Charge densities and charge noise in mesoscopic conductors

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Abstract. We introduce a hierarchy of density of states to characterize the charge distribution in a mesoscopic conductor. At the bottom of this hierarchy are the partial density of states which represent the contribution to the local density of states if both the incident and the out-going scattering channel is prescribed. The partial density of states play a prominent role in measurements with a scanning tunneling microscope on multiprobe conductors in the presence of current flow. The partial density of states determine the degree of dephasing generated by a weakly coupled voltage probe. In addition the partial density of states determine the frequency-dependent response of mesoscopic conductors in the presence of slowly oscillating voltages applied to the contacts of the sample. The partial density of states permit the formulation of a Friedel sum rule which can be applied locally. We introduce the off-diagonal elements of the partial density of states matrix to describe charge fluctuation processes. This generalization leads to a local Wigner–Smith life-time matrix.

Keywords. Density of states; injectivity; emissivity; voltage probe; inelastic scattering; absorption and emission; Bardeen formula; Friedel sum rule; mesoscopic electron transport.

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1. Introduction

The characterization of the charge distribution and its fluctuations are a central aspect of electrical conduction theory. In this work we are concerned with mesoscopic conductors, structures which are so small and cooled to such low temperatures that the wave nature of electron motion becomes apparent. Three recent reviews provide an entry to the literature of this very active field [1–3]. Of interest is the charge distribution in such a conductor and its fluctuations under equilibrium and non-equilibrium condition. The charge distribution is an interesting quantity in itself. However, in addition, it is important for the solution of a number of problems. We mention here only a few: Already, in the equilibrium state, the charge distribution needs to be known to determine the effective equilibrium one-electron potential. It is this potential which determines the scattering properties of the conductor and thus the conductance coefficients. If voltages are applied which drive the conductor away from the equilibrium state, typically, the charge distribution also undergoes a bias dependent modification. Thus the charge distribution is needed to find the non-linear I–V characteristic of an electrical conductor. Nanoscopic contacts to a sample measure local density of states and thus charge distribution. Knowledge of the charge distribution is essential for the discussion of the dynamic conductance like the ac-conductance or photon
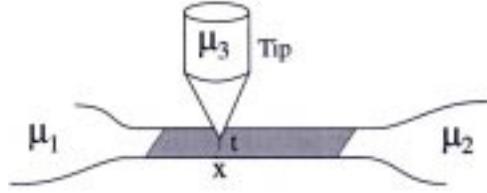
Figure 1. Mesoscopic conductor with a tunneling contact with coupling energy t at x. After ref. [10].

assisted transport. The charge distribution also determines the capacitance coefficients of various spatial regions within the mesoscopic structure and also vis-a-vis nearby gates.

2. Local partial density of states

It is the purpose of this work to present a discussion of the charge distribution [4,5] and the charge noise [6] based on the scattering approach. Similar to the discussion of linear transport [7–9], we view the sample as a target which transmits or reflects electrical carriers into the contacts connected to the sample. A particular example [10] of a structure of interest here is shown in figure 1. For purely elastic scattering the sample is described by a scattering matrix **s**. We label the different contacts to the sample by $\alpha = 1, 2, \dots$. Each contact is treated as a perfect wave guide which permits the definition of incoming and out-going quantum channels. Each contact has at a given energy a set of quantum channels with quantum numbers labeled m. The scattering matrix element $s_{\alpha m, \beta n}$ relates the out-going current amplitude in contact α in channel m to the incoming current amplitude in contact β in channel n. For the following discussion it is useful to introduce the submatrix $\mathbf{s}_{\alpha\beta}$ which combines all scattering matrix elements with the same contact indices. This is a matrix of dimension $M_\alpha x M_\beta$ for a conductor with M_α open scattering channels in contact α and M_β open channels in contact β. We will now show that the equilibrium and non-equilibrium charge distribution can be described with the help of a hierarchy of density of states. On top of this pyramid is the local density of states. At the bottom of this pyramid are the *local partial density of states* [4,6,10,11]

$$\nu(\alpha, \mathbf{r}, \beta) = -\frac{1}{4\pi i} \text{Tr} \left[\mathbf{s}_{\alpha\beta}^\dagger \frac{\delta \mathbf{s}_{\alpha\beta}}{e\delta U(\mathbf{r})} - \frac{\delta \mathbf{s}_{\alpha\beta}^\dagger}{e\delta U(\mathbf{r})} \mathbf{s}_{\alpha\beta} \right] \tag{1}$$

which give the contribution to the local density of states at point $\mathbf{r}$ of carriers incident in contact β and leaving the conductor through contact α. In eq. (1) the trace represents a summation over the channel indices. In the partial density of states we specify both the incident contact (a pre-selection) and the exiting contact (a post-selection). The local partial density of states is obtained by investigating the change of the scattering matrix due to a small additional potential perturbation $\delta U(\mathbf{r})$ at point $\mathbf{r}$.

On the next higher level in the pyramid of density of states are the *injectivities* and *emissivities*. The injectivity of contact β gives the contribution to the density of states of

carriers entering the conductor through β irrespective of the contact through which they leave the sample. The injectivity $\nu(\mathbf{r}, \beta)$ into point $\mathbf{r}$ of contact β is obtained by summing all partial density of states $\nu(\alpha, \mathbf{r}, \beta)$ over the first contact index,

$$\nu(\mathbf{r}, \beta) = -\frac{1}{4\pi i} \sum_\alpha \mathrm{Tr} \left[\mathbf{s}_{\alpha\beta}^\dagger \frac{\delta \mathbf{s}_{\alpha\beta}}{e\delta U(\mathbf{r})} - \frac{\delta \mathbf{s}_{\alpha\beta}^\dagger}{e\delta U(\mathbf{r})} \mathbf{s}_{\alpha\beta} \right]. \tag{2}$$

Using the unitarity of the scattering matrix we can also write for the injectivity,

$$\nu(\mathbf{r}, \beta) = -\frac{1}{2\pi i} \sum_\alpha \mathrm{Tr} \left[\mathbf{s}_{\alpha\beta}^\dagger \frac{\delta \mathbf{s}_{\alpha\beta}}{e\delta U(\mathbf{r})} \right]. \tag{3}$$

The emissivity of point $\mathbf{r}$ into contact α is that portion of the local density of states which consists of carriers which leave the sample through the contact α irresepctive of the contact through which they entered the sample. It is obtained by summing the partial density of states over the second contact index β. Taking into account the unitarity of the scattering matrix $\mathbf{s}$ we find

$$\nu(\alpha, \mathbf{r}) = -\frac{1}{2\pi i} \sum_\beta \mathrm{Tr} \left[\mathbf{s}_{\alpha\beta}^\dagger \frac{\delta \mathbf{s}_{\alpha\beta}}{e\delta U(\mathbf{r})} \right]. \tag{4}$$

At the top of this pyramid of density of states is the local density of states. For the local density of states we impose no restriction as to where the carriers come from nor as to where they will go in the future. The local density of states is thus the sum over all local partial density of states. In particular it is also the sum of all injectivities or the sum of all emissivities,

$$\nu(\mathbf{r}) = \sum_\beta \nu(\mathbf{r}, \beta) = \sum_\alpha \nu(\alpha, \mathbf{r}) \tag{5}$$

and is thus given by

$$\nu(\mathbf{r}) = -\frac{1}{2\pi i} \sum_{\alpha\beta} \mathrm{Tr} \left[s_{\alpha\beta}^\dagger \frac{\delta s_{\alpha\beta}}{e\delta U(\mathbf{r})} \right]. \tag{6}$$

We will later show the usefulness of these density of states. Here we only briefly mention the magnetic field symmetry. Since in a uniform field the scattering matrix has the reciprocity symmetry $\mathbf{s}_{\alpha\beta}(B) = \mathbf{s}_{\alpha\beta}(-B)$, we see that the partial density of states have the symmetry $\nu_B(\alpha, \mathbf{r}, \beta) = \nu_{-B}(\beta, \mathbf{r}, \alpha)$. Similarly, the injectivities and emissivities are related by reciprocity $\nu_B(\mathbf{r}, \alpha) = \nu_{-B}(\alpha, \mathbf{r})$ whereas the local density of states is an even function of the magnetic field $\nu_B(\mathbf{r}) = \nu_{-B}(\mathbf{r})$. Figure 2 shows the local density of states, the injectivity and the ratio of the injectivity to the local density of states for the simple case of a delta function barrier in an otherwise perfect ballistic one-channel wire connecting contacts 1 and 2. For additional simple examples we refer the reader to refs [10–12]. Partial density of states in disordered structures are evaluated numerically in ref. [13].
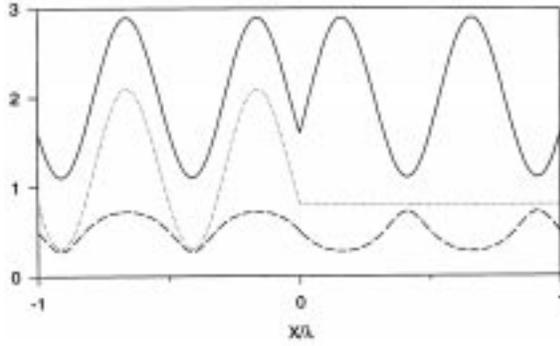
Figure 2. The local density of states $v(x)$ (solid line), the injectivity $v(x, 1)$ of contact 1 (dotted line) (both in units of $1/hv$), and the ratio of these two densities $v(x, 1)/v(x)$ (dashed line) of a one-dimensional wire with a δ barrier at $x = 0$ which has a strength that leads to a transmission probability of $T = 0.8$. The coordinate x is in units of the Fermi wavelength λ. After ref. [10].

3. Global partial density of states

Often we are interested not in the density of states at a given point but in a certain volume Ω. Of course the partial density of states in Ω are obtained simply by integrating the local partial density of states over the volume of interest. Of particular interest are the density of states of the entire sample. In this case the surface of the volume Ω will intersect the leads connected to the sample. Suppose now these intersections coincide with our specification of the scattering matrix. The phases which occur in the scattering matrix $\mathbf{s}_{\alpha\beta}$ are the phases which are accumulated through the scattering between the intersection S_α of Ω in lead α and the intersection of S_β in lead β. Under these circumstances a simplification of the above expressions is possible, since the functional derivative with respect to the local potential and the integration over Ω can be replaced by an energy derivative

$$-\int_\Omega \mathrm{d}\mathbf{r}^3 \frac{\delta}{e\delta U(\mathbf{r})} \rightarrow \frac{\mathrm{d}}{\mathrm{d}E}. \tag{7}$$

For the *global* density of states (density of states of the entire sample) we find the partial density of states

$$N(\alpha, \mathbf{r}, \beta) = \frac{1}{4\pi i} \mathrm{Tr} \left[\mathbf{s}_{\alpha\beta}^\dagger \frac{\mathrm{d}\mathbf{s}_{\alpha\beta}}{\mathrm{d}E} - \frac{\mathrm{d}\mathbf{s}_{\alpha\beta}^\dagger}{\mathrm{d}E} \mathbf{s}_{\alpha\beta} \right] \tag{8}$$

from which we obtain the injectance of contact α

$$N(\mathbf{r}, \beta) = \frac{1}{2\pi i} \sum_\alpha \mathrm{Tr} \left[\mathbf{s}_{\alpha\beta}^\dagger \frac{\mathrm{d}\mathbf{s}_{\alpha\beta}}{\mathrm{d}E} \right] \tag{9}$$

the emittance into contact α,

$$N(\alpha) = \frac{1}{2\pi i} \sum_\beta \mathrm{Tr} \left[\mathbf{s}^\dagger_{\alpha\beta} \frac{\mathrm{d}\mathbf{s}_{\alpha\beta}}{\mathrm{d}E} \right] \tag{10}$$

and the global density of states

$$N = \sum_\alpha N(\alpha) = \frac{1}{2\pi i} \sum_{\alpha\beta} \mathrm{Tr} \left[\mathbf{s}^\dagger_{\alpha\beta} \frac{\mathrm{d}\mathbf{s}_{\alpha\beta}}{\mathrm{d}E} \right]. \tag{11}$$

The scattering matrix is unitary and all its eigenvalues $\lambda_i = \exp(i\zeta_i)$ are on the unit circle. In terms of these eigenvalues we have

$$N = \frac{1}{2\pi} \sum_i \frac{\mathrm{d}\zeta_i}{\mathrm{d}E} = \frac{1}{2\pi} \frac{\mathrm{d}}{\mathrm{d}E} \log[\det(\mathbf{s})], \tag{12}$$

where $\det(\mathbf{s})$ is the determinant of the scattering matrix.

Equation (12) is a familiar expression of the density of states [14–16]. We recall it here to emphasize that it is an approximate expression for the density of states of a mesoscopic conductor. In nuclear scattering theory [14,15] it is turned into an exact expression, not by considering the total density of states like we have done but the excess density of states in comparison to a free problem and by taking the volume of interest to infinity. (The problem with and without a scattering object are compared.) In contrast to our type of scattering problems (for instance for a multiprobe mesoscopic conductor) there is no reasonably defined free problem and similarly it would be meaningless to consider the volume of interest to become infinitely large. Therefore in mesoscopic physics the exact expression for the density of states of the sample is [4,11]

$$N = \int_\Omega \mathrm{d}\mathbf{r}^3 \nu(\mathbf{r}) = -\frac{1}{2\pi i} \int_\Omega \mathrm{d}\mathbf{r}^3 \sum_{\alpha\beta} \mathrm{Tr} \left[s^\dagger_{\alpha\beta} \frac{\delta s_{\alpha\beta}}{e \delta U(\mathbf{r})} \right] \tag{13}$$

whereas the more familiar expression (12) is an approximation.

Except in very special cases the two expressions for the local density need not to be distinguished. However the difference is important when WKB does not hold. For instance using eq. (12), the density of states inside a rectangular tunneling barrier of height U_0 diverges to $E^{-1/2}$ as the kinetic energy E of the incident particles tends to zero. If one uses eq. (13) one finds (the much more reasonable result) that the density of states is finite and vanishes as $E^{1/2}$ for small energies [17]. The distinction between energy derivatives and potential derivatives is familiar from the discussion of characteristic tunneling times [17–20]. For a discussion of the connection between the local partial density of states and characteristic tunneling times we refer the reader to ref. [21].

4. Absorption and emission of particles: Injectivities and emissivities

We next present a simple example which illustrates the usefulness of the densities of states introduced above. Suppose the potential has in some small volume element Ω a small imaginary part [22–24]. Then the potential is $U(\mathbf{r})$ outside Ω but is $U(\mathbf{r}) - i\hbar\Gamma$ inside Ω. To

proceed we take into account that the scattering matrix is a functional of the potential and expand the scattering matrix to first order in Γ. This gives the transmission and reflection probabilities in the presence of a small absorption [22]

$$T_{\alpha\beta}(\Gamma) = T_{\alpha\beta} \left(1 - \int_{\Omega} d\mathbf{r}\, \Gamma\, \nu(\alpha, \mathbf{r}, \beta) \right), \tag{14}$$

where $T_{\alpha\beta}$ is the transmission probability of the scattering problem without absorption if α and β are different. If α and β are equal, we find a reflection probability

$$R_{\alpha\alpha}(\Gamma) = R_{\alpha\alpha} \left(1 - \int_{\Omega} d\mathbf{r}\, \Gamma\, \nu(\alpha, \mathbf{r}, \alpha) \right). \tag{15}$$

Thus in the presence of absorption the reflection and transmission probabilities are 'diminished' according to the partial density of states. Consider now the carriers streaming from contact β into the sample in a narrow energy interval dE. The incident current I_{in} must be equal to the sum of the transmitted current I_T, the reflected current I_R and the absorbed current I_Γ,

$$I_{in} = I_T + I_R + I_\Gamma. \tag{16}$$

Taking into account that the total incident current from contact α is $I_\beta = (e/h)M_\beta dE$, and also taking into account that $\sum_{\alpha \neq \beta} T_{\alpha\beta} + R_{\beta\beta} = M_\beta$ we find that the total absorbed flux is given by the sum

$$I_\Gamma = \int_{\Omega} d\mathbf{r}\, \Gamma\, \nu(\mathbf{r}, \beta). \tag{17}$$

Thus the absorbed flux is determined by the injectivity of contact β into the volume of interest.

Another way of determining the absorbed flux proceeds as follows: The absorbed flux is proportional to the integrated density of particles in the region of absorption. The density of particles can be found from the scattering state $\psi_{\beta m}(\mathbf{r})$ which describes carriers incident from contact β in the channel m. The wave function is normalized such that it has unit amplitude in the incident channel. We assume that all incident channels in contact β are filled equally. The absorbed flux is thus [22]

$$I_\Gamma(\beta) = \int d\mathbf{r}\, \Gamma \sum_m \frac{1}{h v_\beta} |\psi_{\beta m}(\mathbf{r})|^2. \tag{18}$$

Note here that the density of states $1/h v_{\beta m}$ of the asymptotic scattering region appears. $v_{\beta m}$ is the velocity of carriers in the incident channel. Thus we have found a wave function representation for the injectivity. Comparing eqs (15) and (14) gives

$$\nu(\mathbf{r}, \beta) = \sum_m \frac{1}{h v_{\beta m}} |\psi_{\beta m}(\mathbf{r})|^2. \tag{19}$$

The total local density of states $\nu(\mathbf{r})$ at point $\mathbf{r}$ is obtained by considering carriers incident from both contacts.

There is now an interesting additional problem to be addressed. Instead of a potential which acts as a carrier sink (as an absorber) we can ask about a potential which acts as a carrier source. Obviously, all we have to do to turn our potential into a carrier source is to change the sign of the imaginary part of the potential. As a consequence of a carrier source in the volume Ω we should observe a particle current into all contacts of our sample. To find these currents we consider a small energy interval at the energy of interest. The total current injected into the sample in Ω is

$$I_{\text{in}}(y) = \int_{\Omega} d\mathbf{r} \, \Gamma \, \nu(\mathbf{r}). \tag{20}$$

Taking into account that the incident current is normalized to 1 the current $I_{\text{out}}(\beta)$ in contact β due to a carrier source in Ω is given by

$$I_{\text{out}}(\alpha) = (e/h)dE \left[M_\alpha - R_{\alpha\alpha}(\Gamma) - \sum_{\beta \neq \alpha} T_{\alpha\beta}(\Gamma) \right] \tag{21}$$

due to the modification of both the transmission and reflection coefficients. Using eqs (14) and (15) (with Γ replaced by $-\Gamma$) gives

$$I_{\text{out}}(\alpha) = - \int_{\Omega} d\mathbf{r} \, \Gamma \sum_{\beta} \nu(\alpha, \mathbf{r}, \beta) = - \int_{\Omega} d\mathbf{r} \, \Gamma \, \nu(\alpha, \mathbf{r}). \tag{22}$$

The current in contact α is determined by the *emissivity* $\nu(\alpha, \mathbf{r})$ of the region Ω into contact α.

We conclude this section with a remark of caution. The partial densities are not necessarily positive as we would expect from the usual density of states. (A simple example of an (asymmetric) resonant double barrier shows that one of the diagonal elements $\nu(\alpha, \mathbf{r}, \alpha)$ has a range of energies where it is negative [22]. Note that this implies that a small absorption inside a sample can *increase* the reflection probability). The fact that the partial density of states are not necessarily positive is a consequence of over specification: both the incident and the exiting channels are prescribed. In contrast, the injectivities and emissivities are, however, always positive. The proof is given by eq. (17).

5. Generalized Bardeen formulae

It is well-known that with a scanning tunneling microscope (STM) we can measure the local density of states [25]. STM measurements are typically performed in a two terminal geometry, in which the tip of the microscope represents one contact and the sample provides another [25]. Here we are interested in the transmission probability from an STM tip into the contact of a sample with two or more contacts as shown in figure 1. Geometries which use more than one tunneling tip are also of interest [26,27]. Thus we deal with a multiterminal transmission problem [10]. If we denote the contacts of the sample by a Greek letter $\alpha = 1, 2, \ldots$ and use *tip* to label the contact of the STM tip, we are interested in the tunneling probabilities $T_{\alpha\text{tip}}$ from the tip into contact α of the sample. In this case the STM tip acts as carrier source. Similarly we ask about the transmission probability $T_{\text{tip}\alpha}$ from a sample contact to the tip. In this case the STM tip acts as a carrier sink. Earlier

work has addressed this problem either with the help of electron wave dividers [28,29], or by applying the Fermi golden rule [8]. Recently, Gramespacher and the author [10] have returned to this problem and have derived expressions for these transmission probabilities from the scattering matrix of the full multiprobe problem [9] (sample plus tip). For a tunneling contact with the density of states ν_{tip} which couples locally at the point x with a coupling energy $|t|$ they found

$$T_{\text{tip},\alpha} = 4\pi^2 \nu_{\text{tip}} |t|^2 \nu(x,\alpha), \tag{23}$$

$$T_{\alpha\text{tip}} = 4\pi^2 \nu(\alpha,x) |t|^2 \nu_{\text{tip}}. \tag{24}$$

In a multiterminal sample the transmission probability from a contact α to the STM tip is given by the injectivity of contact α into the point x and the transmission probability from the tip to the contact α is given by the emissivity of the point x into contact α. Equations (23) and (24) when multiplied by the unit of conductance e^2/h are generalized Bardeen conductances for multiprobe conductors. Since the local density of states of the tip is an even function of magnetic field and since the injectivity and emissivity are related by reciprocity we also have the reciprocity relation $T_{\text{tip},\alpha}(B) = T_{\alpha,\text{tip}}(-B)$.

The presence of the tip also affects the transmission and the reflection at the massive contacts of the sample. The first order in the coupling energy $|t|^2$ of these probabilities are given by

$$T_{\alpha\beta}^{\text{tip}} = T_{\alpha\beta} - 4\pi^2 \nu(\alpha,x,\beta) |t|^2 \nu_{\text{tip}}. \tag{25}$$

Here the upper index tip indicates that this transmission probability is calculated in the presence of the tip. $T_{\alpha\beta}$ without an upper index is the transmission probability in the absence of the tip. The correction to the transmission probabilities $\alpha \neq \beta$ and reflection probabilities $\alpha = \beta$ is determined by the partial densities of states, the coupling energy and the density of states in the tip. Note that if these probabilities are placed in a matrix then each row and each column of this matrix adds up to the number of quantum channels in the contacts.

6. Voltage probe and inelastic scattering

Consider a two-probe conductor much smaller than any inelastic or phase breaking length. The conductance of such a conductor can then be said to be coherent and its conductance is at zero temperature given by the Landauer formula $G = (e^2/h)T$, where T is the probability for transmission from one contact to the other. How is this result affected by events which break the phase or by events which cause inelastic scattering? To investigate this question ref. [30] proposes an additional (third) contact to the sample. The third probe acts as a voltage probe which has its potential adjusted in such a way that there is no net current flowing into this additional probe, $I_3 = 0$. The current at the third probe is set to zero by floating the voltage $\mu_3 = eV_3$ at this contact to a value for which I_3 vanishes. The third probe acts, therefore, like a *voltage probe*. Even though the total current at the voltage probe vanishes individual carriers can enter this probe if they are at the same time replaced

by carriers emanating from the probe [30]. Entering and leaving a contact are *irreversible* processes, since there is no definite phase relationship between a carrier that enters the contact and a carrier that leaves a contact. In a three probe conductor, the relationship between currents and voltages is given by $I_\alpha = \sum_\beta G_{\alpha\beta} V_\beta$ where the $G_{\alpha\beta}$ are the conductance coefficients. Using the condition $I_3 = 0$ to find the potential V_3 and eliminating this potential in the equation for I_2 or I_1 gives for the two-probe conductance in the presence of the voltage probe

$$G = - \left(G_{21} + \frac{G_{23}G_{31}}{G_{31} + G_{32}} \right). \tag{26}$$

For a very weakly coupled voltage probe (see figure 1) we can use eqs (23)–(25). Taking into account that $G_{\alpha\beta} = -(e^2/h)T_{\alpha\beta}^{\text{tip}}$ for $\alpha \neq \beta$ we find

$$G = \frac{e^2}{h} \left(T - 4\pi^2 |t|^2 \left[\nu(2,x,1) - \frac{\nu(2,x)\nu(x,1)}{\nu(x)} \right] \right). \tag{27}$$

Here $\nu(x)$ is the local density of states at the location of the point at which the voltage probe couples to the conductor. Equation (27) has a simple interpretation [30]. The first term T is the transmission probability of the conductor in the absence of the voltage probe. The first term inside the brackets proportional to the local partial density of states gives the reduction of coherent transmission due to the presence of the voltage probe. The second term in brackets is the incoherent contribution to transport due to inelastic scattering induced by the voltage probe. It is proportional to the injectivity of contact 1 at point x. A fraction $\nu(2,x)/\nu(x)$ of the carriers which reach this point, proportional to its emissivity, are scattered forward and, therefore, contribute to transport. Notice the different signs of these two contributions. The effect of inelastic scattering (or dephasing) can either enhance or diminish transport, depending on whether the reduction of coherent transmission (first term) or the increase due to incoherent transmission (second term) dominates.

Instead of a voltage probe, we can also use an optical potential to simulate inelastic scattering or dephasing. However, in order to preserve current, we must use both an absorbing optical potential (to take carriers out) and an emitting optical potential (to reinsert carriers). The absorbed and re-emitted current must again exactly balance each other [31]. From eq. (15) it is seen that the coherent current is again diminished by $\Gamma\nu(2,x,1)$, i.e. by the partial density of states at point x. The total absorbed current is proportional to $\Gamma\nu(x,1)$, the injectance of contact 1 into this point. As shown in §4 a carrier emitting optical potential at x generates a current $-\Gamma\nu(1,x)$ in contact 1 and generates a current $-\Gamma\nu(2,x)$ in contact 2. It produces a total current $-\Gamma\nu(x)$. If the generated and the absorbed current are equal we have to normalize the emitting optical potential [21] such that it generates a total current proportional to $\Gamma\nu(x,1)$. The current produced by an optical potential normalized in such a way is thus $-\Gamma\nu(2,x)\nu(x,1)/\nu(x)$. The sum of the two contributions [21] – the absorbed current and the re-emitted current gives an overall transmission (or conductance) which is given by eq. (27) with $4\pi|t|^2$ replaced by Γ.

Thus the weakly coupled voltage probe (which has built-in current conservation) and a discussion based on optical potentials coupled with a current conserving re-insertion of carriers are equivalent [31]. There are discussions in the literature which invoke optical potentials but do not re-insert carriers. Obviously, such discussions violate current conservation. Even if current is conserved, the partitioning of the reinserted carriers has to be

done as described above. Otherwise such fundamental properties like the Onsager symmetry are violated [32].

We would like to point out that there is in general no reason that tunnel contacts and absorption and re-emission with the help of imaginary potentials lead to identical results. The equivalence rests on a particular description of the voltage probe. There are many different ways of coupling a tunnel contact and our description of the voltage probe given here is not unique. The claim can only be that for sufficiently weak optical absorption and re-insertion of carriers there exists *one* voltage probe model which gives the same answer.

7. The Friedel sum rule

The connection between the phase shift of scattering elements and the charge is known as Friedel sum rule. It is most often stated as a global relation between the charge in an energy interval dE and the derivatives of the scattering phases with respect to energy as

$$\mathrm{d}Q/\mathrm{d}E = \frac{e}{2\pi} \sum_i \frac{\mathrm{d}\zeta_i}{\mathrm{d}E} = \frac{e}{2\pi} \frac{\mathrm{d}}{\mathrm{d}E} \log[\det(\mathbf{s})]. \tag{28}$$

From the discussion at the end of §4 it is evident that this relation is not exact since in the applications envisioned here the scattering matrix and the phases are calculated for a finite volume Ω. Thus whenever WKB does not hold eq. (28) will also not hold. The exact relation follows from eq. (19) and eqs (5) and (6) and is given by

$$\nu(\mathbf{r}) = \sum_{\beta m} \frac{1}{h v_{\beta m}} |\psi_{\beta m}(\mathbf{r})|^2 = -\frac{1}{2\pi i} \sum_i \frac{\delta \zeta_i}{e \delta U(\mathbf{r})}$$

$$= -\frac{1}{2\pi i} \sum_{\alpha\beta} \mathrm{Tr} \left[s^\dagger_{\alpha\beta} \frac{\delta s_{\alpha\beta}}{e \delta U(\mathbf{r})} \right]. \tag{29}$$

This relation is *locally* exact and by integration can be applied to any volume of interest. Application of eq. (28) to situations in which WKB does not hold has already given rise to statements in the literature that the Friedel sum rule does not apply in mesoscopic conductors [33].

8. The charge response to an internal potential

We next discuss problems for which the self-consistent adjustment of the potential is important. With this goal in mind we first investigate the variation of the local carrier density $\delta n(\mathbf{r})$ in response to a local potential variation $\delta U(\mathbf{r}')$ at a point $\mathbf{r}'$. This variation is given by the Lindhard function, $\delta n(\mathbf{r}) = - \int \mathrm{d}\mathbf{r}'^3 \Pi(\mathbf{r},\mathbf{r}') e\delta U(\mathbf{r}')$. This function plays an important role if we want to determine the carrier distribution self-consistently. Since the local charge density at equilibrium is $n(\mathbf{r}) = \int \mathrm{d}E \nu(\mathbf{r}) f(E)$, it follows immediately that the Lindhard function is given by

$$\Pi(\mathbf{r},\mathbf{r}') = - \int \mathrm{d}E \frac{\delta \nu(\mathbf{r})}{e \delta U(\mathbf{r}')} f(E). \tag{30}$$

This response now involves second order functional derivatives of the scattering matrix. It can be simplified, if we are interested in potential variations not on the microscopic scale but only over distances large compared to a Fermi wavelength λ_F. In that case we can integrate the Lindhard function over its second argument over a volume that is large compared to a Fermi wavelength and use the WKB formula which replaces the functional derivative with respect to $U(\mathbf{r}')$ with an energy derivative. This gives

$$\Pi(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') \int dE \frac{d\nu(\mathbf{r})}{dE} f(E). \tag{31}$$

Partial integration with respect to the energy E gives

$$\Pi(\mathbf{r}',\mathbf{r}) = \delta(\mathbf{r}'-\mathbf{r}) \int dE \nu(\mathbf{r}) \left(-\frac{df(E)}{dE} \right). \tag{32}$$

Over sufficiently large distances the Lindhard function is determined by the local density of states.

9. The local charge response of a mesoscopic conductor

Consider a small deviation $\delta\mu_\alpha = \mu_\alpha - \mu$ of the electrochemical potential μ_α of contact α away from its equilibrium value μ. At fixed internal potential this increases the carrier density inside the conductor by $\delta n(\mathbf{r}) = \nu(\mathbf{r},\alpha)\delta\mu_\alpha$. This injected charge generates due to the Coulomb interaction an electrostatic response $\delta U(\mathbf{r})$ which via the Lindhard function will also give a contribution to the charge density. Thus the local carrier density is [5]

$$\delta n(\mathbf{r}) = \sum_\alpha \nu(\mathbf{r},\alpha)\delta\mu_\alpha - \int d\mathbf{r}'^3 \Pi(\mathbf{r}',\mathbf{r})\delta U(\mathbf{r}'). \tag{33}$$

Suppose all potentials $\delta\mu_\alpha$ applied to the conductor are increased by the same amount $\delta\mu$. Since the state of a conductor can only be changed by voltage differences it follows that the electrostatic potential also increases by $\delta U(\mathbf{r}') = \delta\mu$ and that $\delta n(\mathbf{r}) = 0$. As a consequence of this gauge invariance we have [5]

$$\sum_\alpha \nu(\mathbf{r},\alpha) = \nu(\mathbf{r}) = \int d\mathbf{r}'^3 \Pi(\mathbf{r}',\mathbf{r}). \tag{34}$$

The spatial integral over one of the arguments of the Lindhard function is equal to the local density of states. Note that eq. (30) is a symmetric function of its spatial arguments.

To bring the determination of the local charge response to an end, we must now insert eq. (33) into the Poisson equation and solve for the potential $\delta U(\mathbf{r}')$. Suppose that a test charge at point $\mathbf{r}'$ generates at point $\mathbf{r}$ a potential $g(\mathbf{r},\mathbf{r}')$. Here $g(\mathbf{r},\mathbf{r}')$ is the Green's function of the Poisson equation with a non-local screening kernel determined by the Lindhard function mentioned above. The injected charge $e\nu(\mathbf{r},\alpha)\delta\mu_\alpha$ generates the potential $u_\alpha(\mathbf{r})\delta\mu_\alpha$ where the characteristic potential [5] $u_\alpha(\mathbf{r})$ is given by

$$u_\alpha(\mathbf{r}) = \int d\mathbf{r}'^3 g(\mathbf{r},\mathbf{r}')\nu(\mathbf{r}',\alpha). \tag{35}$$

The injectivity is the source term of the characteristic potential $u_\alpha(\mathbf{r})$. With the help of the characteristic potentials the internal potential can be expressed in linear response to the applied electrochemical potentials. Using this, the local carrier distribution is found to be

$$\delta n(\mathbf{r}) = \sum_\alpha v^{\text{tot}}(\mathbf{r}, \alpha) \delta \mu_\alpha \tag{36}$$

with a screened density of states [5]

$$v^{\text{tot}}(\mathbf{r}, \alpha) = v(\mathbf{r}, \alpha) - \int d\mathbf{r}'^3 d\mathbf{r}''^3 \Pi(\mathbf{r}, \mathbf{r}') g(\mathbf{r}', \mathbf{r}'') v(\mathbf{r}'', \alpha). \tag{37}$$

Equation (36) provides a gauge invariant description of the local carrier density in response to small variations of the potentials applied to the contacts of the sample. The total variation of the charge is zero, $\int_\Omega d\mathbf{r} \delta n(\mathbf{r}) = 0$, for a volume Ω that is sufficiently large (encloses the entire sample).

10. Dynamic conductance

In this section we discuss briefly as an additional application of partial density of states the ac-conductance of mesoscopic systems. We consider a conductor with an arbitrary number of contacts labeled by a Greek index $\alpha = 1, 2, 3....$ The problem is to find the relationship between the currents $I_\alpha(\omega)$ at frequency ω measured at the contacts of the sample in response to a sinusoidal voltage with amplitude $V_\beta(\omega)$ applied to contact β. The relationship between currents and voltages is given by a dynamical conductance matrix [4,5] $G_{\alpha\beta}(\omega)$ such that $I_\alpha(\omega) = \sum_\beta G_{\alpha\beta}(\omega) V_\beta(\omega)$. All electric fields are localized in space. The overall charge on the conductor is conserved. Consequently, current is also conserved and the currents depend only on voltage differences. Current conservation implies $\sum_\alpha G_{\alpha\beta} = 0$ for each β. In order that only voltage differences matter, the dynamical conductance matrix has to obey $\sum_\beta G_{\alpha\beta} = 0$ for each α. We are interested here in the low frequency behavior of the conductance and therefore we can expand the conductance in powers of the frequency [5]

$$G_{\alpha\beta}(\omega) = G_{\alpha\beta}^0 - i\omega E_{\alpha\beta} + K_{\alpha\beta} \omega^2 + O(\omega^3). \tag{38}$$

Here $G_{\alpha\beta}^0$ is the dc-conductance matrix. $E_{\alpha\beta}$ is called the *emittance* matrix and governs the displacement currents. $K_{\alpha\beta}$ gives the response to second order in the frequency. All matrices $G_{\alpha\beta}^0, E_{\alpha\beta}$ and $K_{\alpha\beta}$ are real.

We focus here on the emittance matrix $E_{\alpha\beta}$. The conservation of the total charge can only be achieved by considering the long-range Coulomb interaction. To first order in frequency it is precisely the charge distribution given by eq. (36) which counts. Reference [5] finds for the emittance matrix

$$E_{\alpha\beta} = e^2 \left[\int d\mathbf{r} v(\alpha, \mathbf{r}, \beta) - \int d\mathbf{r}' d\mathbf{r} v(\alpha, \mathbf{r}') g(\mathbf{r}', \mathbf{r}) v(\mathbf{r}, \beta) \right]. \tag{39}$$

Here the first term which is proportional to the integrated partial density of states is the ac-response at low frequencies which we would have in the absence of interactions. The

second term has the following simple interpretation: an ac-voltage applied to contact β would (in the absence of interactions) lead to a charge built up at a point $\mathbf{r}$ given by the injectivity of contact β. Due to interaction, this charge generates at point $\mathbf{r}'$ a variation in the local potential which then induces a current in contact α proportional to the emissivity of this point into contact α. Note, that if screening is local (over a length scale of a Thomas Fermi wavelength) we have $g(\mathbf{r}', \mathbf{r}) = \delta(\mathbf{r}' - \mathbf{r})v^{-1}(\mathbf{r})$. In this limit the close connection between eqs (39) and (24) is then obvious. We have to refer the reader to reviews [34,35] for a more extended discussion and for references to specific applications of eq. (39).

A closely related development which could be discussed here is a theory of quantum pumping in small systems. In quantum pumping one is interested in the current generated as two parameters (like gate voltages, magnetic flux) which modulate the system to be varying sinusoidally but out of phase. Brouwer [36], Avron *et al* [37], and Polianski and Brouwer [38] developed a theory which is based on the slow modulation of the partial densities of states.

11. Partial density of states matrix

So far we have been interested in the charge distribution inside a mesoscopic conductor which is established in response to changes in the external parameters, such as a voltage applied to the contact of the sample. Similar to the dynamic fluctuations of the current away from its average value, we can also ask about the fluctuations of the charge away from its average value. Spontaneous dynamic fluctuations of current and charge can have many sources in an electrical conductor. Here we are concerned with contributions which are fundamental in the sense that they cannot be avoided. Nyquist or thermal noise cannot be avoided at any elevated temperature. A second source, shot noise results from the granularity of charge (the charge quantization) and the quantum mechanical uncertainty arises whenever there are different possible outcomes of a scattering process [3] (such as the possibility of a particle to be either reflected or transmitted).

To describe the charge fluctuations due to carriers in the conductor [6], we consider the Fermi field

$$\hat{\Psi}(\mathbf{r},t) = \sum_{\alpha m} \int dE \frac{\psi_{\alpha m}(\mathbf{r},E)}{(hv_{\alpha m}(E))^{1/2}} \hat{a}_{\alpha m}(E) \exp(-iEt/\hbar), \tag{40}$$

which annihilates an electron at point $\mathbf{r}$ and time t. The Fermi field eq. (40) is built up from all the scattering states $\psi_{\alpha m}(\mathbf{r},E)$ which have unit incident amplitude in contact α in channel m. The operator $\hat{a}_{\alpha m}(E)$ annihilates an incident carrier in the reservoir α in channel m. $v_{\alpha m}$ is the velocity in the incident channel m in the reservoir α. The local carrier density at point $\mathbf{r}$ and time t is determined by $\hat{n}(\mathbf{r},t) = \hat{\Psi}^{\dagger}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)$. We will investigate the density operator in the frequency domain, $\hat{n}(\mathbf{r},\omega)$. Using the Fermi field we find

$$\hat{n}(\mathbf{r},\omega) = \sum_{\alpha m \beta n} \int dE \frac{1}{(hv_{\alpha m}(E))^{1/2}} \frac{1}{(hv_{\beta n}(E + \hbar\omega))^{1/2}}$$
$$\times \psi^{*}_{\alpha m}(\mathbf{r},E)\psi_{\beta n}(\mathbf{r},E + \hbar\omega)\hat{a}^{\dagger}_{\alpha m}(E)\hat{a}_{\beta n}(E + \hbar\omega). \tag{41}$$

This equation defines the *density of states matrix* $\nu_{\beta\gamma}(\mathbf{r})$ with elements

$$v_{\gamma\delta mn}(\mathbf{r},E,E+\hbar\omega) = h^{-1}(v_{\gamma m}(E)v_{\delta n}(E+\hbar\omega))^{-1/2}$$
$$\times \psi_{\gamma m}^*(\mathbf{r},E)\psi_{\delta n}(\mathbf{r},E+\hbar\omega). \tag{42}$$

If we form a vector $\mathbf{a}_\alpha$ with the annihilation operators of the (incoming) channels in contact $\mathbf{a}_\alpha$ the local density operator in the low frequency limit can be expressed with the help of this matrix in the following way:

$$\hat{n}(\mathbf{r},\omega) = \sum_{\alpha\beta} \int dE \hat{\mathbf{a}}_\alpha^\dagger(E) v_{\alpha\beta}(\mathbf{r})\hat{\mathbf{a}}_\beta(E+\hbar\omega). \tag{43}$$

It is now very convenient and instructive to consider an expression for the density operator not in terms of wave functions but more directly in terms of the scattering matrix. In the zero-frequency limit, ref. [6] introduces the matrix

$$v_{\beta\gamma}(\alpha,\mathbf{r}) = -\frac{1}{4\pi i}\left[\mathbf{s}_{\alpha\beta}^\dagger\frac{\delta\mathbf{s}_{\alpha\gamma}}{e\delta U(\mathbf{r})} - \frac{\delta\mathbf{s}_{\alpha\beta}^\dagger}{e\delta U(\mathbf{r})}\mathbf{s}_{\alpha\gamma}\right]. \tag{44}$$

All quantities in this expression are evaluated at the Fermi energy E. The matrix elements of eq. (42) are connected to the matrices $v_{\beta\gamma}(\alpha,\mathbf{r})$ (and thus to wave functions) via [6]

$$v_{\gamma\delta}(\mathbf{r}) = \sum_\alpha v_{\beta\gamma}(\alpha,\mathbf{r}) = -\frac{1}{2\pi i}\sum_\alpha \left(s_{\alpha\beta}^\dagger\frac{\delta s_{\alpha\gamma}}{e\delta U(\mathbf{r})}\right). \tag{45}$$

Equation (45) is a *local* Wigner–Smith life-time matrix [14].

Equation (45) was given in ref. [6] and a derivation of this relation with the help of an optical potential is given in detail in ref. [35]. The relation between scattering states and the Green's function of the Schrödinger equation on one hand and its connection to the scattering matrix on the other hand can also be used [39,40]. Recently Schomerus *et al* [41] proposed yet another way to proceed by using not the overall scattering matrix but scattering matrices for different portions of the system.

It is important to realize that in an electrical conductor charge fluctuations are not free but are screened like the average charge density. Inserting eq. (43) into the Poisson equation with the non-local screening kernel determines a potential operator [6]

$$\hat{u}_{\alpha\beta}(\mathbf{r},\omega) = \int d\mathbf{r}' g(\mathbf{r},\mathbf{r}')\hat{\mathbf{a}}_\alpha^\dagger(E) v_{\alpha\beta}(\mathbf{r}')\hat{\mathbf{a}}_\beta(E+\hbar\omega). \tag{46}$$

In random phase approximations the potential fluctuations give rise to induced charge fluctuations. Thus the true low frequency charge fluctuations in a conductor are determined by the contribution of the bare charge fluctuations and the induced charge fluctuations. This gives rise to a charge fluctuation operator [6]

$$\hat{v}_{\alpha\beta}^{\text{tot}}(\mathbf{r},\omega) = \hat{v}_{\alpha\beta}(\mathbf{r},\omega) - \int d\mathbf{r}'\Pi(\mathbf{r},\mathbf{r}')\hat{u}_{\alpha\beta}(\mathbf{r}',\omega). \tag{47}$$

Equation (47) permits a gauge invariant discussion of charge fluctuations in mesoscopic conductors. Equation (47) has been used in ref. [6] to obtain the second order in frequency term of the ac-conductance (see eq. (38)). For a capacitive structure this defines a novel resistance which determines the dissipative effects in charging and discharging a

mesoscopic conductor. Pedersen, van Langen and the author [42] investigated the current induced into a nearby gate due to charge fluctuations in quantum point contacts and chaotic cavities. More recently, the charge fluctuations in two nearby mesoscopic conductors [43] were treated and the effect of quantum dephasing due to charge fluctuations was calculated within this approach [35,44]. Often self-consistent effects are neglected [39,45]. Charge correlations at two contacts capacitively coupled to a mesoscopic structure are investigated in ref. [46].

Integration of eq. (45) over the volume of the sample gives the global Wigner–Smith life-time matrix. In contrast to the local Wigner–Smith matrix the properties of the (global) Wigner–Smith life-time matrix have received wider attention. In recent years the focus has been on the calculation of the entire distribution function of delay times [47] for structures whose dynamics is in the classical limit chaotic (chaotic cavities) and of one-dimensional wires [41,48,49]. While in many cases an analysis of the global density is quite sufficient, in disordered structures, since screening is local, it is clearly desirable to proceed from the local density and to investigate the properties of the local Wigner–Smith matrix given here.

12. Discussion

We have discussed a hierarchy of density of states as they occur in open multiprobe meso-scopic conductors. We have illustrated that a small absorption or a small emission of particles leads naturally to the appearance of these density of states. We have shown that the transmission probabilities through weakly coupled contacts, like the STM, is related to these densities. We have shown that a weakly coupled voltage probe, describing inelastic scattering or a dephasing process can be described in terms of these densities. We have given a formulation of the Friedel sum rule which holds even when the conditions for the WKB approximation do not apply. We have also pointed out that the ac-conductance of a mesoscopic conductor at small frequencies can be formulated in terms of these densities of states. Furthermore, we have indicated that it is useful to consider also the off-diagonal elements of the partial density of states matrix since this permits a description of fluctuation processes. This consideration has led us to the local Wigner–Smith life-time matrix. We have emphasized that for many problems in electrical conductors, it is necessary to consider the effect of screening. We have treated screening in a simple one-loop random phase approximation.

The partial density of states which we have used here provide a classification with respect to the contact (and/or channel) index of the scattering matrix. In problems with high spatial symmetry [50] we can also envision a classification with respect to the local momentum. Interest in spin transport will require spin resolved partial density of states. In hybrid normal superconducting systems [51] a resolution of both electron and hole density of states is conceptually useful [52,53].

The description of electrical conduction processes in terms of transmission and reflection probabilities has become well-known. The fact that we can also express densities with the help of scattering matrices makes the scattering approach applicable not only to dc-transport but to a much wider range of electrical transport phenomena.

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