to be natural to use the conservation law to eliminate the need of computing GPDOS \textit{externally}. This will be our approach.

Using the electric current conservation relation of Eq. (2) and the injectance formula\cite{8} of $\sum_\alpha D_{\alpha\beta}$, we have

$$
\sum_\alpha \left[ \frac{dN_{\alpha\beta}}{dE} - D_{\alpha\beta} \right] = \sum_\alpha \left[ \frac{dN_{\alpha\beta}}{dE} - \int \frac{dn_{\alpha\beta}}{dE} d^3r \right] = 0 .
$$

(4)

This is consistent with the relationship between the GPDOS and local PDOS (LPDOS)

$$
\frac{dN_{\alpha\beta}}{dE} = \int \frac{dn_{\alpha\beta}(r)}{dE} d^3r
$$

(5)

where

$$
\frac{dn_{\alpha\beta}(r)}{dE} = -\frac{1}{4\pi i} \int dE \left( -\frac{d\delta}{dE} \right) \text{Tr} \left[ s_{\alpha\beta} \frac{\delta s_{\alpha\beta}}{e\delta U(r)} - \frac{\delta s_{\alpha\beta}}{e\delta U(r)} s_{\alpha\beta} \right].
$$

(6)

is the LPDOS\cite{10}. Hence the GPDOS can be computed \textit{locally} through Eq. (6) if we can obtain LPDOS. In general, for 2D systems it is very difficult if not impossible to obtain LPDOS using Eq. (6) since a complicated functional derivative
must be evaluated. In 2D this functional derivative can only be computed for specially simple systems\[12\].

For 1D systems, on the other hand, as shown in Ref. \[10\] simplification to the LPDOS formula Eq. (3) can be obtained (see Ref.\[10\] for details) via the Fisher-Lee relation\[17\] between the scattering matrix and the retarded Green’s function:

\[ s_{\alpha\beta} = -\delta_{\alpha\beta} + i\hbar\sqrt{v_{\alpha}v_{\beta}}G(x_\alpha, x_\beta) \] (7)

where \(x_\alpha\) is the boundary of the scattering region. The functional derivative of the Green’s function \(\delta G/\delta U\) is given by\[10\]

\[ \frac{\delta G(x_{\alpha}, x_{\beta})}{\delta U(x)} = G(x_{\alpha}, x)G(x, x_{\beta}) \] (8)

Furthermore one can prove that for 1D systems the following relation is true\[10\],

\[ G(x_{1}, x)G(x, x_{2}) = G(x_{1}, x_{2})G(x, x) \] (9)

for \(x_{1} < x < x_{2}\). Using Eqs. (7) - (9), it is not difficult to derive\[10\], for 1D systems, the following expressions for the LPDOS

\[ \frac{dn_{\alpha\beta}(\mathbf{r})}{dE} = \frac{1}{2} T_{\alpha\beta} \frac{dn(\mathbf{r})}{dE} \] (10)

for \(\alpha \neq \beta\) and

\[ \frac{dn_{\beta\beta}(\mathbf{r})}{dE} = \frac{dn_{\beta}(\mathbf{r})}{dE} - \frac{1}{2} \sum_{\alpha \neq \beta} T_{\alpha\beta} \frac{dn(\mathbf{r})}{dE} \] (11)

where \(T_{\alpha\beta}\) is the transmission coefficient from lead \(\beta\) to \(\alpha\). In these results, the local DOS \(dn_{\beta}(\mathbf{r})/dE\) is defined as

\[ \frac{dn_{\beta}(\mathbf{r})}{dE} = \sum_{\alpha} \frac{dn_{\alpha\beta}(\mathbf{r})}{dE} \] (12)

which is called the injectivity and it measures the additional local charge density brought into the sample at point \(\mathbf{r}\) by the oscillating chemical potential at probe \(\beta\). In general, the injectivity can be expressed in terms of the scattering wavefunction as\[11\]

\[ \frac{dn_{\beta}(\mathbf{r})}{dE} = \int dE \left( -\frac{df}{dE} \right) \sum_{n} \frac{\left| \Psi_{\beta n}(\mathbf{r}) \right|^{2}}{hv_{\beta n}} , \] (13)

where \(v_{\beta n}\) is the velocity of carriers at the Fermi energy at mode \(n\) in probe \(\beta\). A related quantity, \(dn_{\alpha}(\mathbf{r})/dE\), called emissivity, describes the local density of
states of carriers at point $r$ which are emitted by the conductor at probe $\alpha$. It is defined as

$$\frac{dn_\alpha(r)}{dE} = \sum_\beta \frac{dn_{\alpha\beta}(r)}{dE}.$$  \hfill (14)

It has been shown\cite{9} that in the absence of a magnetic field the injectivity is equal to the emissivity. In the presence of a magnetic field the microreversibility of the scattering matrix implies that the emissivity into contact $\alpha$ in magnetic field $B$ is equal to the injectivity of contact $\alpha$ if the magnetic field is reversed\cite{9},

$$\frac{dn_\alpha(r, B)}{dE} = \frac{d\bar{n}_\alpha(r, -B)}{dE}. \hfill (15)$$

Finally, $dn/r/dE$ is the local DOS given by

$$\frac{dn(r)}{dE} = \sum_{\alpha\beta} \frac{dn_{\alpha\beta}(r)}{dE}. \hfill (16)$$

From these results, one is able to calculate the LPDOS via Eq. (10) and (11) using the scattering wavefunctions.

For 2D systems, the Fisher-Lee relation is of the form\cite{18}

$$s_{an\beta m} = -\delta_{an\beta m} + i\hbar \sqrt{v_{an} v_{\beta m}} \int \int G(x_\alpha, y_\alpha, x_\beta, y_\beta) \chi_{an}(y_\alpha) \chi_{\beta m}(y_\beta) dy_\alpha dy_\beta \hfill (17)$$

where $\chi_{an}$ is the transverse wavefunction in lead $\alpha$. In 2D, the equations similar to Eq. (10) and (11) do not seem to apply. This is because Eq.(9) does not hold in 2D\cite{19}. However, since in a general 2D case one can not obtain analytical expressions for the scattering matrix and numerical computation are usually needed, it is thus enough to have a numerical prescription for calculating the LPDOS. Our numerical method makes use of a mathematical identity

$$\frac{ds_{\alpha\beta}}{dV} = \int d^3 r \, \delta s_{\alpha\beta} \delta U(r), \hfill (18)$$

where $ds_{\alpha\beta}/dV$ is calculated as follows\cite{20, 9, 12}: adding a constant potential $V$ in the scattering volume and computing the scattering matrix formally to get $s_{\alpha\beta} = s_{\alpha\beta}(V)$, then taking the derivative and putting $V = 0$. Numerically the derivative can be easily carried out using finite differencing.

Using Eqs.(18), (5), and (6), the GPDOS is completely expressed by local quantities determined inside the scattering volume thus can be computed accurately for any system sizes,

$$\frac{dN_{\alpha\beta}}{dE} = -\frac{1}{4\pi i} \int dE (- \frac{df}{dE}) T Tr \left[ s_{\alpha\beta}^\dagger \frac{ds_{\alpha\beta}}{dV} - \frac{ds_{\alpha\beta}}{dV} s_{\alpha\beta}^\dagger \right]. \hfill (19)$$
This equation is also valid in 1D. In the following, we shall compute the emittance from Eq. (1) using the Eq. (19) for GPDOS. To obtain the quantity \( D_{\alpha\beta} \) we shall use the Thomas-Fermi approximation, in which case \( D_{\alpha\beta} \) is easily calculable\(^1\),\(^8\) from Eqs. (13), (14), (15), and (16),

\[
D_{\alpha\beta} = \int d^3r \frac{(dn_\alpha(r)/dE)(dn_\beta(r)/dE)}{dn(r)/dE} .
\]  \((20)\)

To illustrate the numerical procedure, we have computed the emittance of a T-junction quantum wire under the multi-mode and finite temperature conditions. The same system has been examined before for the single mode and zero temperature situation\(^4\) using externally computed GPDOS \( i.e. \) Eq. (3)), thus the results here also provide an useful comparison. As shown in Fig. (1), the wire has two probes extending to \( x = \pm\infty \) while the scattering region is provided by the T-junction as shown being bounded by the two dotted lines. We assume that the boundaries of this ballistic conductor are hard walls, \( i.e. \) the potential \( V = \infty \). Inside the conductor the potential is zero. From now on we set \( \hbar = 1 \) and \( m = 1/2 \) to fix our units.

Fig. (2) shows the emittance \( E_{11} \) versus incoming energy \( E \) in the first subband at zero temperature, where the GPDOS is computed using Eq. (19) (solid line) or using Eq. (3) (dotted line). The difference in the two curves comes solely from the difference in GPDOS. Notice that near the second subband the divergence in the dotted curve is removed by using the locally computed GPDOS Eq. (19) as shown by the solid curve. As discussed previously\(^5\) and shown in Fig. (2), there is also a divergence near \( E = E_1 \) where \( E_1 = \pi^2 \) is the first subband energy, if using the externally computed GPDOS. This problem is also overcome using Eq. (19) as shown by the solid curve. In fact since all quantities are computed locally if using Eq. (19), there is no need for any correction terms to the DOS. In Fig. (3a) we plot the emittance \( E_{11} \) up to the 2nd subband energy for three different temperatures \( T = 0.005E_1 \) (dotted line), \( 0.05E_1 \) (dashed line), and \( 0.1E_1 \) (solid line). The inset shows the same quantity up to 3rd subband. We have also depicted the dwell time \( \tau_{d1} \) (dashed line) in Fig. (3b) together with the DC conductance (solid line) and the emittance \( E_{11} \) at zero temperature (dotted line). There are eight resonant states located near the peaks of the dwell time. The behavior of the emittance \( E_{11} \) near the resonant energies \( \mathcal{E}_5 \) (the 5th one) and \( \mathcal{E}_6 \) (the 6th) which are basically inductive are different from that near the other resonant energies which are capacitive. This behavior is useful in explaining the resonance behavior in the transmission coefficient near resonant energies \( \mathcal{E}_5 \) and \( \mathcal{E}_6 \). For instance, from the dwell time we know that near \( \mathcal{E}_5 \) there is a resonant
state. However, it is not clear whether it is a resonant transmission or resonant reflection since the DC conductance has a sharp peak and a dip very close to each other. The fact that the emittance near $E_5$ is inductive indicates that it is a resonant transmission. Finally, as the temperature is turned on, the peaks or valleys in the emittance curve diminish gradually. When the temperature reaches $T = 0.2E_1$, the interference pattern is washed out completely. This is expected since a finite temperature tends to smear out the quantum resonances.

In summary, we have proposed a numerical procedure and formula for computing the global partial density of states which is precise for any finite scattering volume of a quantum conductor. As GPDOS plays a most important role in the AC transport theory, our result provides a useful tool for further numerical investigations of the dynamic admittance. In this formulation the electric current conservation is satisfied automatically. This formulation, especially Eq. (18), also applies to the non-linear transport[16, 12]. Applying the new procedure to a T-shaped junction, the divergences of the emittance at each subband edge are removed.

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Figure Captions

Figure 1. Schematic plot of the quantum wire system: The wire width, the side-sub width, and height are fixed at $W = 1$. The two dotted lines separate the scattering region from the two probes.

Figure 2. The emittance $E_{11}$ versus incoming energy $E$ in the first subband at zero temperature, where the GPDOS is calculated using Eq.(19) (solid line) or using Eq.(3) (dotted line).

Figure 3. Figure (3a): the emittance $E_{11}$ versus energy for three difference temperatures $T = 0.005E_1$ (dotted line), $0.05E_1$ (dashed line), and $0.1E_1$ (solid line), up to the second subband. Inset, the same quantity up to the third subband. Figure (3b): the conductance $G_{11}$ (solid line), the dwell time (dashed line), and the emittance $E_{11}$ at zero temperature (dotted line) where the dwell time and the emittance have been scaled by a factor of eight to fit in one figure.
