From the Kubo formula to variable range hopping

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Consider a multichannel closed ring with disorder. In the semiclassical treatment its conductance is given by the Drude formula. Quantum mechanics challenge this result both in the limit of strong disorder (eigenstates are not quantum-ergodic in real space) and in the limit of weak disorder (eigenstates are not quantum-ergodic in momentum space). Consequently the analysis of conductance requires going beyond linear response theory, leading to a resistor network picture of transitions between energy levels. We demonstrate that our semi-linear response theory provides a firm unified framework from which the "hopping" phenomenology of Mott can be derived.

I. INTRODUCTION

The theory for the conductance of *closed* mesoscopic rings has attracted a lot of interest[1,2,3,4,5,6,7,8,9,10,11,12]. In a typical experiment[13] a collection of mesoscopic rings are driven by a time dependent magnetic flux $\Phi(t)$ which creates an electro-motive-force (EMF) $-\dot{\Phi}$ in each ring. Assuming that Ohm's law applies, the induced current is $I = -G\dot{\Phi}$ and consequently Joule's law gives

$$\dot{\mathcal{W}} \;=\; G\,\dot{\Phi}^2 \;=\; \text{rate of energy absorption} \qquad (1)$$

where G in this context is called the conductance. For diffusive rings the Kubo formula leads to the Drude formula for G. A major challenge in past studies was to calculate the weak localization corrections to the Drude result, taking into account the level statistics and the type of occupation[10,11,12]. It should be clear that these corrections do not challenge the leading order Kubo-Drude result.

One wonders what happens to the Drude result if the disorder becomes weak (ballistic case) or strong (Anderson localization case). In both cases the individual eigenfunction become non ergodic: a typical eigenfunction do not fill the whole accessible phase space. In the ballistic case a typical eigenfunction is not ergodic over the open modes in momentum space, while in the strong localization case it is not ergodic over the ring in real space.

Lack of quantum ergodicity implies that the perturbation matrix is very structured and/or sparse. Consequently the calculation of G requires a non-trivial extension of linear response theory (LRT). Such extension has been proposed in Ref.[14] and later termed "semi linear response theory" (SLRT)[15]. Within SLRT it is still assumed that the transitions between levels are given by Fermi-golden-rule, but a resistor network analogy is used in order to calculate the overall absorption. In order to have non-zero absorption we must have *connected sequences of transitions*. Thus the calculation of the energy absorption in Eq.(1) is somewhat similar to solving a percolation problem. The "percolation" is in energy space rather than in real space.

In a previous work we have worked out results for G in the case of a ballistic ring[16]. In this work we would like to explore the other extreme case of strong disorder. If we go to the literature we find a strange twist. For the AC conductance Mott[17] (see also[18]) has used the Kubo formula in order to predict $\sim \omega^2|\log(\omega)|^{d+1}$ dependence of the conductivity, where $d = 1, 2, 3$ is the dimensionality of the sample. On the other hand for the DC calculation Mott has abandoned the Kubo formalism and has adopted a phenomenological variable range hopping (VRH) picture[19], which can be regarded as an approximation for a more elaborated (but still phenomenological) resister network picture[20,21,22]. The "ad hoc" approach to hopping is obviously bothering. For example it is not clear whether the effect of low frequency noisy driving should treated like "low temperature" or like "small frequency"[23]. The main purpose of this Letter is to explain that the hopping picture is a natural outcome of SLRT, and hence can be regarded as a natural extension of LRT. This automatically resolves such conceptual problems, and opens the way for further refinements of the theory.

The outline of this Letter is as follows: We summarize the LRT and the SLRT recipes for the calculation of the conductance. Then we demonstrate that all the known results for the conductance can be derived from the same theoretical framework, without any extra assumptions.

II. THE MODEL PARAMETERS:

We consider a ring of length L and mean free path ℓ. The particles are non-interacting "spinless" electrons with charge e. The Fermi energy and the Fermi velocity are E_F and $v_{\rm F}$ respectively. The one-particle density of states at the Fermi energy is

$$\varrho_{\rm F} = \text{GeometricFactor} \times \mathcal{M}\frac{L}{\pi\hbar v_{\rm F}} \qquad (2)$$

The number of open modes $\mathcal{M}$ reflects the cross section of the ring. The GeometricFactor depends on the dimensionality $d = 1, 2, 3$ and equals unity for $d = 1$ network systems. In what follows, for sake of presentation, and without loss of generality, we set in all expressions the $d = 1$ geometric factor, and use units such that $\hbar = 1$.

The mean level spacing is $\Delta = \varrho_{\rm F}^{-1}$. This is the "small" energy scale. We also have the "Thouless energy" or its equivalent which we denote as Δ_b. For ballistic ring $\Delta_b = \mathcal{M}\Delta$ is associated with the time scale $L/v_{\rm F}$, while

in the diffusive regime $\Delta_b = (\ell/L)\mathcal{M}\Delta$ is associated with the ergodic time. In the strong disorder regime we shall see that the relevant time scale for our analysis is the breaktime t^* which is related to the localization length ℓ_ξ.

Within the framework of both LRT and SLRT it is essential to realize that the combined effect of the driving and the environment is to *"broaden"* the energy levels and to induce *"relaxation"*. Accordingly we distinguish between Γ which can be interpreted as the dephasing or decoherence rate (analogous to $1/T_2$ in NMR studies), and $\gamma_{\rm rlx}$ which is the relaxation rate (analogous to $1/T_1$ in NMR studies). We assume that Γ is much larger than Δ but much smaller compared with Δ_b. We also assume that the driving source is "essentially DC driving". This means that the driving frequency is much smaller compared with Δ_b. LRT applies whenever the driven transitions are much slower compared with the relaxation rate. SLRT is an extension of LRT that applies in the opposite circumstances, namely if the relaxation process can be neglected during the time that the absorption rate get stabilized. This is explained in length in[14], and will be emphasized again in a later paragraph.

III. THE SEMICLASSICAL LRT CALCULATION:

The semiclassical Kubo formula once expressed with the velocity-velocity correlation function is

$$G = \varrho_{\rm F} \times \frac{1}{2}\left(\frac{e}{L}\right)^2 \int_{-\infty}^{\infty} \langle v(t)v(0)\rangle dt \tag{3}$$

where v is the velocity of the particle along the ring. For the purpose of later reference we note that Eq.(1) [with Eq.(3) substituted] is easily generalized to the case where the driving is noisy. Instead of a multiplication by $\dot{\Phi}^2$ we have in general an integration over the all the Fourier components of the driving. Namely,

$$\dot{\mathcal{W}} = \varrho_{\rm F} \times \frac{1}{2}\left(\frac{e}{L}\right)^2 \int_{-\infty}^{\infty} d\omega\, \tilde{F}(\omega)\, \tilde{C}(\omega) \tag{4}$$

where $\tilde{C}(\omega)$ is the Fourier transform of the velocity-velocity correlation function, and $\tilde{F}(\omega)$ is the power spectrum of $\dot{\Phi}(t)$.

The Kubo formula parallels the expression for the spatial diffusion coefficient, which is the integral over the velocity-velocity correlation function:

$$\mathcal{D} = \frac{1}{2}\int_{-\infty}^{\infty} \langle v(t)v(0)\rangle dt \tag{5}$$

In the case of pure DC driving ($F(\omega) = \dot{\Phi}^2\delta(\omega)$) one obtains the Einstein relation:

$$G = \varrho_{\rm F}\left(\frac{e}{L}\right)^2 \mathcal{D} \tag{6}$$

If the driving is noisy, then in general $G > \varrho_{\rm F}(e/L)^2\mathcal{D}$. This reflects the simple observation that an insulator ($\mathcal{D} \sim 0$) may have a finite AC conductance (finite $\dot{\mathcal{W}}$).

IV. THE QUANTUM LRT CALCULATION:

Eq.(4) is formally valid also in the quantum mechanical case, and can be regarded as the outcome of the Fermi-Golden-rule picture. However one should use the proper expression for $\tilde{C}(\omega)$, taking into account the levels statistics and the level broadening:

$$\tilde{C}_{\rm qm}(\omega) = R(\omega)\tilde{C}_{\rm cl}(\omega) \tag{7}$$

$$\tilde{C}(\omega) \approx \delta_\Gamma(\omega) \star \tilde{C}_{\rm qm}(\omega) \tag{8}$$

where $R(\omega)$ takes care for the level statistics, $\delta_\Gamma(\omega)$ is the line shape of the level broadening, and $\star$ indicates a convolution. It should be clear that with pure DC driving Eq.(4) gives zero due to the discreteness of the energy spectrum, unless there is some mechanism that "broadens the levels" so as to have effectively a continuum. It is customary to express the quantum version of the Kubo formula using the matrix elements of the velocity operator:

$$G = \pi\hbar\left(\frac{e}{L}\right)^2 \sum_{n\neq m} |v_{mn}|^2\ \delta_T(E_n - E_F)\ \delta_\Gamma(E_m - E_n) \tag{9}$$

The T broadened delta should be interpreted as the derivative of the Fermi occupation function, while the functional shape of the Γ broadened delta function will be discussed later.

V. THE QUANTUM SLRT CALCULATION:

A loose way to write the last expression is

$$G = \pi\hbar\left(\frac{e}{L}\right)^2 \varrho_{\rm F}^2\ \langle\langle |v_{nm}|^2\rangle\rangle \tag{10}$$

The interpretation of $\langle\langle ...\rangle\rangle$ within the framework of the tradition LRT is implied by Eq.(9). It involves the specification of the level broadening parameter Γ and of the occupation temperature T.

The implicit assumption in LRT is that the driving induced transitions are much slower compared with the environmentally induced relaxation. In other words it is assumed that the relaxation is very effective in "killing" any quantum effect that goes beyond first order perturbation theory. SLRT, unlike LRT is aimed in taking account also the opposite circumstances in which the possibility to make connected sequences of transitions becomes essential in order to get absorption[14]. Following[15,16] we regard the energy levels as the nodes of a resistor network. We define

$$\mathsf{g}_{nm} = 2\varrho_{\rm F}^{-3}\ \frac{|v_{nm}|^2}{(E_n - E_m)^2}\ \delta_\Gamma(E_m - E_n) \tag{11}$$

Then it is argued that $\langle\langle |v_{nm}|^2\rangle\rangle^{-1}$ is the resistivity of the network. It is a simple exercise to verify that if all the matrix elements are the same, say $|v_{nm}|^2 = \sigma^2$, then $\langle\langle |v_{nm}|^2\rangle\rangle = \sigma^2$ too. But if the matrix is structured or sparse then $\langle\langle |v_{nm}|^2\rangle\rangle$ is in general much smaller compared with the RMS value of the matrix elements.

VI. LEVEL BROADENING:

Neither LRT nor SLRT are self contained without the specification of the level broadening. For the purpose of analysis we can regard the environmental fluctuations as a noisy driving source. This driving source induces decoherence: It can be argued (see for example Ref.[24]) that the effect of decoherence is to multiply the velocity-velocity correlation function by an exponential factor $\exp(-\Gamma|t|)$. This means that

$$\delta_\Gamma(\omega) \approx \frac{1}{\pi}\frac{\Gamma}{\omega^2+\Gamma^2} \tag{12}$$

It can be further argued[24] that an estimate of the rate Γ can be obtained using the Fermi golden rule (FGR):

$$\Gamma = \int_{-\infty}^{\infty} d\omega\, \tilde{F}(\omega)\, \tilde{C}_{\rm qm}(\omega) \tag{13}$$

where $\tilde{F}(\omega)$ is the power spectrum of the environmentally induced noise. At low temperatures (see later) the noise power spectrum is effectively very narrow. Schematically we can write $\tilde{F}(\omega)=\epsilon^2\delta_T(\omega)$, where ϵ is the noise amplitude, and T is the temperature.

The FGR expression Eq.(13) parallels Eq.(4), and can be expressed using the matrix elements of the perturbation as in Eq.(9), or it can be written loosely in the style of Eq.(10):

$$\Gamma = \epsilon^2 \times 2\pi\hbar \left(\frac{e}{L}\right)^2 \varrho_{\rm F}\ \langle\langle |v_{nm}|^2\rangle\rangle \tag{14}$$

The latter version is common in elementary textbooks (the FGR calculated decay rate is proportional to the squared matrix element times the density of states). It is implicit in this expression that the FGR transitions $\delta(E_m-E_n)$ have a width (broadening) which is determined by the normalized power spectrum of the environmental fluctuations.

So far we simply re-stated the standard textbook version of FGR using our notations. But it should be clear that the naive application of the FGR recipe is as problematic as the the naive application of the Kubo formula[25]: the first order (transient) transitions to "neighboring" states are not enough in order to get a non-transient decay. Rather, the possibility to have *connected sequences* of transitions is essential in order to have a long time decay. Thus we conclude that an analogous SLRT recipe, with g_{nm} defined in a similar fashion as in Eq.(11), should be applied in order to determine the long time value of Γ. We point out again that in the calculation of Γ the role of the broadened delta is played by the normalized power spectrum of the environmental fluctuations. This means that at low temperatures (see further discussion in a later paragraph) we have in the Γ oriented version of Eq.(11) a thermally broadened delta function $\delta_T(E_m-E_n)$.

VII. MODERATE DISORDER:

The effect of hard chaos or disorder is to randomize the velocity. Within the framework of the semiclassical LRT calculation we always get the Drude formula irrespective of the strength of the disorder. Following Drude it is customary to write

$$\langle v(t)v(0)\rangle\Big|_{\rm cl} = v_{\rm F}^2 \exp\left[-2\left(\frac{v_{\rm F}}{\ell}\right)|t|\right] \tag{15}$$

or equivalently

$$\tilde{C}_{\rm cl}(\omega) = v_{\rm F}^2\ \frac{(2v_{\rm F}/\ell)}{\omega^2+(2v_{\rm F}/\ell)^2} \tag{16}$$

This leads to the Drude result

$$G = \frac{e^2}{2\pi\hbar}\mathcal{M}\frac{\ell}{L} \tag{17}$$

Once we turn to the quantum calculation, we have to be more careful. For moderate disorder the eigenfunctions are ergodic, and therefore the distinction between the LRT recipe and the SLRT recipe is not important. Furthermore, using a random wave conjecture for the eigenstates, one recovers the Drude expression $\tilde{C}_{\rm cl}(\omega)$ as an approximation for the quantum $\tilde{C}(\omega)$. In order to do a better job, the spectral function $R(\omega)$ is introduced. This function takes into account the level statistics: for large ω it equals unity, while for small ω it reflects the repulsion between levels. The "level broadening" effect is taken care of by the convolution with $\delta_\Gamma(\omega)$, as indicated in Eq.(8). The standard LRT regime is having $\Delta \ll \Gamma \ll \Delta_b$. In this regime the introduction of $R(\omega)$ implies so-called weak localization corrections to the Drude result. These are found to be of order Δ/Γ. See Refs.[10,11,12], and also[26] for the "quantum chaos" point of view.

VIII. WEAK DISORDER:

The SLRT recipe for the calculation of G can be regarded as an extension of the LRT recipe. The results of SLRT become very different from those of LRT once the perturbation matrix v_{nm} is either structured or sparse. The case of weak disorder (ballistic case) has been analyzed in a previous Letter[16]. In the non trivial ballistic regime ($1 \ll \ell/L \ll \mathcal{M}$) each eigenfunctions occupy a large but finite fraction of open modes. One may say that the eigenfunctions are "localized" in mode space. This lack of quantum-ergodicity implies sturctures and sparsity. Consequently the SLRT result is not merely a small weak localization correction: the leading order result is no longer Drude. In what follows we address the other extreme case of strong disorder (Anderson localization case). Also here we are going to see that the leading order result is not Drude.

IX. STRONG DISORDER:

The first step is to figure out how $R(\omega)$ look like for a system with strong localization. The initial spread of a wavepacket is diffusive with $\langle (x(t)-x(0))^2\rangle = 2\mathcal{D}_0 t$ where $\mathcal{D}_0 = v_{\rm F}\ell$. But for long time $\langle (x(t)-x(0))^2\rangle = \ell_\xi^2$, where ℓ_{xi} is the localization length. This implies a breaktime at $t^* = \ell_\xi^2/\mathcal{D}_0$, and therefore the velocity-velocity correlation function is modified in the frequency range $|\omega| < (1/t^*)$. Namely, the above implies

$$R(\omega)\Big|_{\rm global} \;\approx\; \frac{1}{1+(t^*\omega)^{-2}} \tag{18}$$

Further considerations which are based on Mott's picture of resonances imply an extra $|\log\omega|^{d+1}$ factor at small frequencies. We can argue in advance that this type of correction has no importance in SLRT because it reflects a very sparse contribution to the perturbation matrix, that cannot lead to connected sequences of transitions.

Even if we eliminate Mott's resonances, still the low frequency behavior of $\tilde{C}(\omega)$ reflects a very sparse matrix $|v_{nm}|^2$. Within the framework of SLRT the sparse component of $|v_{nm}|^2$ does not contribute to the diffusion. Only the non-sparse component allows *connected sequences of transitions*. We argue that the non sparse component is obtained by multiplying $\tilde{C}_{\rm cl}(\omega)$ by

$$R(\omega)\Big|_{\rm effective} \;\approx\; \exp\left[-\left(\frac{\Delta_\xi}{|\omega|}\right)^{1/d}\right] \tag{19}$$

The reasoning is as follows: The matrix elements of states n that are located within range $|x_n - x_m| < r$ from a given state m constitute a connected grid with spacing $\Delta_r = (L/r)^d\Delta$ and typical value $|v_{nm}| \propto \exp(-r/\ell_\xi)$. From the equation $\Delta_r = \omega$ we deduce that the "volume" of states that contribute a connected grid for ω transitions has a radius $r = (\Delta/\omega)^{1/d}L$. Hence we deduce the above formula, where $\Delta_\xi = (L/\ell_\xi)^d\Delta$.

X. THE HOPPING PICTURE:

Assuming that the coherence time $\tau_\gamma = 1/\Gamma$ is much smaller compared with the breaktime t^* we observe that the $d\omega$ integral of Eq.(4) with (7-8) and the Lorentzian of (12) is dominated by the tail $[\omega > (1/t*)]$ leading to the result

$$\mathcal{D} \;\approx\; \Gamma t^*\mathcal{D}_0 \;=\; \frac{(\ell_\xi)^2}{\tau_\gamma} \tag{20}$$

This is as expected from heuristic considerations. It describes a random walk hopping process with steps of size ℓ_ξ and time τ_γ.

The issue is to obtain an explicit expression for Γ. Thermal noise is "white" at high temperatures ($F(\omega) \propto T$), with a very large temperature-independent cutoff frequency. In such case Eq.(13) implies $\Gamma \propto T$ which is not very interesting. Low temperature noise, unlike white noise, has an exponentially decaying emission tail, and consequently, it has effectively a very narrow span of frequencies:

$$F(\omega) \;\sim\; \exp\left(-\frac{|\omega|}{T}\right) \tag{21}$$

In the above expression we have neglected ω^α term whose exponent depends of the detailed spectral properties of the bath. The calculation of Γ with Eq.(13) involves a $d\omega$ integral over

$$\exp\Big[-\frac{|\omega|}{T}\Big] \times \exp\Big[-\left(\frac{\Delta_\xi}{|\omega|}\right)^{1/d}\Big] \tag{22}$$

This is mathematically equivalent to the VRH integral[19]. There the optimization is over the range of the hopping r, while here it is over the associated frequency ω. The optimal frequency is $\omega \propto T^{d/(d+1)}$ leading to the VRH estimate $\mathcal{D} \propto \exp[(-T_0/T)^{1/(1+d)}]$ where T_0 is a constant. It should be clear that the VRH estimate is an approximation for the resistor network calculation with Eq.(11). The VRH estimate works quite well for $d > 1$, but gives the wrong exponent ($T^{-1/2}$) for $d = 1$. The correct exponent (T^{-1}) in the latter case is implied by the absence of percolation.

XI. CONCLUSIONS:

We have established that SLRT provides a firm unified framework for the calculation of the conductance. Ad hock phenomenology is not required in order to establish the resistor network "hopping" picture, from which Mott's VRH approximation is derived. It should be clear that the generalized resistor network picture of SLRT is not limited to the strong disorder regime: it allows *on equal footing* the calculation of the conductance in the other extreme case of ballistic motion. The importance of this approach is also in its potential capabilities: being a natural extension of LRT it also allows, in principle, the incorporation of many-body effects. In the latter case the calculation of conductance is reduced, as in LRT, to the analysis of the matrix elements of the current operator, whatever are the interactions involved.

XII. ACKNOWLEDGMENT:

The apparent inconsistency between the hopping/VRH picture and the Kubo AC/DC formalism, and the question how to reconcile between them, have been pointed out by Michael Wilkinson in the late nineties. The issue has been raised again in his 2005 visit in BGU, while discussing the extension of the Kubo formalism that has been presented in Ref.[14]. This discussion has initiated further refinement of the theory[15]

in collaboration with him and with Bernhard Mehlig. The belief that the theory can give hopping/VRH has been shared by all of us and was implicitly expressed in[15]. Prior to submission of this manuscript I have been notified that during the last year MW and BM have made independently further progress on SLRT in general and possibly on this issue in particular (undocumented). The research was supported by a grant from the DIP, the Deutsch-Israelische Projektkooperation.

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