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Local density of states from transmission amplitudes in multichannel systems

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We consider phase-coherent electron transport in the multichannel case with time-reversal symmetry. The two-terminal conduction, as described by the Landauer-Büttiker theory, can be considered to take place in parallel in independent channels: the so-called *eigenchannels*. We extend the known relationship between the local density of states (LDOS) and phase of the transmission amplitude in one dimension to the multichannel case, and derive a simple explicit expression for the LDOS as a sum of individual eigenchannel contributions. A simple expression for the LDOS that can be used for numerical calculations is given. We show how this formalism can be useful in the description of the electronic states and conductance of metallic nanocontacts. [S0163-1829(98)51124-1]

The density of states (DOS) that do not originate from localized states can be obtained from the scattering properties of a quantum system.[1] It has been shown by Avishai and Band[2] that the DOS of a one-dimensional system is simply related to the phase of the transmission amplitude. In this paper we show how this relationship can be extended in a simple way to the multidimensional case using the concept of eigenchannels.

We consider a general two-terminal phase-coherent conductor in the linear-response regime with time-reversal symmetry. We denote the two terminals by 1 and 2 and label the transmission and reflection amplitude matrices for states originating from terminal 1 by $\mathbf{t}_{12}$ and $\mathbf{r}_{11}$ and accordingly for terminal 2. The conductance is obtained from the multichannel Landauer-Büttiker formula,[3]

$$G = G_0 \ \mathrm{Tr}[\mathbf{t}^{\dagger}{}_{12}\mathbf{t}_{12}](E_F). \tag{1}$$

Only states at the Fermi energy (E_F) are considered at zero temperature.

The local density of states (LDOS) can be split into two parts dN_t/dE and dN_r/dE, describing states that are being transmitted between 1 and 2, and states that are reflected. These can be classified according to the originating terminal, and we end up with a sum of four terms,[4]

$$\frac{dN}{dE}(E,\vec{r}) = \frac{dN_t}{dE}(E,\vec{r}) + \frac{dN_r}{dE}(E,\vec{r}),$$

$$\frac{dN_t}{dE} = -\frac{1}{2\pi}\left(\mathrm{Im\,Tr}\left[\mathbf{t}_{12}^{\dagger}\frac{\delta \mathbf{t}_{12}}{\delta V(\vec{r})}\right] + \mathrm{Im\,Tr}\left[\mathbf{t}_{21}^{\dagger}\frac{\delta \mathbf{t}_{21}}{\delta V(\vec{r})}\right]\right), \tag{2}$$

$$\frac{dN_r}{dE} = -\frac{1}{2\pi}\left(\mathrm{Im\,Tr}\left[\mathbf{r}_{11}^{\dagger}\frac{\delta \mathbf{r}_{11}}{\delta V(\vec{r})}\right] + \mathrm{Im\,Tr}\left[\mathbf{r}_{22}^{\dagger}\frac{\delta \mathbf{r}_{22}}{\delta V(\vec{r})}\right]\right),$$

where V is the scattering potential. The partition into the four so-called *partial* LDOS is important, e.g., in the discussion of ac transport[4,5] or the effect of finite dc bias. Here we will focus on the total transmitted and reflected parts of LDOS (dN_t/dE, dN_r/dE).

In the case of time reversal symmetry:

$$\mathbf{t}_{21} = \mathbf{t}_{12}^{T}, \quad \mathbf{r}_{11}^{T} = \mathbf{r}_{11}, \quad \mathbf{r}_{22}^{T} = \mathbf{r}_{22}, \tag{3}$$

so the two terms in the transmitted LDOS will be equal.

Eigenchannels[6] are special orthogonal linear combinations of the incoming (outgoing) states in terminal 1(2) with a fixed energy and correspond to transmission eigenstates. Recently these have been addressed experimentally[7] as well as theoretically[8,9] in order to elucidate the nature of conduction in atomic-scale metal point contacts (nanocontacts).

Consider the incoming eigenchannels in terminal 1 determined by the columns in the *unitary* matrix $\mathbf{U_1}$:

$$\mathbf{U_1}^{\dagger}\ \mathbf{t}_{12}^{\dagger}\mathbf{t}_{12}\ \mathbf{U_1} = \mathrm{diag}\{|\tau_n|^2\}. \tag{4}$$

Using this special basis, the Landauer-Büttiker formula reduces to a sum of contributions from each eigenchannel,

$$G = G_0 \sum_n \ |\tau_n|^2. \tag{5}$$

We will for simplicity assume that τ_n are all different and differ from zero. For the physical systems we have in mind this is not a crucial restriction.

Now consider the outgoing eigenchannels in 2 given by the columns in $\mathbf{U_2}$ (denoted by $\mathbf{U_{2n}}$):

$$\mathbf{U_2} = \mathbf{t}_{12}\ \mathbf{U_1}\ \mathrm{diag}\{1/\tau_n\}. \tag{6}$$

$\mathbf{U}_2$ will also be unitary ($\mathbf{U_2}^{\dagger}\ \mathbf{t}_{12}\mathbf{t}_{12}^{\dagger}\ \mathbf{U_2} = \mathrm{diag}\{|\tau_n|^2\}$). An incoming state from terminal 1 given by the nth column $\mathbf{U_{1}}_n$, will end up in terminal 2 in the linear combination given by $\tau_n \mathbf{U_{2}}_n$ according to Eq. (6). For simplicity we choose all phase information to be contained in the $\mathbf{U}$'s using $|\tau_n|$ in Eq. (6) (Ref. 10), i.e.,

$$\mathbf{t}_{12} = \mathbf{U_2}\ \mathrm{diag}\{|\tau_n|\}\mathbf{U_1}^{\dagger}. \tag{7}$$

Inserting Eq. (7) in the expression for the transmitted LDOS yields

$$\frac{dN_t}{dE}(\vec{r}) = \frac{1}{\pi}\sum_n\ |\tau_n|^2 \left(\frac{\delta\theta_n}{\delta V(\vec{r})}\right). \tag{8}$$

Here the transmitted LDOS is split into eigenchannel contributions. We have introduced a quantity corresponding to the derivative of the phase of each eigenchannel given by

$$\frac{\delta\theta_n}{\delta V(\vec{r})} = \frac{1}{i}\left(\frac{\delta \mathbf{U}^*_{\mathbf{2}n}}{\delta V(\vec{r})}\cdot\mathbf{U}_{\mathbf{2}n} - \frac{\delta \mathbf{U}^*_{\mathbf{1}n}}{\delta V(\vec{r})}\cdot\mathbf{U}_{\mathbf{1}n}\right). \tag{9}$$

Now we consider the reflected part of the LDOS. Due to current conservation, $\mathbf{t}^{\dagger}_{12}\mathbf{t}_{12}+\mathbf{r}^{\dagger}_{11}\mathbf{r}_{11}=\mathbf{I}$, so $\mathbf{r}^{\dagger}_{11}\mathbf{r}_{11}$ will be diagonal in the basis in 1 described by $\mathbf{U_1}$,

$$\mathbf{U}^{\dagger}_{\mathbf{1}}\mathbf{r}^{\dagger}_{11}\mathbf{r}_{11}\mathbf{U_1} = \mathrm{diag}\{|\rho_n|^2\}, \tag{10}$$

where $|\rho_n|^2 = 1-|\tau_n|^2$. Consider $\mathbf{X}$ defined by

$$\mathbf{X} = \mathbf{U}^T_{\mathbf{1}}\mathbf{r}_{11}\mathbf{U_1} = \mathbf{X}^T, \tag{11}$$

$$\mathbf{X}^{\dagger}\mathbf{X} = \mathbf{X}\mathbf{X}^{\dagger} = \mathrm{diag}\{|\rho_n|^2\}. \tag{12}$$

Due to the time-reversal symmetry, $\mathbf{X}$ is symmetric [Eq. (11)] and normal [Eq. (12)]. From this and the assumption that all $|\rho_n|$ are different it follows that $\mathbf{X}$ is diagonal:

$$\mathbf{r}_{11} = \mathbf{U}^*_{\mathbf{1}}\ \mathrm{diag}\{\rho_n\}\ \mathbf{U}^{\dagger}_{\mathbf{1}}. \tag{13}$$

Inserting this expression in the partial LDOS related to $\mathbf{r}_{11}$ we obtain

$$-\frac{1}{2\pi}\mathrm{Im\ Tr}\left[\mathbf{r}^{\dagger}_{11}\frac{\delta\mathbf{r}_{11}}{\delta V(\vec{r})}\right] = -\frac{1}{2\pi}\sum_n\ \mathrm{Im}\left(\rho^*_n\frac{\delta\rho_n}{\delta V(\vec{r})}\right) - \frac{1}{i\pi}\sum_n\ |\rho_n|^2\left(\frac{\delta\mathbf{U}^*_{\mathbf{1}n}}{\delta V(\vec{r})}\cdot\mathbf{U}_{\mathbf{1}n}\right). \tag{14}$$

In the case of the reflected LDOS in terminal 2 we note that due to the time-reversal symmetry ($\mathbf{t}_{12}\mathbf{t}^{\dagger}_{12}+\mathbf{r}_{22}\mathbf{r}^*_{22}=\mathbf{I}$), $\mathbf{U_2}$ will diagonalize $\mathbf{r}_{22}\mathbf{r}^*_{22}$. Using the same arguments as for $\mathbf{r}_{11}$, we can write

$$\mathbf{r}_{22} = \mathbf{U}^{\dagger}_{\mathbf{2}}\ \mathrm{diag}\{\tilde{\rho}_n\}\ \mathbf{U}^*_{\mathbf{2}}. \tag{15}$$

We have that $|\rho_n| = |\tilde{\rho}_n|$, however, the phase of ρ_n and $\tilde{\rho}_n$ will in general differ. The $\mathbf{r}_{22}$ term reads

$$-\frac{1}{2\pi}\mathrm{Im\ Tr}\left[\mathbf{r}^{\dagger}_{22}\frac{\delta\mathbf{r}_{22}}{\delta V(\vec{r})}\right] = -\frac{1}{2\pi}\sum_n\ \mathrm{Im}\left(\tilde{\rho}^*_n\frac{\delta\tilde{\rho}_n}{\delta V(\vec{r})}\right) + \frac{1}{i\pi}\sum_n\ |\rho_n|^2\left(\frac{\delta\mathbf{U}^*_{\mathbf{2}n}}{\delta V(\vec{r})}\cdot\mathbf{U}_{\mathbf{2}n}\right). \tag{16}$$

We can relate the phase of ρ_n and $\tilde{\rho}_n$ using the unitarity of the $\mathbf{S}$ matrix ($\mathbf{t}^{\dagger}_{21}\mathbf{r}_{11}+\mathbf{r}^{\dagger}_{22}\mathbf{t}_{12}=0$) combined with time-reversal symmetry ($\mathbf{t}^*_{12}\mathbf{r}_{11}+\mathbf{r}^*_{22}\mathbf{t}_{12}=0$). Using Eqs. (7), (13), and (15) we obtain

$$\rho_n\ =\ -\tilde{\rho}^*_n. \tag{17}$$

Using this we arrive at the following simple result for the reflected part of the LDOS,

$$\frac{dN_r}{dE}(\vec{r}) = \frac{1}{\pi}\sum_n\ (1-|\tau_n|^2)\left(\frac{\delta\theta_n}{\delta V(\vec{r})}\right), \tag{18}$$

and together with Eq. (8) we have the total LDOS:

$$\frac{dN}{dE}(\vec{r}) = \sum_n\ \frac{dN_n}{dE}(\vec{r}) = \frac{1}{\pi}\sum_n\ \left(\frac{\delta\theta_n}{\delta V(\vec{r})}\right). \tag{19}$$

These simple equations for the total [Eq. (19)], transmitted [Eq. (8)], and reflected LDOS [Eq. (18)], are the main results of this paper. They generalize the single-channel result by Avishai and Band[2] to the multichannel case. It shows that we can obtain the total LDOS from the individual eigenchannel components of the transmitted LDOS [Eq. (8)] by dividing each eigenchannel contribution by $|\tau_n|^2$. Thus the total LDOS is simply expressed using the transmission amplitude matrix $\mathbf{t}$ instead of the full $\mathbf{S}$ matrix in the case of time-reversal symmetry.

We end this general discussion by noting that the transmitted part of LDOS for eigenchannel n alternatively can be obtained from

$$|\tau_n|^2\left(\frac{\delta\theta_n}{\delta V(\vec{r})}\right) = -\,\mathrm{Im}\left(\mathbf{U_1}^{\dagger}\mathbf{t}^{\dagger}_{12}\frac{\delta\mathbf{t}_{12}}{\delta V(\vec{r})}\mathbf{U_1}\right)_{nn}. \tag{20}$$

This expression does not involve $\mathbf{U_2}$, and is therefore more convenient for numerical calculations. The total LDOS can in principle be obtained by dividing the right-hand side of Eq. (20) by $|\tau_n|^2$. However, in actual numerical calculations only the contributions to the total LDOS from eigenchannels with a certain size of $|\tau_n|$ are accessible in this way. But in many situations one is especially interested in the LDOS close to a ''bottleneck'' in the potential where the LDOS is contributed only by the few eigenchannels with the highest $|\tau_n|$. In such cases Eq. (20) can be employed to obtain the total LDOS, as demonstrated below.

Now we turn to a concrete example where we can apply the general formalism. Several papers have lately addressed the special electronic structure of metal nanocontacts and its effect on their mechanical behavior.[11–15] In these studies the adiabatic approximation has been applied.[16,17] This approximation is valid in the limit of a slowly (on the scale of the Fermi wavelength) varying confining potential. In this limit the eigenchannels correspond to the local transverse energy eigenstates along the nanocontact; the columns of $\mathbf{U_1}$ will simply contain these at the point where the scattering region is connected to terminal 1. If we denote this point by z_1 (the transmission amplitudes $\mathbf{t}_{12}$ are defined with respect to the starting and ending points: z_1 and z_2, see Fig. 1), i.e.,

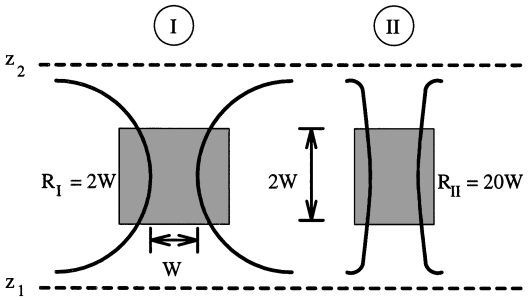

FIG. 1. The shapes of the two-dimensional hard-wall potentials. I: Radius of curvature comparable to the width, $R=2W$. II: Radius of curvature at the narrowest point much larger than the width, $R=20W$. LDOS is integrated over the gray volume ($\mathcal{V}$) centered around the thinnest point ($z_b-z_a=2W$). The transmission amplitudes are defined with respect to the borderline between the scattering region and terminals 1 and 2 at z_1 and z_2, respectively.

$$\langle x,y|\mathbf{U_{1}}_n\rangle=\phi_{n,z_1}(x,y), \tag{21}$$

and similarly for $\mathbf{U_2}$ except for the phase θ_n containing all information about the propagation through the wire,

$$\langle x,y|\mathbf{U_{2}}_n\rangle=e^{i\theta_n}\,\phi_{n,z_2}(x,y). \tag{22}$$

The adiabatic limit θ_n defined in Eq. (22) corresponds to the θ_n in Eq. (9). This follows from the fact that the local transverse wave functions ($\phi_{n,z_1},\phi_{n,z_2}$) do not depend on the potential inside the scattering region.

Using WKB we may write the phase (in a.u.),

$$\theta_n=\int_{z_1}^{z_2}dz\ \sqrt{2[E_F-\varepsilon_n(z)]}, \tag{23}$$

where $\varepsilon_n(z)$ is the quantized transverse energies along the nanocontact. In order to compute the LDOS integrated over a certain volume $\mathcal{V}$, we simply replace the functional derivative in Eq. (9) by the normal derivative with respect to a constant shift of the potential inside $\mathcal{V}$. This procedure has recently been used in numerical calculations of DOS (Ref. 5) from the full **S** matrix. In the WKB approximation this simply corresponds to a shift in $\varepsilon_n(z)$ by dV and we obtain from Eq. (19) (including now a factor of 2 for spin),

$$\int_{\mathcal{V}}d\vec{r}\,\frac{dN_n}{dE}(E,\vec{r})=\frac{2}{\pi}\mathrm{Re}\int_{z_a}^{z_b}dz\,\frac{1}{\sqrt{2[E-\varepsilon_n(z)]}}, \tag{24}$$

where the volume $\mathcal{V}$ extends from z_a to z_b inside the nanocontact. This formula, based on the adiabatic approximation and WKB, has been employed for nanocontacts with a straight boundary[12,13,15] (constant ε_n) or including the finite curvature in the variation of $\varepsilon_n(z)$.[11,14]

We will now compare the numerical result for the total DOS of the individual eigenchannels with the corresponding WKB result for a simple two-dimensional example. Here we shall especially focus on the adiabatic approximation and study the effect of a finite curvature of the contact. We consider two types (Fig. 1): Type I with a radius of curvature (R) comparable to the width (W) at the thinnest point ($R=2W$), and type II with a radius of curvature much larger than the width ($R=20W$) corresponding to low and high degree of adiabaticity, respectively. For this illustrative purpose we use free-electron electrodes and a confining potential in the hard-wall limit.[18] The total LDOS is integrated over a volume (gray in Fig. 1) around the narrowest part of the constriction. We use Eq. (20) to calculate the phase derivative and we include channels with eigenchannel transmissions $|\tau_n|^2$ larger than 10^{-12}. This procedure agrees with the total DOS obtained from the full **S** matrix within a few percent.

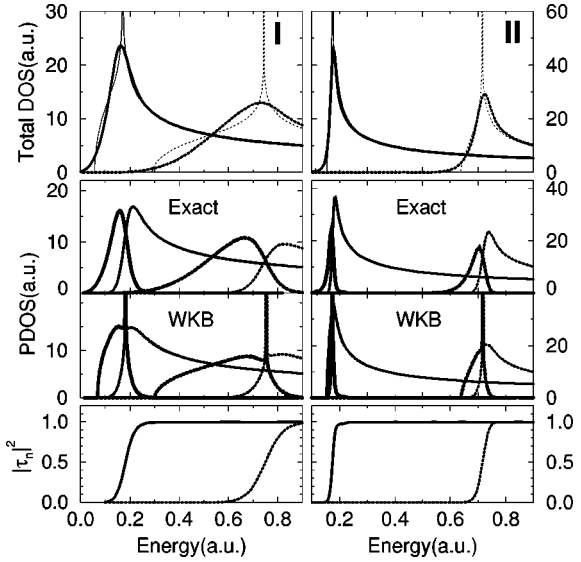

FIG. 2. Upper: The total DOS inside the gray volume ($\mathcal{V}$) in Fig. 1 of potential I and II calculated from Eq. (20). The thick solid and dotted lines are for 1 and 2 eigenchannels, respectively. The thin lines correspond to WKB [Eq. (24)]. Middle: Partial DOS: Reflected [Eq. (18), thick lines] and transmitted [Eq. (8)] parts of DOS inside $\mathcal{V}$ for 1 (solid) and 2 (dotted) eigenchannels. The exact and WKB [using Eq. (23)] results are shown. These sum up to the total DOS in the upper panel. Lower: Transmission probabilities $|\tau_n|^2$ for the 1 and 2 eigenchannels.

In Fig. 2 we show the results for potential I with the smallest curvature, i.e., the least adiabatic potential. In this case, as expected, the difference between the WKB and the exact result is most striking. The WKB results exhibit a logarithmic divergence at the channel opening, and converge to the exact result in the high-energy limit. The reflected DOS is seen to play a large role in this case. The transmitted and reflected part of DOS (middle panel) are rather symmetric around the channel closing ($\tau_n=0.5$); the electron density does not decrease suddenly as the channel is closed, but is transferred slowly from transmitting to reflected states inside $\mathcal{V}$. The low-energy part of the reflected DOS is controlled by the evanescent tails of the wave functions reaching into $\mathcal{V}$ while the high energy cutoff is due to the onset of transmission. For comparison we also show the result where we use the WKB phase [Eq. (23)] instead of the exact.

The reflected DOS becomes less significant for the more adiabatic potential (II); it does not contribute as much as the transmitted part around the opening of a channel and the electron density inside $\mathcal{V}$ drops steeply as the channel is closed. In this case the agreement with WKB becomes more pronounced. We note that for a fixed radius of curvature the discrepancy between the WKB and the exact result will increase with channel number as the width of the transition between open and closed channels increases.[17]

Recently, there has been interest in the electronic contribution to the tensile forces in the metallic nanocontacts.[11–15] We can now, in general, associate a thermodynamic potential (Ω) with each eigenchannel (in the limit of zero temperature),

$$\Omega_n = \int_{-\infty}^{E_F} (\varepsilon - E_F) \left(\frac{dN_n}{dE}(\varepsilon) \right) d\varepsilon, \tag{25}$$

and a tensile force due to each eigenchannel ''bond'' $F_n = -\delta\Omega_n / \delta L$, where L is the elongation parameter of the nanocontact. Within the adiabatic approximation and WKB the drastic change in the DOS around the channel closings leads to fluctuations in the tensile force with a magnitude close to the one found experimentally.[19] It is, however, clear that the one-electron potentials of nanocontacts in general will vary on the atomic scale that is comparable to the Fermi wavelength. Thus DOS can differ from the adiabatic WKB result in a significant way, as illustrated by our simple example, and calculations beyond the adiabatic WKB treatment are necessary in order to confirm the adiabatic estimates. Our formalism can provide a general framework for these discussions and discussions of conductance in atomic-scale systems in general, e.g., combined with first-principles calculations.[20]

In conclusion we have shown how the components of LDOS can be written as a sum of contributions from the individual eigenchannels. By defining a derivative of the eigenchannel phase, this result extends the one-dimensional result by Avishai and Band[2] to the multichannel case in a simple way. For ''bottleneck'' potentials this method can be used in numerical calculations to obtain the total DOS from the transmission matrix. As an example, we have discussed how this formalism is relevant for metal nanocontacts. Especially, we have shown that the (partial) LDOS, conductance, and tensile force (electronic contribution only) can be written as a sum over individual eigenchannel contributions.

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