On observing electron-electron attraction
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Abstract: In a startling discovery it has been recently found that certain density of states can become negative in mesoscopic systems wherein electrons can travel back in time. We give a brief introduction to the hierarchy of density of states in mesoscopic systems as we want to point out some robust phenomenon that can be experimentally observed with our present day technologies. They can have direct consequences on thermodynamic effects and also can provide indirect evidence of time travel. Essentially certain members of the hierarchy become negative in these regimes and that has consequences.

Introduction
We will look at a novel approach to response of a mesoscopic sample to applied fields. We will provide a brief introduction to a hierarchy of Friedel sum rule like formulas that consist of local partial density of states, emissivity, injectivity, injectance, emittance, partial density of states, and finally the well known local density of states and the density of states. Except for the last two there are no known analogues for bulk systems that are treated within the scope of statistical mechanics. And then we will show how the lower members of the hierarchy play a crucial role in determining observations related to an STM tip probing a mesoscopic sample without making an actual contact and by making a contact. It has been proved recently [1] that some members of this hierarchy can become negative because partial electrons in these states can move back in time. And we will present here some simple ways to probe that experimentally and related consequences.

The system
In the figure 1 we show a typical mesoscopic sample which is the shaded region. It can have several leads attached to it that are indexed \( \alpha, \beta, \gamma, \delta \), etc and the shaded region between the leads retain single particle quantum coherence. As has been already hinted in the section above these lead indices appear in all the formulas to be discussed below showing the importance of these leads in mesoscopic systems. The \( \beta \)th lead is drawn in a special way signifying the tip of an STM tip. The STM tip can have four possible functions. First is that it does not make an actual contact and also does not draw or deliver any current but can locally change the electrostatic potential at a point \( \mathbf{r} \). Second is that it does not make a contact but can draw or deliver a current via quantum tunneling. Third is that it makes an actual contact and becomes like any other lead. Fourth is that it makes a contact and yet does not draw or deliver a current because its chemical potential is so adjusted. Below we will detail and define the hierarchy of density of states and then discuss some applications with respect to this schematic diagram of the sample.
Fig. 1. We show a mesoscopic set up where there are many leads $\alpha, \beta, \gamma, \delta$ etc., attached to a sample. The lead $\beta$ is special in the sense that it is an STM tip that can deliver (or draw) current to (or from) a particular point $\mathbf{r}$ in the sample. All other leads (minimum one other) are fixed and draw (or deliver) current from (or to) the sample.

### Hierarchy of mesoscopic formulas

In this section we discuss a hierarchy of relations between scattering phase shifts and DOS. It starts with Larmor precession time given as

$$\tau_{lpt}(E, \alpha, \mathbf{r}, \gamma) = -\frac{\hbar}{4\pi i |s_{\alpha\gamma}(E)|^2} \left[ s_{\alpha\gamma}^* \frac{\delta s_{\alpha\gamma}}{\epsilon \delta U(\mathbf{r})} - \frac{\delta s_{\alpha\gamma}^*}{\epsilon \delta U(\mathbf{r})} s_{\alpha\gamma} \right]$$  \hspace{1cm} (1)

A detailed derivation of this formula is given in reference [1]. $\frac{\delta s_{\alpha\gamma}}{\epsilon \delta U(\mathbf{r})}$ is a functional derivative of $s_{\alpha\gamma}$ with respect to the local potential $U(\mathbf{r})$. Thus we define local partial density of states (LPDOS) $\rho_{lpd}$ in the same sense as it is defined on a 1D line as $\frac{|s_{\alpha\gamma}(E)|^2}{\hbar} \tau_{lpt}$.

$$\rho_{lpd}(E, \alpha, \mathbf{r}, \gamma) = \frac{1}{4\pi i} \left[ s_{\alpha\gamma}^* \frac{\delta s_{\alpha\gamma}}{\epsilon \delta U(\mathbf{r})} - \frac{\delta s_{\alpha\gamma}^*}{\epsilon \delta U(\mathbf{r})} s_{\alpha\gamma} \right]$$  \hspace{1cm} (2)

One may see this from the theory of Green’s function whose imaginary part gives the time of propagation as well as the number of states accessed in the propagation within a factor of $\hbar$. The $|s_{\alpha\gamma}(E)|^2$ is also easy to understand. Electrons in an ensemble are indistinguishable fermions that occupy one state each at zero temperature. At a given incident energy $E$, electrons that are incident along input channel $\gamma$ form a quantum ensemble. Every member of the ensemble is not scattered to output channel $\alpha$. But those that are scattered to output channel $\alpha$, are done with an amplitude of $s_{\alpha\gamma}$ which means for unit incident flux there are exactly $|s_{\alpha\gamma}|^2$ of them and each of them occupy a state. Doubling the input flux in $\gamma$ will double the number of electrons that are scattered to channel $\alpha$ as long as we are not in the limiting situation of a completely filled band. We cannot get linear superposition of states in the input channels.
that can be argued \[1\]. Note that \( \rho_{lpd} \) is only defined between two prescribed leads which in the above formula are \( \alpha \) and \( \gamma \). As per convention of matrix multiplication the second index \( \gamma \) is always the incoming channel and the first index \( \alpha \) is the outgoing as the scattering matrix connects the outgoing wave vector to the incoming wave vector. Numerical simulations \[3\] suggest that Eq. 2 is also valid in presence of electron-electron interaction in the sample. We get partial density of states by integrating (physically this implies averaging) \( \rho_{lpd}(E, \alpha, r, \gamma) \) over the spatial coordinates of the sample.

\[
\rho_{lpd}(E, \alpha, \gamma) = -\frac{1}{4\pi i} \int_{\Omega} d^3r \left[ s_{\alpha\gamma}^* \frac{\delta s_{\alpha\gamma}}{e\delta U(r)} - \frac{\delta s_{\alpha\gamma}^*}{e\delta U(r)} s_{\alpha\gamma} \right]
\]

(3)

Here \( \Omega \) stands for the spatial region of the sample that is the shaded area in figure 1. To get injectivity \( \rho_i \) of a specific lead \( \gamma \) we sum \( \rho_{lpd} \) in Eq. 2 over all possible outgoing channels \( \alpha \).

\[
\rho_i(E, r, \gamma) = -\frac{1}{4\pi i} \sum_{\alpha} \left[ s_{\alpha\gamma}^* \frac{\delta s_{\alpha\gamma}}{e\delta U(r)} - \frac{\delta s_{\alpha\gamma}^*}{e\delta U(r)} s_{\alpha\gamma} \right]
\]

(4)

Similarly to get emissivity \( \rho_e \), we sum \( \rho_{lpd} \) in Eq. 2 over all possible incoming channels \( \gamma \).

\[
\rho_e(E, \alpha, r) = -\frac{1}{4\pi i} \sum_{\gamma} \left[ s_{\alpha\gamma}^* \frac{\delta s_{\alpha\gamma}}{e\delta U(r)} - \frac{\delta s_{\alpha\gamma}^*}{e\delta U(r)} s_{\alpha\gamma} \right]
\]

(5)

Injectivity (or emissivity) is an important member of the hierarchy. It is like a correlation function between two spatial points \( \gamma \) and coordinate \( r \) where the lead index \( \gamma \) is actually a spatial index signifying the spatial point where the lead is attached. Hopefully, something like an STM tip can affect a single point \( r \) in its closest approximation and can be used to change the local potential at a point infinitesimally (i.e., \( \delta U(r) \)) without any tunneling between the tip and the sample. If such an STM tip delivers a current into the sample where the current can leave through one or many leads then the current delivered can be related to injectivity of the STM tip \( \beta \). Such a set up can be made and injectivity can be measured. However, the definition of injectivity holds in general even when a lead is partially bringing current and partially taking current away with some imbalance between the two. But here we are talking about the specific experimental set up that is explained in more detail in Fig 1. We have shown \[1\] that injected current will see this DOS in the hierarchy. What \( \rho_i \) in Eq. 4 means is that for those particular electrons that are coming from lead \( \gamma \) irrespective of to which lead it is going, the relevant part of DOS at the point \( r \) is \( \rho_i(E, \gamma, r) \).

Injectivity or emissivity can be integrated over \( r \) to give higher members of the hierarchy called injectance and emittance. Injectance can thus be defined as from Eq. 4 (or from Eq. 3)

\[
\rho(E, \gamma) = -\frac{1}{4\pi i} \int_{\Omega} d^3r \sum_{\alpha} \left[ s_{\alpha\gamma}^* \frac{\delta s_{\alpha\gamma}}{e\delta U(r)} - \frac{\delta s_{\alpha\gamma}^*}{e\delta U(r)} s_{\alpha\gamma} \right]
\]

(6)

Local density of states (LDOS) can be defined by summing the RHS of Eq. 2 over \( \alpha \) and \( \gamma \).

\[
\rho_{ld}(E, r) = -\frac{1}{4\pi i} \sum_{\alpha\gamma} \left[ s_{\alpha\gamma}^* \frac{\delta s_{\alpha\gamma}}{e\delta U(r)} - \frac{\delta s_{\alpha\gamma}^*}{e\delta U(r)} s_{\alpha\gamma} \right]
\]

(7)
Integrating this over \( r \) we obtain

\[
\rho_d(E) = -\frac{1}{4\pi i} \sum_{\alpha \gamma} \int_{\text{sample}} d^3r \left[ s^*_\alpha \frac{\delta s_{\alpha \gamma}}{\delta U(r)} - \frac{\delta s^*_\alpha}{\delta U(r)} s_{\alpha \gamma} \right] \tag{8}
\]

\[
\rho_d(E) = -\frac{1}{2\pi} \sum_{\alpha \gamma} \int_{\text{sample}} d^3r \left[ |s_{\alpha \gamma}|^2 \frac{\delta \theta_{\alpha \gamma}}{\delta U(r)} \right] \tag{9}
\]

This is the mesoscopic version of Friedel sum rule that relates scattering phase shift to DOS. In this equation too we get the functional derivative of the scattering phase shift with respect to the local potential \( r \) along with an integration over \( r \) and so this is not of much use to an experimentalist or theory as \( U(r) \) is unknown. One may consider the following substitution

\[
\int_{\text{global}} dr \frac{\delta}{\delta U(r)} = -\frac{d}{dE} \tag{10}
\]

On substituting this in Eq. 9 we get the FSR that appears in textbooks but this substitution is an approximation. Eq. 10 implies that the global integration on LHS means the potential can be increased (or decreased) by a constant amount globally which is identical to not shifting the potential but decreasing (or increasing) the incident energy. An experimentalist can easily achieve this by changing the Fermi energy but what appears in Eq. 9 is not a global integration but a sample integration. For a large bulk system one need not make a difference between the two but for a mesoscopic system we may only write

\[
\int_{\text{sample}} dr \frac{\delta}{\delta U(r)} \approx -\frac{d}{dE} \tag{11}
\]

Thus

\[
\rho_d(E) \approx \frac{1}{2\pi} \sum_{\alpha \gamma} \left[ |s_{\alpha \gamma}|^2 \frac{d\theta_{\alpha \gamma}}{dE} \right] \tag{12}
\]

As we have discussed, injectance is essentially an injected current. We know injected current is of the form \( nev \) or differential current is \( \frac{dn}{dE} evdE \). Electronic charge \( e \) can be set to unity and if properly normalized wave-functions are taken then we can also drop the \( v \) factor making injected current to be \( \frac{dn}{dE} \) at an energy \( E \). Now that can be determined from internal wavefunction when just the \( \gamma \)th lead carries current into the system and all other leads take current away from the system. That gives

\[
\rho(E, \gamma) = \int_{\text{sample}} dx dy \sum_{k \gamma} |\psi(x, y, \gamma)|^2 \delta(E - E_{\gamma, k}) = \int d^3r \sum_{\alpha} -\frac{1}{2\pi} \left[ |s_{\alpha \gamma}|^2 \frac{\delta s_{\alpha \gamma}}{\delta U(r)} \right] \tag{13}
\]

In 1D it was argued that the correction term to the substitution in Eq. 11 can be determined to give

\[
\rho(E, 1) = \frac{1}{2\pi} \left[ |r|^2 \frac{d\theta_r}{dE} |t|^2 \frac{d\theta_t}{dE} + \frac{m_e |r|}{\hbar k^2} \sin(\theta_r) \right] \tag{14}
\]
which means the last term is the correction term to the semiclassical formula due to interference effects. If we consider a semi-classical regime where the electron behaves like a classical particle then $\sin(\theta_r)$ goes to zero and we recover the textbook FSR (in fact in practice ensemble averaging washes out any dependence on $\sin(\theta_r)$ and make large systems effectively behave semi-classically).

Mesoscopic response

In this section we will consider a particular case wherein the sample is connected to only two leads $\alpha$ and $\gamma$ as shown in Fig. 2. The STM tip is again called the lead $\beta$. Let us consider the situation when the tip of $\beta$ is not making a physical contact with the sample but close enough to deliver (or draw) a current to (or from) the sample by tunneling. The two leads $\alpha$ and $\gamma$ have fixed chemical potentials $\mu_\alpha$ and $\mu_\gamma$, respectively. It is their chemical potentials that determine if current will go from $\alpha$ to $\gamma$ or the reverse and we assume $\mu_\gamma > \mu_\alpha$. So now if the STM tip is close to a point of the sample whose coordinate is say, $r$, then we can find that the transmission probability of the STM tip is strongly dependent on the exact coordinate $r$ and is given by the following expressions that correspond to different cases.

$$T_{\beta\alpha} = 4\pi^2 \nu_\beta |t|^2 \rho_i(E, r, \alpha) \quad (16)$$
$$T_{\alpha\beta} = 4\pi^2 \nu_\beta |t|^2 \rho_i(E, \alpha, r) \quad (17)$$
$$T_{\beta\gamma} = 4\pi^2 \nu_\beta |t|^2 \rho_i(E, r, \gamma) \quad (18)$$
$$T_{\gamma\beta} = 4\pi^2 \nu_\beta |t|^2 \rho_i(E, \gamma, r) \quad (19)$$

For example, $T_{\beta\alpha}$ is contribution of lead $\alpha$ to emission taking place through lead $\beta$ and it is proportional to the injectivity of lead $\alpha$ to the remote point $r$. Others can be similarly interpreted. Here $\nu_\beta$ is the density of states in the lead $\beta$ that couple to the states at the point $r$ through the coupling parameter $t$. Details of this can be found in reference [2]. Eqs. 16 and 18 correspond to current drawn by the lead $\beta$ while Eqs. 17 and 19 corresponds to that delivered by lead $\beta$. So the individual formulas are not of much physical significance as the total current emitted through lead $\beta$ will be ($T_{\beta\alpha} + T_{\beta\gamma} - T_{\alpha\beta} - T_{\gamma\beta}$).

Now coming back to the set up in Fig. 2 again with the lead $\beta$ not making an actual contact but allowing tunneling to or from the sample we want to address the issue of current flowing from $\gamma$ to $\alpha$. The lead $\beta$ thus interacts with the quantum states in the sample at the local point $r$ and changes the quantum states in the sample which is viewed as decoherence of the states in the sample. So the role of $\beta$ is to provide or remove electrons from the system by tunneling as well as causing some decoherence. At $0^\circ$K, consider a current going from lead $\gamma$ to lead $\alpha$ in the energy interval $(\mu_\gamma - \mu_\alpha)$, then the coherent current is a measurable quantity that is proportional to [2]

$$|S_{\gamma\alpha}^f|^2 = |S_{\alpha\gamma}|^2 - 4\pi^2 |t|^2 \nu_\beta \rho_{pd}(E, \alpha, r, \gamma) \quad (20)$$

This measurable quantity therefore directly depends on the local partial density of states. Here $|S_{\gamma\alpha}^f|^2$ is the transmission probability from $\gamma$ to $\alpha$ when $\beta$ is
Fig. 2 The STM tip making an actual contact with the sample at point $r$ and $\mu_\beta$ is so adjusted that there is no net current flowing through the STM tip. One can put an Aharonov-Bohm flux through the sample as well.

present and $|S_{\alpha\gamma}|^2$ is that when $\beta$ is removed. Transmission probability multiplied by a factor $\frac{e^2}{h}$ gives the measured conductance. So $|S_{\alpha\gamma}|^2$ and $|S_{\alpha\gamma}|^2$ are both measurable and so in relative proportions $\rho_{lpd}(E, \alpha, r, \gamma)$ is also measurable. It suggests that in quantum mechanics one can ascribe a real number to the point $r$ for a process in which an electron goes from initial state $\gamma$ to a final state $\alpha$ that contributes to the partial density of states at the point $r$ for the process. So this is a local formulation of quantum mechanics. Intuitively, one would think that $\rho_{lpd}$ is positive definite and so the conductance in presence of the lead $\beta$ is always less than that in the coherent situation. Here it is difficult to isolate the effect of decoherence due to lead $\beta$. Never the less, recent works show that $\rho_{lpd}$ can be designed to be negative \[1\] by creating Fano resonances and using this set up we can confirm its negativity.

In a situation wherein the probe $\beta$ makes an actual contact with the sample we get a three probe set up and also the probe $\beta$ is made like a voltage probe in the sense that its chemical potential is so adjusted that it does not draw any net current from or into the system. This leads to the celebrated Landauer-Buttiker three probe conductance given by

$$G = -G_{\alpha\gamma} - \frac{G_{\alpha\beta}G_{\beta\gamma}}{G_{\beta\alpha} + G_{\beta\gamma}}$$ \hspace{1cm} (21)

Here

$$G_{\alpha\beta} = \frac{e^2}{h} |S_{\alpha\beta}|^2 \hspace{0.5cm} \text{for} \hspace{0.5cm} \alpha \neq \beta \hspace{0.5cm} \text{etc.}$$ \hspace{1cm} (22)

This formula can be rewritten in terms of the hierarchy of the density of states in the following way \[2\].

$$G = \frac{e^2}{h} \left( |S_{\alpha\gamma}|^2 - 4\pi^2 |t|^2 \rho_{lpd}(\alpha, r, \gamma) + 4\pi^2 |t|^2 \rho_{e}(\alpha, r) \rho_{i}(r, \gamma) \rho_{ld}(r) \right)$$ \hspace{1cm} (23)

Note that in the above formula if the lead $\beta$ is completely removed then $|t|^2 = 0$ and we will be left with only the first of the three terms. This is
the standard two probe Landauer conductance formula. So the three terminal formula of Eqn.(21) is now restated in the form of Eqn.(23). The second term comes with a negative sign and unless $\rho_{lpd}$ is designed to be negative, accounts for the loss of coherent electrons due to the lead $\beta$. This loss affects only those partial electrons that are going from $\gamma$ to $\alpha$, coherently. It is proportional to the local partial density of states at the point $r$ means again it is related to only those partial electrons going from $\gamma$ to $\alpha$ at the point $r$.

The lost coherent electrons will be reinjected into the system as after all the lead $\beta$ is not carrying away any net current from the system. The fraction of reinjected electrons going towards $\alpha$ will not be the same as that going towards $\gamma$. So the question arises what will be the ratio and this will again be determined by the members of the hierarchy. This contribution is the third term separately written below and it is in fact the incoherent contribution in the conductance from $\gamma$ to $\alpha$.

$$4\pi^2|t|^2 \frac{\rho_e(\alpha, r) \rho_i(r, \gamma)}{\rho_{ld}(r)}$$ (24)

Note that it is proportional to injectivity of lead $\gamma$ to the remote point $r$ and its larger value can only enhance incoherent current going from $\gamma$ to $\alpha$. The ratio $\frac{\rho_e(\alpha, r)}{\rho_{ld}(r)}$ also determine this current. Emissivity of the remote point $r$ to lead $\alpha$ will enhance this incoherent current. Thus the coherent 2nd term and the incoherent third term can be easily measured separately as the coherent term will depend on an Aharonov-Bohm flux while the incoherent term will not. And again if the second term is designed to be negative its negativity can be experimentally confirmed.

To understand the denominator in Eq. 24 let us consider the following. Total number of incoherent electrons reinjected at the point $r$ must be

$$4\pi^2|t|^2 \frac{\rho_e(\alpha, r) \rho_i(r, \gamma)}{\rho_{ld}(r)} + 4\pi^2|t|^2 \frac{\rho_e(\gamma, r) \rho_i(r, \gamma)}{\rho_{ld}(r)}$$ (25)

$$= 4\pi^2|t|^2 \frac{(\rho_e(\alpha, r) + \rho_e(\gamma, r)) \rho_i(r, \gamma)}{\rho_{ld}(r)}$$ (26)

The first term in Eq. 25 is just the term in Eq. 24 and gives the fraction of reinjected incoherent electrons at $r$ that goes to $\alpha$ and the second term is that which goes to $\gamma$. Which means Eq. 26 give the total reinjected incoherent current from $\beta$. Given the fact that $\rho_e(\alpha, r) + \rho_e(\gamma, r) = \rho_{ld}(r)$, the total reinjected incoherent current in Eq. 26 is simply proportional to $\rho_i(r, \gamma)$. This is the quantity that has to be balanced against the chemical potential of the lead $\beta$ so that lead $\beta$ does not draw or deliver any net current. This is a situation wherein we are at 0$^0$K and in the regime of incident energy $E$ being such that $\mu_\gamma > E > \mu_\alpha$. In this regime there is no injectance from lead $\alpha$.

**Summary**

Now $\rho_{lpd}$ in the second term of Eq. 23 that involves electrons going from $\gamma$ to $\alpha$ via the point $r$, is obviously a coherent term. While the third term involves a product of two terms coming from two different processes and so do not involve electrons that are directly going from $\gamma$ to $\alpha$. The electrons contributing to $\rho_i(r, \gamma)$ can be different from the electrons contributing to $\rho_e(\alpha, r)$. 

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So Aharonov-Bohm effect can be used to separately measure these two terms. Strangely enough if $\rho_{lpd}$ is made negative then the second term in Eq. 23 becomes positive implying the system draws in coherent electrons to the point $r$ instead of loosing them to the voltage probe and this can be considered as experimental proof of electron-electron attraction due to change of sign of density of states. This can be also interpreted as loosing coherent electrons in reverse time The same signature can also be seen from Eq. 20 which too can be experimentally verified. A negative number of states accommodating negatively charged electrons can behave as a positive charge cloud.

References

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