Quantum pumping and dissipation: From closed to open systems

Doron Cohen

Department of Physics, Ben-Gurion University, Beer-Sheva 84105, Israel
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Current can be pumped through a closed system by changing parameters (or fields) in time. The Kubo formula allows one to distinguish between dissipative and nondissipative contributions to the current. We obtain a Green function expression and an *S*-matrix formula for the associated terms in the generalized conductance matrix: the "geometric magnetism" term that corresponds to adiabatic transport, and the "Fermi golden rule" term which is responsible for the irreversible absorption of energy. We explain the subtle limit of an infinite system, and demonstrate the consistency with the formulas by Landauer and Büttiker, Prétre and Thomas. We also discuss the generalization of the fluctuation-dissipation relation, and the implications of the Onsager reciprocity.

Linear response theory (LRT) is the traditional theoretical tool for dealing with the response of driven systems.[1–4] It offers an expression (the Kubo formula) for the generalized susceptibility, and hence for the generalized conductance matrix. It has been realized that in the adiabatic limit the Kubo formula reduces to an expression for "geometric magnetism."[5] In case of electrical current calculation the latter gives the "adiabatic transport" of charge.[6,7] Outside the adiabatic regime the response includes an additional "dissipation" term.[8] The latter determines the rate of irreversible energy absorption, which is caused by Fermi golden rule transitions between energy levels.

Recently there has been much interest in analyzing the response of *open systems* that are connected to reservoirs. The analysis has been based on the *S*-matrix formalism, leading to the Landauer formula,[2,3] and more generally to the Büttiker, Prétre, and Thomas (BPT) formula.[9] A major motivation for the present work is the realization that the relation between the BPT formula and the Kubo formula has not been clarified. In particular, the notion of "adiabatic pumping" in the context of an open system has been left obscured, and some confusion has arose regarding the role of dissipation in the pumping process.[8,10,11]

The purpose of the present work is to analyze the response of *closed isolated systems*,[11,12] and in particular to consider the special limit of an infinite system (no reservoirs!). Thus we are going to construct a bridge between the LRT formulation and the BPT formula. This is of great practical importance, because the assumed open geometry of the *S*-matrix formulation is in many cases an idealization. It is clear that Kubo formula allows a straightforward incorporation of finite-size, external noise, environmental, and possibly also many-body effects. A major step in constructing this bridge, had been taken up in Ref. 13, where the authors start with the Kubo formula for the electrical conductivity and end up with the Landauer formula which relates the conductance to the transmission of the device. We are going to see that the general case, which deals with the *generalized* conductance matrix and hence incorporates adiabatic transport, is much more subtle.

Consider a *closed isolated system* whose Hamiltonian $\mathcal{H}$ depends on several control parameters x_j. An example is presented in Fig. 1, where x_1 and x_2 are gate voltages and x_3 is the magnetic flux through the loop. The generalized forces are conventionally defined as $F^k = -\partial \mathcal{H}/\partial x_k$. Note that F^3 is the electrical current. In LRT[1] the first-order contribution to $\langle F^k \rangle$ is related to $x_j(t)$ by a causal response kernel $\alpha^{kj}(t-t')$. The Kubo expression for this response kernel is $\alpha^{kj}(\tau) = \Theta(\tau) K^{kj}(\tau)$, where $K^{kj}(\tau) = (i/\hbar) \times \langle [F^k(\tau), F^j(0)] \rangle$ and $\Theta(\tau)$ is the step function. The Fourier transform of $\alpha^{kj}(\tau)$ is the generalized susceptibility $\chi^{kj}(\omega)$. The generalized conductance matrix is

$$G^{kj} = \lim_{\omega \to 0} \frac{\text{Im}[\chi^{kj}(\omega)]}{\omega} = \int_0^\infty K^{kj}(\tau)\tau d\tau. \tag{1}$$

Thus in the limit of zero frequency the nontrivial part of the response can be written as a generalized Ohm's law

$$\langle F^k \rangle = -\sum_j G^{kj}\dot{x}_j \equiv (-\boldsymbol{\eta}\cdot\dot{x} - \boldsymbol{B}\wedge\dot{x})_k, \tag{2}$$

where following Ref. 5 the generalized conductance matrix is written as a sum of a symmetric matrix $\boldsymbol{\eta}^{kj} = \boldsymbol{\eta}^{jk}$ that represents the dissipative response, and an antisymmetric matrix $\boldsymbol{B}^{kj} = -\boldsymbol{B}^{jk}$ that represents the nondissipative response (also called geometric magnetism).
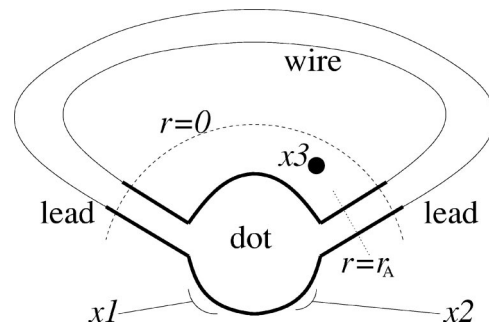

FIG. 1. Illustration of a closed system. The dot potential is controlled by gate voltages x_1 and x_2. The flux through the loop is $x_3 = \Phi$. The scattering region ($r < 0$) is represented by an S matrix. The length L of the wire is assumed to be very large.

For a device as in Fig. 1, and zero-temperature occupation of noninteracting (spinless) fermions, we find below that the dissipative part of the response is

$$\boldsymbol{\eta}^{kj} = \frac{\hbar}{\pi} \text{tr}[F^k \text{Im}[\mathsf{G}^+] F^j \text{Im}[\mathsf{G}^+]] \tag{3}$$

$$= \frac{\hbar}{4\pi} \text{tr}\left[\frac{\partial S^\dagger}{\partial x_i} \frac{\partial S}{\partial x_j}\right], \tag{4}$$

where $\mathsf{G}^\pm = 1/(E - \mathcal{H} \pm i0)$ are Green functions of the corresponding open system, and $\text{Im}[\mathsf{G}^+] = -i(1/2)(\mathsf{G}^+ - \mathsf{G}^-)$. For the nondissipative part of the response we find

$$\boldsymbol{B}^{kj} = -\frac{i\hbar}{2\pi} \text{tr}[F^k(\mathsf{G}^+ + \mathsf{G}^-)F^j \text{Im}[\mathsf{G}^+]] \tag{5}$$

$$= \frac{e}{4\pi i} \text{tr}\left[P_A\left(\frac{\partial S}{\partial x_j}S^\dagger - \frac{\partial S^\dagger}{\partial x_j}S\right)\right] + \boldsymbol{B}^{3j}_{\text{intrf}}, \tag{6}$$

where the second equality holds for $k = 3$, and allows the determination of the electrical current $\langle F^3 \rangle$ via a specified lead A. The last term is defined in Eq. (26). The projector P_A restricts the trace operation to be over the specified lead channels. In the absence of magnetic field the remaining component is $\boldsymbol{B}^{12} = 0$, while $\boldsymbol{\eta}^{31} = \boldsymbol{\eta}^{32} = 0$ as expected from the Onsager reciprocity relations (see last paragraph). Disregarding the last term in Eq. (6), the sum of Eqs. (6) and (4) for $k = 3$ coincides with the BPT formula, which can be written in our notations as

$$\boldsymbol{G}^{3j} = \frac{e}{2\pi i} \text{tr}\left(P_A \frac{\partial S}{\partial x_j}S^\dagger\right) \quad [\text{BPT}]. \tag{7}$$

We show later that this reduces for $j = 3$ to the Landauer formula which relates the electrical conductance G^{33} to the transmission of the device.

Below we explain how to derive the expressions for $\boldsymbol{\eta}^{kj}$ and $\boldsymbol{B}^{kj}$ starting from the Kubo formula Eq. (1). Later we discuss further physical implications of our results. Assuming zero-temperature Fermi occupation up to energy E_F, standard textbook procedure[1-4] leads to

$$\boldsymbol{\eta}^{kj}|_\Gamma = \pi\hbar \sum_{n,m} F^k_{nm} \overline{\delta(E_F - E_m)} F^j_{mn} \overline{\delta(E_F - E_n)}, \tag{8}$$

where the overline indicates that the δ functions are smeared. If the system were not isolated, the "broadening" Γ of the energy levels would be determined by the interaction with the external environment.[4] But we assume a closed *isolated* system. Still we argue[8] that in case of a quantized *chaotic* system the levels acquire an effective width $\Gamma = ((\hbar \sigma_F / \Delta^2) |\dot{x}|)^{2/3} \Delta$, where Δ is the mean level spacing, and σ_F is the root-mean-square value of the near-diagonal matrix elements (see remark[14]). Therefore we find two possibilities: In the adiabatic regime ($\Gamma \ll \Delta$) the dissipative conductance is zero ($\boldsymbol{\eta} = 0$), while in the nonadiabatic regime ($\Gamma > \Delta$) the dissipative conductance acquires a well-defined finite value, which is *not* sensitive to Γ, and can be calcu-

lated using Eq. (3). A similar claim holds regarding $\boldsymbol{B}^{kj}$, but the details are much more subtle. We start with the standard expression[5,11]

$$\boldsymbol{B}^{kj}|_{\Gamma=0} = 2\hbar \sum_n f(E_n) \sum_{m(\neq n)} \frac{\text{Im}[F^k_{nm} F^j_{mn}]}{(E_m - E_n)^2}, \tag{9}$$

where $f(E)$ is the Fermi occupation function (later we take the limit of zero temperature). Incorporating Γ, and exploiting the antisymmetry of the numerator with respect to $n \Leftrightarrow m$ interchange we get

$$\boldsymbol{B}^{kj}|_\Gamma = \sum_{n,m} \frac{-i\hbar F^k_{nm} F^j_{mn}}{(E_m - E_n)^2 + (\Gamma/2)^2}(f(E_n) - f(E_m)). \tag{10}$$

The numerator, on an average, depends mainly on the difference $r = m - n$, and it is nonnegligible within a bandwidth $|E_m - E_n| < \Delta_b$. We further discuss the bandwidth issue in the next paragraph, and explain that in the limit of a very long wire $\Delta \ll \Gamma \ll \Delta_b$. This means that in this limit Γ serves like the infinitesimal $i0$ in the definition of the Green functions $\mathsf{G}^\pm$. Consequently, the sum in Eq. (10), which is of the form $\sum_{n,m} g(n-m)(f(E_n) - f(E_m)) = \sum_r rg(r)$, leads after some straightforward algebra to Eq. (5).

Formally there is an optional derivation that leads to Eqs. (3) and (5). The kernel $K^{ij}(\tau)$ is related to the symmetrized correlation function $C^{ij}(\tau) = \langle \frac{1}{2}[F^i(\tau)F^j(0) + F^j(0)F^i(\tau)]\rangle$. The quantum-mechanical derivation of this subtle relation is discussed in Appendix D of Ref. 11. If we use this relation we get from Eq. (1) an extremely simple (and useful) result

$$\boldsymbol{G}^{kj} = \frac{1}{\Delta} \int_0^\infty C^{kj}(\tau) d\tau, \tag{11}$$

which can be regarded as the generalization of the *fluctuation dissipation relation*. The fluctuations are described by $\tilde{C}^{kj}(\omega)$ which is defined as the Fourier transform of $C^{ij}(\tau)$. It follows from this definition that

$$\tilde{C}^{kj}(\omega) = \frac{2\pi\hbar}{\Delta}\overline{F^k_{nm}F^j_{mn}}\bigg|_{E_n - E_m \approx \hbar\omega}. \tag{12}$$

For the device of Fig. 1 the mean level spacing is $\Delta \propto 1/L$, where L is the length of the wire. The above relation implies that the bandwidth of the mn matrix is $\Delta_b \sim \hbar/\tau_{cl}$, where the classical correlation time τ_{cl} is determined by the chaotic motion inside the dot. It is also clear that $\tilde{C}^{ij}(\omega) \propto 1/L$, and therefore $\sigma_F^2 \propto (1/L)^2$. Hence we get that $\Gamma \propto (1/L)^{1/3}$, implying that the limit $L \to \infty$ (keeping constant Fermi energy) is nonadiabatic, and that $\Delta \ll \Gamma \ll \Delta_b$. Assuming for simplicity that there is no magnetic field, one easily derives the expressions

$$\boldsymbol{G}^{33} = \frac{1}{2\Delta}\tilde{C}^{33}(\omega \sim 0), \tag{13}$$

$$G^{3j} = \frac{1}{\Delta} \int_{-\infty}^{\infty} \Im \left[\frac{\widetilde{C}^{3j}(\omega)}{\omega} \right] \frac{d\omega}{2\pi} \quad \text{for } j=1,2, \qquad (14)$$

which are equivalent to those obtained in the preceding paragraph. Note that $C^{3j}(\tau)$ with $j=1,2$ is antisymmetric with respect to τ, and therefore $-i\widetilde{C}^{3j}(\omega)/\omega$ is a real symmetric function.

We turn back to the formal derivation. We want to get exact expressions for the elements of the conductance matrix, for the device of Fig. 1, in the nonadiabatic limit of large L. The location of the particle is specified by $\boldsymbol{r} = (\mathsf{r},s)$, where r is the coordinate along the ring and s is a transverse coordinate. Optionally we can specify the location along a lead using a radial coordinate r, while the surface coordinate s distinguishes different points that have the same r. We shall refer to $r=0$ as the boundary of the scattering region. The channel basis is defined as $\langle \mathsf{r},s|a,r\rangle = \chi_a(s)\delta(\mathsf{r} - \mathsf{r}_a(r))$, where a is the channel index. The wave function in the lead regions can be expanded as follows:

$$|\Psi\rangle = \sum_{a,r} (C_{a,+} e^{ik_a r} + C_{a,-} e^{-ik_a r})|a,r\rangle. \qquad (15)$$

Following[3] we define an operator which can be identified with the imaginary part of the self-energy of the interaction of the dot with the leads

$$\hat{\Gamma} = \sum_a |a,0\rangle \hbar v_a \langle a,0| = \delta(r) \otimes \sum_a |a\rangle \hbar v_a \langle a|, \qquad (16)$$

where $v_a = (\hbar k_a / \text{mass})$ is the velocity in channel a. The matrix elements of the second term in Eq. (16) are

$$\hat{\Gamma}(s,s') = \sum_a \chi_a(s) \hbar v_a \chi_a(s'). \qquad (17)$$

Using standard procedure [see Sec. (3.4) of Ref. 3] the Green function in the leads, inside the scattering region ($r<0$), can be expressed using the S matrix

$$\mathsf{G}^+(r,s|0,s') = -i\sum_{a,b} \chi_b(s) \frac{1}{\sqrt{\hbar v_b}}$$

$$\times (e^{-ikr} + Se^{ikr})_{ba} \frac{1}{\sqrt{\hbar v_a}} \chi_a(s'), \qquad (18)$$

where $k = \text{diag}\{k_a\}$ is a diagonal matrix. Now we are fully equipped to convert Eq. (3) into an S-matrix expression. Using the identities [for Eq. (19) below see Ref. 3]

$$\text{Im}[\mathsf{G}^+] = -\tfrac{1}{2} \mathsf{G}^+ \hat{\Gamma} \mathsf{G}^- = -\tfrac{1}{2} \mathsf{G}^- \hat{\Gamma} \mathsf{G}^+, \qquad (19)$$

$$\frac{\partial \mathsf{G}^\pm}{\partial x_j} = -\mathsf{G}^\pm F^j \mathsf{G}^\pm, \qquad (20)$$

we obtain

$$\boldsymbol{\eta}^{kj} = \frac{\hbar}{4\pi} \text{tr} \left[\frac{\partial \mathsf{G}^+}{\partial x_j} \hat{\Gamma} \frac{\partial \mathsf{G}^-}{\partial x_j} \hat{\Gamma} \right]. \qquad (21)$$

Using the definition of $\hat{\Gamma}$ and Eq. (18) we get Eq. (4).

The derivation of the S-matrix expression Eq. (6) for $\boldsymbol{B}^{kj}$ is much more subtle, and requires a preliminary discussion of the definition of the current operator. Consider a ring geometry, and assume that the current is driven by the flux Φ. In order to have a better defined model we should specify what is the vector potential $\mathcal{A}(\boldsymbol{r})$ along the ring. We can regard the values of $\mathcal{A}$ at different points in space as independent parameters (think of tight binding model). Their sum [meaning $\oint \mathcal{A}(\boldsymbol{r}) \cdot d\boldsymbol{r}$] should be Φ. So we have to know how Φ is distributed along the ring. This is not just a matter of "gauge choice" because the electric field $\mathcal{E}(\boldsymbol{r}) = -\dot{\mathcal{A}}(\boldsymbol{r})$ is a gauge invariant quantity. The transformation $\mathcal{A} \mapsto \mathcal{A} + \nabla \Lambda(\boldsymbol{r})$ for a time dependent field is not merely a gauge change. A gauge transformation of time dependent field requires a compensating replacement of the scalar potential, which is not the case here. So let us define a flux Φ_A which is associated with a vector potential that is concentrated across a section $\mathsf{r} = \mathsf{r}_A$ of a given lead. For the later derivation it is essential to assume that the section $\mathsf{r} = \mathsf{r}_A$ is contained within the scattering region (see Fig. 1). The generalized force which is associated with Φ_A is $F^3 = I_A$, the current through this section. Namely,

$$I_A = -\frac{\partial \mathcal{H}}{\partial \Phi_A} = \tfrac{1}{2} e (v \, \delta(\mathsf{r} - \mathsf{r}_A) + \delta(\mathsf{r} - \mathsf{r}_A) v) \qquad (22)$$

$$= (e/\hbar)[\hat{\Gamma}_A P^+ - \hat{\Gamma}_A P^-], \qquad (23)$$

where v is the r component of the velocity operator. The last equality involves new definitions. We define

$$\hat{\Gamma}_A = \sum_{a \in A} |a,r_A\rangle \hbar v_a \langle a,r_A|. \qquad (24)$$

We also define projectors P^+ and P^- that project out of the lead wave function, Eq. (15), the outgoing and the ingoing parts, respectively. These projectors commute with $\hat{\Gamma}_A$. Furthermore, note that $P^+ \mathsf{G}^+ = \mathsf{G}^+$, $P^- \mathsf{G}^+ = 0$, and $\mathsf{G}^- P^- = 0$, and so forth. Using these extra identities one obtains the following expression:

$$\boldsymbol{B}^{3j} = \frac{e}{4\pi i} \text{tr} \left[\hat{\Gamma}_A \frac{\partial \mathsf{G}^+}{\partial x_j} \hat{\Gamma} \mathsf{G}^- - \hat{\Gamma}_A \frac{\partial \mathsf{G}^-}{\partial x_j} \hat{\Gamma} \mathsf{G}^+ \right]. \qquad (25)$$

Using the definitions of $\hat{\Gamma}$ and $\hat{\Gamma}_A$, together with Eq. (18), followed by a straightforward algebraic manipulation, one arrives at Eq. (6) with the additional term

$$\boldsymbol{B}^{3j}_{\text{intrf}} = \frac{e}{2\pi} \text{Re} \left[\text{tr} \left(P_A \frac{\partial S}{\partial x_j} e^{i2kr_A} \right) \right], \qquad (26)$$

where P_A is a projector that restrict the trace operation to the $a \in A$ lead channels.

For the simple ring geometry of Fig. 1, we have a left lead ($b \in B$) and a right lead ($a \in A$) channels, and the S matrix can be written as

$$S=\begin{pmatrix} r_{\mathrm{B}} & t_{\mathrm{AB}}e^{-i\phi} \\ t_{\mathrm{BA}}e^{i\phi} & r_{\mathrm{A}} \end{pmatrix}, \quad P_{\mathrm{A}}=\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \qquad (27)$$

where $\phi=e\Phi_{\mathrm{A}}/\hbar$. Using the identity

$$\frac{\partial S}{\partial \Phi_{\mathrm{A}}}=i\frac{e}{\hbar}(P_{\mathrm{A}}S-SP_{\mathrm{A}}) \qquad (28)$$

one can derive the relation that has been stated between Eq. (4), Eq. (6), and the BPT formula Eq. (7). Furthermore, assuming that there is an electro motive force $-\dot{\Phi}_{B}$ which is induced in the other lead, one obtains from BPT $G^{33} =(e^2/2\pi\hbar)\mathrm{tr}(t_{\mathrm{AB}}t_{\mathrm{AB}}^{\dagger})$ which is the Landauer formula. The application of this procedure to multilead systems is a straightforward generalization.

For an *open* system it is evident that the current which is emitted (say) through the right lead does not have to be equal to the current which is absorbed by the left lead. The reason is that charge can be accumulated in the dot region. But for a pumping cycle one realizes that the integrated current (pumped charge) is a well defined (lead independent) quantity. Similar observation holds in case of a *closed* system. Assume for example, that the left lead is blocked. In such case raising the dot potential will cause an emission of charge through the right lead, while the current through the left lead is zero. The emitted charge is accumulated in the "wire." But for a full cycle the original charge distribution is restored, and therefore the integrated charge Q becomes a well-defined (lead independent) quantity. The additional term, Eq. (26), gives a zero net contribution for a full pumping cycle. This term implies that the current is not uniform within the lead. The current has a modulation in the radial direction r, with a spatial period that equals half the de Broglie wavelength at the Fermi energy. This reflects that the net transported current corresponds to translation of a standing wave which is associated with the last occupied level.

More subtle is the value of Q for a full driving cycle. In contrast to a previous wrong statement[10] we have argued[11] that for a strictly adiabatic driving cycle, in the absence of magnetic field, the transported charge Q is at best *approximately* quantized (say $Q\approx 1$ in units of the elementary charge). The deviation is related to the Thouless conductance

of the device, and can be either positive or negative.[11] In contrast to that, with the BPT formula the correction to $Q\approx 1$ is always negative. On the basis of our derivation we can conclude the following: The deviation from quantization in a strictly adiabatic cycle is related to the contribution of the neighboring level. If the degeneracy with this level is located in the plane $(x_1,x_2,x_3=0)$ of the encircling cycle, then the correction is positive. If the encircled degeneracy is off plane, then the correction is negative. The effect of nonadiabaticity $(\Gamma>\Delta)$ is to screen the contribution of the neighboring levels, which is the reason for having always a negative correction from the BPT formula.

The role that dissipation may have in pumping is restricted, merely by the realization that the BPT formula is related to the Kubo formula. The Onsager reciprocity relation imply that in the absence of magnetic field the conductance matrix G^{kj} should be symmetric (antisymmetric) with respect to the permutation of the indexes (k,j), depending on whether F^k and F^j transform (not) in the same way under time reversal. This means that shape deformations lead to dissipation via η^{ij} with $i,j<3$, while the electrical current is determined exclusively by the nondissipative terms B^{31} and B^{32}. This should be contrasted with the response to electromotive force which is purely dissipative. Both the current and the dissipation are exclusively determined by the Ohmic conductance η^{33}. Thus, in the absence of magnetic field, we have a clear cut distinction between the dissipative and the nondissipative contributions to the response.

In summary, starting with the Kubo formalism, we were able to find expressions for the dissipative and for the nondissipative parts of the response, and to illuminate the role of nonadiabaticity in the limiting case of an *infinite* system. In contradiction with past speculations, we were able to demonstrate that the switch to an *open* system does not necessitate an extra dissipative term.

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