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 challenges 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 semilinear response theory provides a firm unified framework from which the "hopping" phenomenology of Mott can be derived.

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I. INTRODUCTION

The theory of the conductance of *closed* mesoscopic rings has attracted a lot of interest.[1–12] In a typical experiment[13] a collection of mesoscopic rings are driven by a time-dependent magnetic flux $\Phi(t)$ which creates an electromotive 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

$$\dot{\mathcal{W}} = G\dot{\Phi}^2 = \text{rate of energy absorption}, \tag{1}$$

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.[10–12] 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 eigenfunctions become nonergodic: a typical eigenfunction does 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.

A lack of quantum ergodicity implies that the perturbation matrix is very structured and/or sparse. Consequently the calculation of G requires a nontrivial extension of linear response theory (LRT). Such an extension has been proposed in Ref. 14 and later termed "semilinear response theory" (SLRT).[15] Within SLRT it is still assumed that the transitions between levels are given by Fermi's golden rule, but a resistor network analogy is used in order to calculate the overall absorption. In order to have nonzero 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 Ref. 18) has used the Kubo formula in order to predict a $\sim\omega^2|\ln(\omega)|^{d+1}$ 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 elaborate (but still phenomenological) resister network picture.[20–22] 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 paper 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 paper is as follows: We summarize the LRT and SLRT recipes for the calculation of the conductance. Then we demonstrate that all known results for the conductance can be derived from the same theoretical framework, without any extra assumptions.

II. MODEL PARAMETERS

We consider a ring of length L and mean free path ℓ. The particles are noninteracting "spinless" electrons with charge e. The Fermi energy and the Fermi velocity are E_F and v_F, respectively. The one-particle density of states at the Fermi energy is

$$\varrho_F = \text{geometric factor} \times \mathcal{M}\frac{L}{\pi\hbar v_F}. \tag{2}$$

The number of open modes, $\mathcal{M}$, reflects the cross section of the ring. The geometric factor depends on the dimensionality $d=1,2,3$ and equals unity for $d=1$ network systems. In what follows, for the 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 $\Delta=\varrho_F^{-1}$. This is the "small" energy scale. We also have the "Thouless energy" or its equivalent which we denote as Δ_b. For a ballistic ring Δ_b

$=\mathcal{M}\Delta$ is associated with the time scale L/v_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 break time 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, which applies in the opposite circumstances—namely, if the relaxation process can be neglected during the time that the absorption rate gets stabilized. This is explained at length in Ref. 14 and will be emphasized again in a later paragraph.

III. SEMICLASSICAL LRT CALCULATION

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

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

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 all the Fourier components of the driving: namely,

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

where $\widetilde{C}(\omega)$ is the Fourier transform of the velocity-velocity correlation function and $\widetilde{F}(\omega)$ 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

$$G = \varrho_F\left(\frac{e}{L}\right)^2 \mathcal{D}. \tag{6}$$

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

IV. QUANTUM LRT CALCULATION

Equation (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 $\widetilde{C}(\omega)$, taking into account the levels statistics and the level broadening:

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

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

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

V. QUANTUM SLRT CALCULATION

A loose way to write the last expression is

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

The interpretation of $\langle\langle\cdots\rangle\rangle$ 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 at 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 Refs. 15 and 16 we regard the energy levels as the nodes of a resistor network. We define

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

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 is self-contained without 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 Fermi's golden rule (FGR):

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

where $\widetilde{F}(\omega)$ 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 $\widetilde{F}(\omega)=\epsilon^2\delta_T(\omega)$, 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 have simply restated the standard textbook version of FGR using our notations. But it should be clear that naive application of the FGR recipe is as problematic as the naive application of the Kubo formula:[25] the first-order (transient) transitions to "neighboring" states are not enough in order to get a nontransient 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 function 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

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

or equivalently

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

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 $\widetilde{C}_{\rm cl}(\omega)$ as an approximation for the quantum $\widetilde{C}(\omega)$. 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 has $\Delta \ll \Gamma \ll \Delta_b$. 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. 10–12 and also Ref. 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 nontrivial ballistic regime $(1 \ll \ell/L \ll \mathcal{M})$ each eigenfunction occupies 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 wave packet 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_ξ is the

localization length. This implies a break time 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

$$R(\omega)\big|_{\text{global}} \approx \frac{1}{1+(t^*\omega)^{-2}}. \tag{18}$$

Further considerations which are based on Mott's picture of resonances imply an extra $|\ln \omega|^{d+1}$ 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, which 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 nonsparse component allows *connected sequences of transitions*. We argue that the nonsparse component is obtained by multiplying $\tilde{C}_{\text{cl}}(\omega)$ by

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

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. HOPPING PICTURE

Assuming that the coherence time $\tau_\gamma=1/\Gamma$ is much smaller compared with the break time t^* we observe that the $d\omega$ integral of Eq. (4) with Eqs. (7) and (8) and the Lorentzian of Eq. (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 a 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 on the detailed spectral properties of the bath. The calculation of Γ with Eq. (13) involves a $d\omega$ integral over

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

This is mathematically equivalent to the VRH integral.[19] There the optimization is over the range of 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 of 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 hoc* 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.

The long-standing puzzle regarding "ac conductance" versus "dc conductance" that was discussed in the Introduction is automatically resolved by our theoretical framework. We claim that there is no crossover from ac conductance to dc conductance as a function of frequency. Rather, we argue that there is a crossover from ac conductance to dc conductance as a function of the driving intensity. Using the terminology of Ref. 14, the crossover is from the "spectroscopic" to the "mesoscopic" result for the conductance: The Kubo formula of LRT applies to a spectroscopic measurement of the conductance, where the driving is assumed to be very weak compared with the relaxation processes. The hopping picture that emerges from SLRT applies to the mesoscopic regime where the relaxation is assumed to be slow compared with the driving-induced transitions.

Note added. The apparent inconsistency between the hopping and VRH pictures and the Kubo ac and dc formalisms, and the question how to reconcile between them, was pointed out by Michael Wilkinson (M.W.) in the late 1990s. The issue was 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 (B.M.). The belief that the theory can give hopping and VRH estimates has been shared by all of us and

was implicitly expressed in Ref. 15. Recently, I was notified that during the last year M.W. and B.M. have made independently further progress on SLRT in general and possibly on this issue in particular (undocumented).

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[1] M. Büttiker, Y. Imry, and R. Landauer, Phys. Lett. **96A**, 365 (1983).
[2] R. Landauer and M. Büttiker, Phys. Rev. Lett. **54**, 2049 (1985).
[3] M. Büttiker, Phys. Rev. B **32**, 1846 (1985).
[4] M. Büttiker, Ann. N.Y. Acad. Sci. **480**, 194 (1986).
[5] Y. Imry and N. S. Shiren, Phys. Rev. B **33**, 7992 (1986).
[6] N. Trivedi and D. A. Browne, Phys. Rev. B **38**, 9581 (1988).
[7] Y. Gefen and D. J. Thouless, Phys. Rev. Lett. **59**, 1752 (1987).
[8] M. Wilkinson, J. Phys. A **21**, 4021 (1988).
[9] M. Wilkinson and E. J. Austin, J. Phys. A **23**, L957 (1990).
[10] B. Reulet and H. Bouchiat, Phys. Rev. B **50**, 2259 (1994).
[11] A. Kamenev, B. Reulet, H. Bouchiat, and Y. Gefen, Europhys. Lett. **28**, 391 (1994).
[12] A. Kamenev and Y. Gefen, Int. J. Mod. Phys. B **9**, 751 (1995).
[13] Measurements of conductance of closed diffusive rings are described by B. Reulet, M. Ramin, H. Bouchiat, and D. Mailly, Phys. Rev. Lett. **75**, 124 (1995).
[14] D. Cohen, T. Kottos, and H. Schanz, J. Phys. A **39**, 11755 (2006).
[15] M. Wilkinson, B. Mehlig, and D. Cohen, Europhys. Lett. **75**, 709 (2006).
[16] S. Bandopadhyay, Y. Etzioni, and D. Cohen, Europhys. Lett. **76**, 739 (2006).
[17] N. F. Mott, Philos. Mag. **22**, 7 (1970).
[18] U. Sivan and Y. Imry, Phys. Rev. B **35**, 6074 (1987).
[19] N. F. Mott and E. A. Davis, *Electronic Processes in Non-crystalline Materials* (Clarendon Press, Oxford, 1971).
[20] A. Miller and E. Abrahams, Phys. Rev. **120**, 745 (1960).
[21] V. Ambegaokar, B. Halperin, and J. S. Langer, Phys. Rev. B **4**, 2612 (1971).
[22] M. Pollak, J. Non-Cryst. Solids **11**, 1 (1972).
[23] M. Wilkinson (private communication); see *Note added*.
[24] D. Cohen, Phys. Rev. A **44**, 2292 (1991).
[25] A detailed SLRT study of the quantum decay problem is in preparation in collaboration with T. Kottos.
[26] O. M. Auslaender and S. Fishman, Phys. Rev. Lett. **84**, 1886 (2000); J. Phys. A **33**, 1957 (2000).