Quantum pumping in closed systems, adiabatic transport, and the Kubo formula

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Quantum pumping in closed systems is considered. We explain that the Kubo formula contains all the physically relevant ingredients for the calculation of the pumped charge (Q) within the framework of linear response theory. The relation to the common formulations of adiabatic transport and "geometric magnetism" is clarified. We distinguish between adiabatic and dissipative contributions to Q. On the one hand we observe that adiabatic pumping does not have to be quantized. On the other hand we define circumstances in which quantized adiabatic pumping holds as an approximation. The deviation from exact quantization is related to the Thouless conductance. As an application we discuss the following examples: classical dissipative pumping by conductance control, classical adiabatic (nondissipative) pumping by translation, and quantum pumping in the double barrier model. In the latter context we analyze a 3 site lattice Hamiltonian, which represents the simplest pumping device. We remark on the connection with the popular S matrix formalism which has been used to calculate pumping in open systems.

I. INTRODUCTION

Linear response theory[1–3] (LRT) is the leading formalism to deal with driven systems. Such systems are described by a Hamiltonian $\mathcal{H}(x)$ where $x(t)$ is a set of time dependent classical parameters ("fields"). The Kubo formula is the corner stone of LRT. It allows the calculation of the response coefficients, and in particular the *conductance matrix* (**G**) of the system. If we know **G**, we can calculate the charge (Q) which is transported through the system during one cycle of a periodic driving. This is called *pumping*.

Pumping of charge in mesoscopic[4] and molecular size devices is regarded as a major issue in the realization of future quantum circuits or quantum gates, possibly for the purpose of quantum computing.

A. Model system

In order to explain the motivation for the present work, and its relation to the published literature, we have to give a better definition of the problem. For presentation purpose we focus on a model system with a ring geometry (Fig. 1). The shape of the ring is controlled by some parameters x_1 and x_2. These parameters can be gate voltages that determine the location of some boundaries, or the height of some barriers. The third parameter is the flux through the ring:

$$x_3 = \Phi \equiv (\hbar/e)\phi. \tag{1}$$

We shall use units such that the elementary charge is $e=1$. Note that the Hamiltonian $\mathcal{H}[x_1(t), x_2(t), x_3(t)]$ has gauge invariance for $\phi \mapsto \phi + 2\pi$. Another system with a ring topology is presents in Fig. 1(b), and its abstraction is represented in Fig. 2(c). The "dot" can be represented by an S matrix that depends on x_1 and x_2. In Fig. 1(d) also the flux x_3 is regarded as a parameter of the dot. If we cut the wire in Fig. 1(d) we get the open two lead geometry of Fig. 1(e). Finally we can put many such units in series (no flux), hence getting the periodic system of Fig. 1(f). In the latter case the Hamiltonian is invariant for unit translations, and therefore

the quasimomentum ϕ is a constant of motion. It follows that the mathematical treatment of a driven periodic structure reduces to an analysis of a driven ring system with flux.

B. Classification of pumps

"Pumping" means that net charge (or maybe better to say "net integrated probability current") is transported through the ring per cycle of a periodic driving. Using the common jargon of electrical engineering this can be described as ac-dc conversion. We distinguish between pumping in open systems [such as in Fig. 1(e)], pumping in closed systems [such as in Fig. 1(d)], and pumping in periodic systems [such as in Fig. 1(f)].
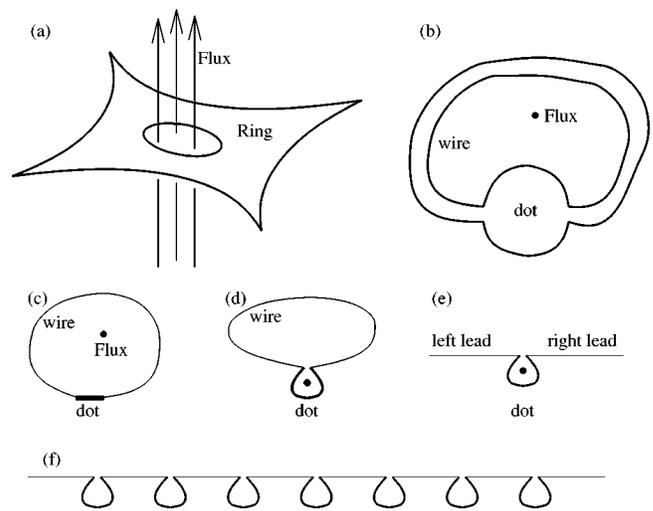

FIG. 1. Illustration of a ring system (a). The shape of the ring is controlled by some parameters x_1 and x_2. The flux through the ring is $x_3 = \Phi$. A system with equivalent topology, and abstraction of the model are presented in (b) and (c). The "dot" can be represented by an S matrix that depends on x_1 and x_2. In (d) also the flux x_3 is regarded as a parameter of the dot. If we cut the wire in (d) we get the open two lead geometry of (e). If we put many such units in series we get the period system in (f).
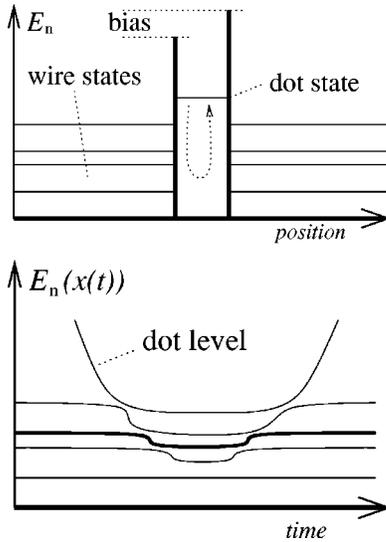
FIG. 2. Schematic illustration of quantum pumping in a closed wire-dot system. The net charge via the third level (thick solid line on the right) is vanishingly small: As the dot potential is lowered an electron is taken from the left side (first avoided crossing), and then emitted back to the left side (second avoided crossing). Assuming that the bias is inverted before the dot potential is raised back, only the second level carry a net charge $Q = \mathcal{O}(1)$.

For a reason that was explained at the end of the previous subsection we regard the last category[5] as mathematically equivalent to the second category. We also regard the first category[6–9] as a special (subtle) limit of the second category: in a follow up paper[10] we demonstrate that in the limit of open geometry the Kubo formula reduces to the S-matrix formula of Büttiker, Prétre, and Thomas.[6]

There are works in the literature regarding "rectification" and "ratchets."[11] These can be regarded as studies of pumping in periodic systems with the connotation of having *damped* non-Hamiltonian dynamics. These type of systems are beyond the scope of the present paper. There is also a recent interest in Hamiltonian ratchets,[12] which is again a synonym for pumping in periodic systems, but with the connotation of having a *nonlinear* pumping mechanism. We are going to clarify what are the conditions for having a *linear* pumping mechanism. Only in case of linear pumping mechanism the Kubo formula can be used, which should be distinguished from the nonlinear mechanism of Ref. 12.

C. Objectives

The purpose of this paper is to explain and demonstrate that the Kubo formula contains all the physically relevant ingredients for the calculation of the charge (Q) which is pumped during one cycle of a periodic driving. In the limit of a very slow time variation (small $\dot{x}$), the emerging picture coincides with the adiabatic picture of Refs. 5,13–15. In this limit the response of the system is commonly described as a nondissipative "geometric magnetism"[15] effect or as adiabatic transport.

A major objective of this paper is to bridge between the adiabatic picture and the more general LRT/Kubo picture,

and to explain how *dissipation* emerges in the quantum mechanical treatment. For one-parameter driving a unifying picture that bridges between the quantum mechanical adiabatic picture and LRT has been presented in Refs. 16–19. A previous attempt[20] had ended in some confusion regarding the identification of the linear response regime, while Ref. 15 avoided the analysis of the mechanism that leads to dissipation in the quantum mechanical case.

The presented (Kubo based) formulation of the pumping problem has a few advantages. It is not restricted to the adiabatic regime; it allows a clear distinction between *dissipative* and *adiabatic* contributions to the pumping; the classical limit is manifest in the formulation; it gives a level by level understanding of the pumping process; it allows the consideration of any type of occupation (not necessarily Fermi occupation); it allows future incorporation of external environmental influences such as that of noise; and it regards the voltage over the pump as electromotive force, rather than adopting the conceptually more complicated view[9] of having a chemical potential difference.

Of particular interest is the possibility to realize a pumping cycle that transfers *exactly* one unit of charge per cycle. In open systems[7,8] this "quantization" holds only approximately, and it has been argued[7] that the deviation from exact quantization is due to the dissipative effect. Furthermore it has been claimed[7] that exact quantization would hold in the strict adiabatic limit, if the system were *closed*. In this paper we would like to show that the correct picture is quite different. We shall demonstrate that the deviation from exact quantization is in fact of adiabatic nature. This deviation is related to the so-called "Thouless conductance" of the device.

D. Examples

We give several examples for the application of the Kubo formula to the calculation of the pumped charge Q: classical dissipative pumping, classical adiabatic pumping (by translation), and quantum pumping in the double barrier model. The last example is the main one. In the context of open geometry it is known as "pumping around a resonance."[8] We explain that this is in fact an diabatic transfer scheme, and we analyze a particular version of this model which is represented by a three site lattice Hamiltonian. This is definitely the simplest pump circuit possible, and we believe that it can be realized as a molecular size device. It also can be regarded as an approximation for the closed geometry version of the two delta potential pump (Fig. 2).[8]

E. Outline

In Sec. II we define the main object of the study, which is the conductance matrix **G** of Eq. (5). The conductance matrix can be written as the sum of a symmetric ($\boldsymbol{\eta}$) and an antisymmetric (**B**) matrices, which are later identified as the dissipative and the adiabatic contributions respectively. In the first part of the paper (Secs. II–VIII) we analyze the adiabatic equation (Sec. III), and illuminate the distinction between its zero order solution (Sec. IV) its stationary first order solution (Sec. V), and its nonstationary solution (Sec.

VI). The outcome of the analysis in Sec. V is Eq. (26) for the conductance matrix **G**. This expression is purely adiabatic, and does not give any dissipation. In order to get dissipation we have to look for a nonstationary solution.

The standard textbook derivation of the Kubo formula [Eq. (29)] for the conductance matrix **G** _implicitly_ assumes a nonstationary solution. We show how to get from it Eq. (30) for $\boldsymbol{\eta}$ and Eq. (31) for **B**. The latter is shown to be identical with the adiabatic result [Eq. (26)]. In Sec. VII we further simplify the expression for $\boldsymbol{\eta}$ leading to the fluctuation-dissipation relation [Eq. (33)].

The disadvantages of the standard textbook derivation of Kubo formula make it is essential to introduce a different route toward Eq. (33) for $\boldsymbol{\eta}$. This route, which is discusssed in Sec. VIII, _explicitly_ distinguishes the dissipative effect from the adiabatic effect, and allows to determine the conditions for the validity of either the adiabatic picture or LRT. In particular it is explained that LRT is based, as strange as it sounds, on perturbation theory to infinite order.

In Sec. IX we clarify the general scheme of the pumping calculation [Eq. (39)]. Secs. X and XI give two simple classical examples. In Sec. XII we turn to discuss quantum pumping, where the cycle is around a chain of degeneracies. The general discussion is followed by presentation of the double barrier model (Sec. XIII). In order to get a quantitative estimate for the pumped charge we consider a three site lattice Hamiltonian (Sec. XIV).

The summary (Sec. XV) gives some larger perspective on the subject, pointing out the relation to the _S_-matrix formalism, and to the Born-Oppenheimer picture. In the Appendixes we give some more details regarding the derivations, so as to have a self-contained presentation.

II. THE CONDUCTANCE MATRIX

Consider the Hamiltonian $\mathcal{H}[\boldsymbol{x}(t)]$, where $\boldsymbol{x}(t)$ is a set of time dependent parameters ("fields"). For presentation, as well as for practical reasons, we assume later a set of three time dependent parameters $\boldsymbol{x}(t) = [x_1(t), x_2(t), x_3(t)]$. We define generalized forces in the conventional way as

$$F^k = -\frac{\partial \mathcal{H}}{\partial x_k}. \tag{2}$$

Note that if x_1 is the location of a wall element, then F^1 is the force in the Newtonian sense. If x_2 is an electric field, then F^2 is the polarization. If x_3 is the magnetic field or the flux through a ring, then F^3 is the magnetization or the current through the ring.

In linear response theory (LRT) the response of the system is described by a causal response kernel, namely,

$$\langle F^k \rangle_t = \sum_j \int_{-\infty}^{\infty} \alpha^{kj}(t - t') x_j(t') dt', \tag{3}$$

where $\alpha^{kj}(\tau) = 0$ for $\tau < 0$. The Fourier transform of $\alpha^{kj}(\tau)$ is the generalized susceptibility $\chi^{kj}(\omega)$. The conductance matrix is defined as

$$G^{kj} = \lim_{\omega \to 0} \frac{\text{Im}[\chi^{kj}(\omega)]}{\omega} = \int_0^{\infty} \alpha^{kj}(\tau) \tau d\tau. \tag{4}$$

Consequently, as explained further in Appendix B, the response in the "dc limit" ($\omega \to 0$) can be written as

$$\langle F^k \rangle = -\sum_j G^{kj} \dot{x}_j. \tag{5}$$

As an example for the applicability of this formula note the following standard examples for one parameter driving: Let $x =$ wall or piston displacement, then $\dot{x} =$ wall or piston velocity, $G =$ friction coefficient, and $F = -G\dot{x}$ is the friction force. Another standard example is $x =$ magnetic flux, $-\dot{x} =$ electromotive force, $G =$ electrical conductance, and hence $F = -G\dot{x}$ is the Ohm law.

It is convenient to write the conductance matrix as $G^{kj} \equiv \eta^{kj} + B^{kj}$, where $\eta^{kj} = \eta^{jk}$ is the symmetric part of the conductance matrix, while $B^{kj} = -B^{jk}$ is the antisymmetric part. In case of having three parameters we can arrange the elements of the antisymmetric part as a vector $\vec{\boldsymbol{B}} = (B^{23}, B^{31}, B^{12})$. Consequently Eq. (5) can be written in abstract notation as

$$\langle \boldsymbol{F} \rangle = -\boldsymbol{\eta} \cdot \dot{\boldsymbol{x}} - \mathbf{B} \wedge \dot{\boldsymbol{x}}, \tag{6}$$

where the dot product should be interpreted as matrix-vector multiplication, which involves summation over the index _j_. The wedge-product also can be regarded as a matrix-vector multiplication. It reduces to the more familiar cross product in the case where we consider three parameters. The dissipation, which is defined as the rate in which energy is absorbed into the system, is given by

$$\dot{\mathcal{W}} = \frac{d}{dt} \langle \mathcal{H} \rangle = -\langle \boldsymbol{F} \rangle \cdot \dot{\boldsymbol{x}} = \sum_{kj} \eta^{kj} \dot{x}_k \dot{x}_j. \tag{7}$$

Only the symmetric part contributes to the dissipation. The contribution of the antisymmetric part is identically zero.

III. THE ADIABATIC EQUATION

The adiabatic equation is conventionally obtained from the Schrodinger equation by expanding the wave function in the _x_-dependent adiabatic basis:

$$\frac{d}{dt}|\psi\rangle = -\frac{i}{\hbar}\mathcal{H}[\boldsymbol{x}(t)]|\psi\rangle, \tag{8}$$

$$|\psi\rangle = \sum_n a_n(t)|n[\boldsymbol{x}(t)]\rangle, \tag{9}$$

$$\frac{da_n}{dt} = -\frac{i}{\hbar}E_n a_n + \frac{i}{\hbar}\sum_m \sum_j \dot{x}_j A^j_{nm} a_m, \tag{10}$$

where following Ref. 13 we define

$$`A_{nm}^j(x) = i\hbar \left\langle n(x) \left| \frac{\partial}{\partial x_j} m(x) \right\rangle \right.. \tag{11}$$

Differentiation by parts of $\partial_j \langle n(x)|m(x)\rangle = 0$ leads to the conclusion that A_{nm}^j is a hermitian matrix. Note that the effect of gauge transformation is

$$|n(x)\rangle \mapsto e^{-i[\Lambda_n(x)/\hbar]}|n(x)\rangle, \tag{12}$$

$$A_{nm}^j \mapsto e^{i[(\Lambda_n - \Lambda_m)/\hbar]} A_{nm}^j + (\partial_j \Lambda_n)\delta_{nm}. \tag{13}$$

Note that the diagonal elements $A_n^j \equiv A_{nn}^j$ are real, and transform as $A_n^j \mapsto A_n^j + \partial_j \Lambda_n$.

Associated with $A_n(x)$ is the gauge invariant two form, which is defined as

$$B_n^{ij} = \partial_i A_n^j - \partial_j A_n^i \tag{14}$$

$$= -2\hbar \, \mathrm{Im}\langle \partial_i n | \partial_j n \rangle \tag{15}$$

$$= -\frac{2}{\hbar} \mathrm{Im} \sum_m A_{nm}^i A_{mn}^j. \tag{16}$$

This can be written in an abstract notation as $\mathbf{B} = \nabla \wedge \mathbf{A}$. Using standard manipulations, namely, via differentiation by parts of $\partial_j \langle n(x)|\mathcal{H}|m(x)\rangle = 0$, we get for $n \neq m$ the expressions

$$A_{nm}^j(x) = \frac{i\hbar}{E_m - E_n} \langle n | \frac{\partial \mathcal{H}}{\partial x_j} | m \rangle \equiv -\frac{i\hbar F_{nm}^j}{E_m - E_n} \tag{17}$$

and hence

$$B_n^{ij} = 2\hbar \sum_{m(\neq n)} \frac{\mathrm{Im}[F_{nm}^i F_{mn}^j]}{(E_m - E_n)^2}. \tag{18}$$

IV. THE STRICTLY ADIABATIC SOLUTION, AND THE BERRY PHASE

We define the perturbation matrix as

$$W_{nm} = -\sum_j \dot{x}_j A_{nm}^j \quad \text{for } n \neq m \tag{19}$$

and $W_{nm}^j = 0$ for $n = m$. Then the adiabatic equation can be rewritten as follows:

$$\frac{da_n}{dt} = -\frac{i}{\hbar}(E_n - \dot{x}A_n)a_n - \frac{i}{\hbar}\sum_m W_{nm}a_m. \tag{20}$$

If we neglect the perturbation W, then we get the strict adiabatic solution

$$e^{-i/\hbar\{\int_0^t E_n[x(t')]dt' - \int_{x(0)}^{x(t)} A_n(x) \cdot dx\}} |n(x(t))\rangle. \tag{21}$$

Due to $A_n(x)$, we have the so called geometric phase. This can be gauged away unless we consider a closed cycle. For a closed cycle, the gauge invariant phase $(1/\hbar)\oint A \cdot \vec{dx}$ is called Berry phase.

With the above zero-order solution we can obtain the following result:

$$\langle F^k \rangle = \langle n(x)| - \frac{\partial \mathcal{H}}{\partial x_k} |n(x)\rangle \tag{22}$$

$$= -\frac{\partial}{\partial x_k} \langle n(x)|\mathcal{H}(x)|n(x)\rangle. \tag{23}$$

In the case of the standard examples that were mentioned previously this corresponds to conservative force or to persistent current. From now on we ignore this trivial contribution to $\langle F^k \rangle$, and look for the a first order contribution.

V. THE STATIONARY ADIABATIC SOLUTION: ADIABATIC TRANSPORT OR "GEOMETRIC MAGNETISM"

For linear driving (unlike the case of a cycle) the $A_n(x)$ field can be gauged away. Assuming further that the adiabatic equation can be treated as parameter independent (that means disregarding the parametric dependence of E_n and W on x) one realizes that Eq. (20) possesses stationary solutions. To first order these are

$$|\psi\rangle = |n\rangle + \sum_{m(\neq n)} \frac{W_{mn}}{E_n - E_m} |m\rangle. \tag{24}$$

Note that in a *fixed-basis representation* the above stationary solution is, in fact, time dependent. Hence the notations $|n[x(t)]\rangle$, $|m[x(t)]\rangle$, and $|\psi(t)\rangle$ are possibly more appropriate.

With the above solution we can write $\langle F^k \rangle$ as a sum of zero order and first order contributions. From now on we ignore the zero order contribution, and go on with the first order contribution

$$\langle F^k \rangle = -\sum_{m(\neq n)} \frac{W_{mn}}{E_n - E_m} \langle n | \frac{\partial \mathcal{H}}{\partial x_k} |m\rangle + \text{c.c.}$$

$$= \sum_j \left(i \sum_m A_{nm}^k A_{mn}^j + \text{c.c.} \right)\dot{x}_j = -\sum_j B_n^{kj}\dot{x}_j. \tag{25}$$

For a general *stationary* preparation, either pure or mixed, one obtains Eq. (5) with

$$G^{kj} = \sum_n f(E_n)B_n^{kj}, \tag{26}$$

where $f(E_n)$ are weighting factors, with the normalization $\Sigma_n f(E_n) = 1$. For a pure state preparation $f(E_n)$ distinguishes only one state n, while for canonical preparation $f(E_n) \propto \exp(-E_n/T)$, where T is the temperature. For a many-body system of non-interacting Fermions $f(E_n)$ can be reinterpreted as the Fermi occupation function, so that $\Sigma_n f(E_n)$ is the total number of particles.

Thus we see that the assumption of a stationary first-order solution leads to a nondissipative (antisymmetric) conductance matrix. This is know as either adiabatic transport[5,14] or

"geometric magnetism."[13] In the later sections we shall discuss the limitations of the above result.

VI. THE NONSTATIONARY SOLUTION: THE KUBO FORMULA

The Kubo formula is an expression for the linear response of a driven system that goes beyond the stationary adiabatic solution of the previous section. The Kubo formula has many type of derivations. One possibility is to use the same procedure as in Section V starting with

$$|\psi(t)\rangle = e^{-iE_n t}|n\rangle$$
$$+ \sum_{m(\neq n)} \left[-i\mathbf{W}_{mn} \int_0^t e^{i(E_n - E_m)t'} dt' \right] e^{-iE_m t}|m\rangle$$

For completeness we give in Appendix A the simplest version of the standard derivation, which is based on a conventional fixed-basis first-order-treatment of the perturbation. The disadvantages are: The standard derivation does not illuminate the underlaying physical mechanisms of the response, the stationary adiabatic limit is not manifest, the fluctuation-dissipation relation is vague, and the validity conditions of the derivation are not clear: no identification of the *regimes*. For now we go on with the conventional approach, but in a later section we refer to the more illuminating approach of Refs. 20 and 16–19. Then we clarify what is the regime (range of $\dot{x}$) were the Kubo formula can be trusted,[18,19] and what is the subregime where the response can be described as nondissipative adiabatic transport.

In order to express the Kubo formula one introduces the following definition:

$$K^{ij}(\tau) = \frac{i}{\hbar} \langle [F^i(\tau), F^j(0)] \rangle. \qquad (27)$$

We use the common interaction picture notation $F^k(\tau) = e^{i\mathcal{H}t} F^k e^{-i\mathcal{H}t}$, where $\mathcal{H} = \mathcal{H}(x)$ with $x = $ const. The expectation value assumes that the system is prepared in a *stationary* state (see previous section). It is also implicitly assumed that the result is not sensitive to the exact value of x. Note that $K^{ij}(\tau)$ has a well defined classical limit. Its Fourier transform will be denoted $\tilde{K}^{ij}(\omega)$.

The expectation value $\langle F^k \rangle$ is related to the driving $x(t)$ by the causal response kernel $\alpha^{ij}(t-t')$. The Kubo expression for this response kernel, as derived in Appendix A, is

$$\alpha^{ij}(\tau) = \Theta(\tau) K^{ij}(\tau), \qquad (28)$$

where the step function $\Theta(\tau)$ cares for the upper cutoff of the integration in Eq. (3). The Fourier transform of $\alpha^{ij}(\tau)$ is the generalized susceptibility $\chi^{ij}(\omega)$. The conductance matrix is defined as

$$G^{ij} = \lim_{\omega \to 0} \frac{\text{Im}[\chi^{ij}(\omega)]}{\omega} = \int_0^\infty K^{ij}(\tau)\tau d\tau. \qquad (29)$$

This can be split into symmetric and antisymmetric components (see derivation in Appendix C) as follows:

$$\eta^{ij} = \tfrac{1}{2}(G^{ij} + G^{ji}) = \frac{1}{2} \lim_{\omega \to 0} \frac{\text{Im}[\tilde{K}^{ij}(\omega)]}{\omega}, \qquad (30)$$

$$B^{ij} = \tfrac{1}{2}(G^{ij} - G^{ji}) = -\int_{-\infty}^\infty \frac{d\omega}{2\pi} \frac{\text{Re}[\tilde{K}^{ij}(\omega)]}{\omega^2}. \qquad (31)$$

The antisymmetric part is identified[15] (Appendix C) as corresponding to the stationary solution Eq. (26) of the adiabatic equation.

VII. THE EMERGENCE OF DISSIPATIVE RESPONSE, AND THE FLUCTUATION-DISSIPATION RELATION

The Kubo formula for the symmetric part of the conductance matrix (η^{ij}) can be further simplified. If we take Eq. (30) literally, then $\eta^{ij} = 0$ due to the simple fact that we have finite spacing between energy levels (see Ref. 21 for a statistical point of view). But if we assume that the energy levels have some finite width Γ, then the smoothed version of $\tilde{K}^{ij}(\omega)$ should be considered. In common textbooks the introduction of Γ is "justified" by assuming some weak coupling to an environment, or by taking the limit of infinite volume. But we are dealing with a strictly isolated finite system, and therefore the meaning of Γ requires serious consideration. We postpone the discussion of this issue to the next section.

If the smoothed version of $\tilde{K}^{ij}(\omega)$ should be used in Eq. (30), then it is possible to obtain η^{ij} from power spectrum $\tilde{C}^{ij}(\omega)$ of the fluctuations. This is called the fluctuation-dissipation relation. The spectral function $\tilde{C}^{ij}(\omega)$ is defined as the Fourier transform of the symmetrized correlation function

$$C^{ij}(\tau) = \langle \tfrac{1}{2}[F^i(\tau)F^j(0) + F^j(0)F^i(\tau)] \rangle. \qquad (32)$$

We use again the interaction picture, as in the definition of $K^{ij}(\tau)$. Also this function has a well defined classical limit.

There are several versions for the fluctuation-dissipation relation. The microcanonical version[15] has been derived using classical considerations, leading to

$$\eta^{ij}|_E = \frac{1}{2} \frac{1}{g(E)} \frac{d}{dE} [g(E) \tilde{C}_E^{ij}(\omega \to 0)]. \qquad (33)$$

In Appendix C we introduce its quantum mechanical derivation. The subscript emphasizes that we assume a microcanonical state with energy E, and $g(E)$ is the density of states. The traditional version of the fluctuation-dissipation relation assumes a canonical state. It can be obtained by canonical averaging over the microcanonical version leading to

$$\eta^{ij}|_T = \frac{1}{2T} \tilde{C}_T^{ij}(\omega \to 0). \qquad (34)$$

VIII. THE VALIDITY OF LINEAR RESPONSE THEORY AND BEYOND

The standard derivation of the dissipative part of the Kubo formula, leading to the fluctuation-dissipation relation (33), is not very illuminating physically. More troubling is the realization that one cannot tell from the standard derivation what are the conditions for its validity. An alternate, physically appealing derivation,[16–19] is based on the observation that energy absorption is related to having diffusion in energy space.[20] In Appendix E we outline the main ingredients of this approach.

It should be clear that the diffusion picture of Appendix E holds only in case of *chaotic systems*. If this diffusion picture does not hold, then also the Kubo formula for η^{ij} does not hold. Driven one-dimensional systems are the obvious example for the failure of linear response theory. As in the case of the kicked rotator (standard map) (Ref. 22) there is a complicated route to chaos and stochasticity: By increasing the driving amplitude the phase space structure is changed. If the amplitude is smaller than a threshold value, then the diffusion is blocked by Kolmogorov-Arnold-Moser curves, and consequently there is not dissipation. Therefore the Kubo formula is not applicable in such cases.

The following discussion of *dissipative response* assumes that we deal with a quantized chaotic system. We would like to discuss the reason and the consequences of having an energy scale Γ. In the standard derivation the assumption of having level broadening as if comes out of the blue. As we already noted it is customary in textbooks to argue that either a continuum limit, or some small coupling to an environment is essential in order to provide Γ. But this is of course just a way to avoid confrontation with the physical problem of having a driven *isolated finite mesoscopic system*. In fact the energy scale Γ is related to the rate ($\dot{x}$) of the driving:

$$\Gamma = \left(\frac{\hbar \sigma}{\Delta^2} |\dot{x}| \right)^{2/3} \times \Delta, \qquad (35)$$

where for simplicity of presentation we assume one parameter driving. We use Δ to denote the mean level spacing, and σ is the root mean square value of the matrix element F_{nm} between neighboring levels. In order to derive the above expression for Γ we have used the result of Ref. 19 (Sec. 17) for the "core width" at the breaktime $t = t_{prt}$ of perturbation theory. The purpose of the present section is to give an optional "pedestrian derivation" for Γ, and to discuss the physical consequences.

Looking at the first order solution Eq. (24) of Sec. V one realizes that it makes sense provided $|W_{mn}| \ll \Delta$. This leads to the adiabaticity condition

$$|\dot{x}| \ll \frac{\Delta^2}{\hbar \sigma}. \qquad (36)$$

If this condition is not satisfied one should go beyond first order perturbation theory (FOPT), in a sense to be explained below. Note that this adiabaticity condition can be written as $\Gamma \ll \Delta$.

The adiabaticity condition (36) can be explained in a more illuminating way as follows: Let us assume that we prepare the system at time $t = 0$ at the level $|n\rangle$. Using *time dependent* FOPT we find out that a stationarylike solution is reached after the Heisenberg time $t_H = 2\pi\hbar/\Delta$. This is of course a valid description provided we do not have by then a breakdown of FOPT. The condition for this is easily found to be $\dot{x} t_H \ll \delta x_c$, where $\delta x_c = \Delta/\sigma$. This leads again to the adiabaticity condition (36).

Another assumption in the derivation of Sec. V was that we can ignore the parametric dependence of E_n and W on x. The adiabaticity condition $t_H \ll \delta x_c / \dot{x}$ manifestly justify such an assumption: We should think of t_H as the transient time for getting a stationarylike state, and we should regard δx_c as the parametric correlation scale.

As strange as it sounds, in order to have dissipation, it is essential to have a breakdown of FOPT. In the language of perturbation theory this implies a required summation of diagrams to *infinite order*, leading to an effective broadening of the energy levels. By iterating FOPT, neglecting interference terms, we get a *Markovian approximation* for the energy spreading process. This leads to the diffusion equation of Appendix E. This diffusion can be regarded as arising from Fermi-golden-rule transitions between energy levels. A simple ad-hoc way to determine the energy level broadening is to introduce Γ as a lower cutoff in the energy distribution which is implied by Eq. (24):

$$|\langle n|\psi\rangle|^2 = \frac{|\hbar \dot{x} F_{mn}|^2}{(E_n - E_m)^4 + (\Gamma)^4}. \qquad (37)$$

This constitutes a generalization of the well known procedure used by Wigner in order to obtain the local density of states.[16,17] However, in the present context we do not get a Lorentzian. The width parameter Γ is determined self-consistently from normalization, leading to Eq. (35) (disregarding numerical prefactor).

We can summarize the above reasoning by saying that there is a *perturbative regime* that includes an adiabatic (FOPT) subregime. Outside of the adiabatic subregime we need *all orders* of perturbation theory leading to Fermi-golden-rule transitions, diffusion in energy space, and hence dissipation. Thus the dissipative part of Kubo formula emerges only in the regime $\Gamma > \Delta$, which is just the opposite of the adiabaticity condition. The next obvious step is to determine the boundary of the perturbative regime. Following Refs. 18,19 we argue that the required condition is $\Gamma \ll \Delta_b$. The bandwidth $\Delta_b \propto \hbar$ is defined as the energy width $|E_n - E_m|$ were the matrix elements F_{nm} are not vanishingly small. If the condition $\Gamma \ll \Delta_b$ is violated we find ourselves in the nonperturbative regime where the Kubo formula cannot be trusted.[18,19]

We still have to illuminate why we can get in the perturbative regime a dissipative *linear* response in spite of the breakdown of FOPT. The reason is having a separation of scales ($\Delta \ll \Gamma \ll \Delta_b$). The nonperturbative mixing on the small energy scale Γ does not affect the rate of first-order transitions between distant levels ($\Gamma \ll |E_n - E_m| \ll \Delta_b$).

Therefore Fermi golden rule picture applies to the description of the coarse grained energy spreading, and we get the linear response.

The existence of the adiabatic regime is obviously a quantum mechanical effect. If we take the formal limit $\hbar \to 0$ the adiabaticity condition $\Gamma \ll \Delta$ breaks down. In fact the *proper* classical limit is *nonperturbative*, because the weaker condition $\Gamma \ll \Delta_b$ does not survive the $\hbar \to 0$ limit. For further details see Refs. 16–19. In the nonperturbative regime the quantum mechanical derivation of Kubo formula is not valid. Indeed we have demonstrated[18] the failure of Kubo formula in case of random-matrix models. But if the system has a classical limit, then Kubo formula still holds in the nonperturbative regime due to *semiclassical* (rather than quantum-mechanical) reasons.

The discussion of *dissipation* assumes a generic situation such that the Schrödinger equation does not have a stationary solution. This means that driven one-dimensional systems are automatically excluded. Another nongeneric possibility is to consider a special driving scheme, such as translation, rotation, or dilation.[23] In such case the time dependent Hamiltonian $\mathcal{H}[x(t)]$ possesses a stationary solution (provided the "velocity" $\dot{x}$ is kept constant). Consequently we do not have a dissipation effect. In Sec. XI we discuss the simplest example of pumping by translation, where the stationary adiabatic solution of Sec. V is in fact exact, and no dissipation arises.

IX. APPLICATION TO PUMPING

So far we have discussed the response for driving in a very general way. From now on we focus on a system with a ring geometry as described in the Introduction, and illustrated in Fig. 1. The shape of the ring is controlled by some parameters x_1 and x_2, and x_3 is the magnetic flux. The generalized force F^3 which is conjugate to the flux is the current. The time integral over the current is the transported charge

$$Q = \oint \langle F^3 \rangle dt. \tag{38}$$

In fact a less misleading terminology is to talk about "probability current" and "integrated probability current." From a purely mathematical point of view it is not important whether the transported particle has an electrical charge.

Disregarding a possible persistent current contribution, the expression for the pumped charge is

$$Q = -\left[\oint \mathbf{G} \cdot dx + \oint \mathbf{B} \wedge dx \right]_{k=3}. \tag{39}$$

If we neglect the first term, which is associated with the dissipation effect, and average the second ("adiabatic") term over the flux, then we get

$$\overline{Q|_{\text{adiabatic}}} = -\frac{1}{2\pi\hbar} \int \int \mathbf{B} \cdot \vec{dx} \wedge \vec{dx}. \tag{40}$$

The integration should be taken over a cylinder of vertical height $2\pi\hbar$, and whose basis is determined by the projection of the pumping cycle onto the (x_1, x_2) plane.

We already pointed out that the Berry phase $(1/\hbar) \oint A_n \cdot \vec{dx}$ is gauge invariant. Therefore from Stokes law it follows that $(1/\hbar) \int \int \mathbf{B} \cdot \vec{dx} \wedge \vec{dx}$ is independent of the surface, and therefore $(1/\hbar) \oiint \mathbf{B} \cdot \vec{dx} \wedge \vec{dx}$ with closed surface should be $2\pi \times$ integer. Integrating over a cylinder, as in Eq. (40), is effectively similar to integrating over a closed surface (because of the 2π periodicity in the vertical direction). This means that the flux averaged Q of Eq. (40) has to be an integer.

The common interest is in pumping cycles in the $\Phi = 0$ plane. This means that the zero order conservative contribution to Q, due to a persistent current, does not exist. Furthermore, from the reciprocity relations (see Appendix B) it follows that $G^{31} = -G^{13}$ and $G^{32} = -G^{23}$, which should be contrasted with $G^{12} = G^{21}$. This means that a pumping cycle in the $\Phi = 0$ plane is purely adiabatic: there is no dissipative contribution to Q. Only the $\vec{B}$ field [second term in Eq. (39)] is relevant to the calculation of the pumped charge, and its vertical component B^{12} vanishes due to the time reversal symmetry.

The absence of dissipative contribution for a cycle in the $\Phi = 0$ plane, does not imply that dissipation is not an issue. The symmetric part of the conductance matrix η^{ij} is in general nonzero, leading to an energy absorption rate which is proportional to $\dot{x}^2$. This implies that the energy absorption per cycle is proportional to $|\dot{x}|$. Therefore we are able to minimize the dissipation effect by making the pumping cycle very slow. Furthermore, if we get into the quantum-mechanical adiabatic regime, then η^{ij} becomes extremely small, and then we can neglect the dissipation effect as long as quantum-mechanical adiabaticity can be trusted.

Whenever the dissipation effect cannot be neglected, one should specify whether or how a *stationary operation* is achieved. In case of pumping in open system the stationary operation is implicitly guaranteed by having equilibrated reservoirs, where the extra energy is dissipated to infinity. In case of pumping in closed system the issue of stationary operation is more subtle: In the adiabatic regime, to the extend that adiabaticity can be trusted, we have a stationary solution to the transport problem, as defined in Sec. V. But outside of the adiabatic regime we have diffusion in energy space (Appendix E) leading to a slow energy absorption (dissipation). Thus a driven system is heated up gradually (though possibly very slowly). Strictly speaking a stationary operation is not achieved, unless the system is in (weak) thermal contact with some large bath. Another way to reach a stationary operation, that does not involve an external bath, is by having an effectively bounded phase space. This is the case with the mixed phase space example which is discussed in Ref. 12. There the stochasticlike motion takes place in a bounded chaotic region in phase space.

X. CLASSICAL DISSIPATIVE PUMPING

Before we discuss the quantum mechanical pumping, it is instructive to bring simple examples for *classical* pumping.

In the following we consider one particle (r) in a two-dimensional ring as in Fig. 1(a).

The first example is for classical *dissipative* pumping. The conductance $G = G^{33}$ can be calculated for this system[24] leading to a mesoscopic variation of the Drude formula. The current is given by Ohm law $I = -G \times \dot{\Phi}$, where $-\dot{\Phi}$ is the electromotive force.

Consider now the following pumping cycle: Change the flux from Φ_1 to Φ_2, hence pumping charge $Q = -G(1) \times (\Phi_2 - \Phi_1)$. Change the conductance from $G(1)$ to $G(2)$ by modifying the shape of the ring. Change the flux from Φ_2 back to Φ_1, hence pumping charge $Q(2) = -G(2) \times (\Phi_1 - \Phi_2)$. Consequently the net pumping is

$$Q = [G(2) - G(1)] \times (\Phi_2 - \Phi_1). \tag{41}$$

Thus we have used the dissipative part of the conductance matrix [first term in Eq. (39)] in order to pump charge. In the quantum mechanical version of this example extra care should be taken with respect to the zero order contribution of the persistent current.

XI. CLASSICAL ADIABATIC PUMPING

The second example is for classical *adiabatic* pumping. The idea is to trap the particle inside the ring by a potential well, and then to make a translation of the trap along a circle. The result of such a cycle is evidently $Q = 1$. We would like to see how this trivial result emerges form the Kubo formula.

Let (r,p) be the canonical coordinate of the particle in the ring, while (x_1,x_2) are the center coordinate of a trapping potential. The Hamiltonian is

$$\mathcal{H}[r,p;x(t)] = \frac{1}{2m}\left[p_\perp^2 + \left(p_\| - \frac{1}{2\pi\sqrt{x_1^2+x_2^2}}\Phi(t)\right)\right]$$
$$+ U_{\text{trap}}[r_1-x_1(t),r_2-x_2(t)], \tag{42}$$

where $p_\|$ and $p_\perp$ are the components of the momentum along the ring and in the perpendicular (transverse) directions. The pumping is done simply by cycling the position of the trap. The translation of the trap is assumed to be along an inside circle of radius R,

$$x(t) = [R\cos(\Omega t), R\sin(\Omega t), \Phi = \text{const}]. \tag{43}$$

In this problem the stationary solution of Sec. V is an exact solution. Namely

$$|\psi(t)\rangle = e^{im\dot{x} \cdot r}|n[x(t)]\rangle, \tag{44}$$

where $|n(x)\rangle \mapsto \psi^{(n)}(r-x)$ are the eigenfunctions of a particle in the trap. Equation (44) is just Galilei transformation from the moving (trap) frame to the laboratory frame.

It is *a priori* clear that in this problem the pumped charge per cycle is $Q = 1$, irrespective of Φ. Therefore the $\vec{B}$ field must be

$$\vec{B} = -\frac{(x_1,x_2,0)}{2\pi(x_1^2+x_2^2)}. \tag{45}$$

This can be verified by calculation via Eq. (18). The singularity along the x_3 axis is not of quantum-mechanical origin: It is not due to degeneracies, but rather due to the diverging current operator ($\partial\mathcal{H}/\partial x_3 \propto 1/\sqrt{x_1^2+x_2^2}$).

XII. QUANTUM PUMPING

We turn now to the quantum-mechanical case. Consider an adiabatic cycle that involves a particular energy level n. This level is assumed to have a degeneracy point at $(x_1^{(0)},x_2^{(0)},\Phi^{(0)})$. It follows that in fact there is a vertical chain of degeneracy points:

$$\text{chain} = (x_1^{(0)},x_2^{(0)},\Phi^{(0)} + 2\pi\hbar \times \text{integer}). \tag{46}$$

These degeneracy points are important for the geometrical understanding of the $\vec{B}$ field, as implied by Eq. (18). Every degeneracy point is similar to a monopole charge. The total flux that emerges from each monopole must be $2\pi\hbar \times$ integer for a reason that was explained after Eq. (40). Thus the monopoles are quantized in units of $\hbar/2$. The $\vec{B}$ field which is created (so to say) by a vertical chain of monopoles may have a different *near field* and *far field* behavior, which we discuss below.

The far field region exists if the chains are well isolated. Later we explain that "far" means $g_T \ll 1$, where g_T is the Thouless conductance. The far field is obtained by regarding the chain as a smooth line. This leads *qualitatively* to the same field as in Eq. (45). Consequently, for a "large radius" pumping cycle in the $\Phi = 0$ plane, we get $|Q| \approx 1$. In the following we are interested in the deviation from exact quantization: If $\phi^{(0)} = 0$ we expect to have $|Q| \geq 1$, while if $\phi^{(0)} = \pi$ we expect $|Q| \leq 1$. Only for the ϕ averaged Q of Eq. (40) we get *exact quantization*.

The deviation from $|Q| \approx 1$ is extremely large if we consider a tight pumping cycle around a $\phi^{(0)} = 0$ degeneracy. After linear transformation of the shape parameters, the energy splitting $\Delta = E_n - E_m$ of the energy level n from its neighboring (nearly degenerated) level m can be written as

$$\Delta = [(x_1-x_1^{(0)})^2 + (x_2-x_2^{(0)})^2 + c^2(\phi-\phi^{(0)})^2]^{1/2} \tag{47}$$

where c is a constant. The monopole field is accordingly

$$\vec{B} = \pm\frac{c}{2}\frac{(x_1-x_1^{(0)},x_2-x_2^{(0)},x_3-x_3^{(0)})}{\left[(x_1-x_1^{(0)})^2 + (x_2-x_2^{(0)})^2 + \left(\frac{c}{\hbar}\right)^2(x_3-x_3^{(0)})^2\right]^{3/2}}, \tag{48}$$

where the prefactor is determined by the requirement of having a single ($\hbar/2$) monopole charge. Assuming a pumping cycle of radius R in the $\Phi = 0$ plane we get from the second term of Eq. (39)

$$Q = -\left[\oint \mathbf{B} \wedge dx\right]_3 = \mp\pi\sqrt{g_T}, \tag{49}$$

where

$$g_T = \frac{1}{\Delta} \frac{\partial^2 \Delta}{\partial \phi^2} = \frac{c^2}{R^2} \qquad (50)$$

is a practical definition for the Thouless conductance in this context. It is used here simply as a measure for the sensitivity of an energy level to the magnetic flux Φ.

What we want to do in the next sections is to interpolate between the near field result, which is $Q = \mathcal{O}(\sqrt{g_T})$, and the far field result, which is $Q = \mathcal{O}(1)$. For this purpose it is convenient to consider a particular model that can be solved exactly.

XIII. THE DOUBLE BARRIER MODEL

A simple example for quantum pumping is the double barrier model. An open geometry version of this model has been analyzed in Ref. 8 using the S matrix approach. The analogous closed geometry version is obtained by considering a one-dimensional ring with two delta barriers. As we are going to explain below, the pumping process in this model can be regarded as a particular example of an adiabatic transfer scheme: The electrons are adiabatically transferred from state to state one by one as in "musical chair game."

The two delta barriers version of the double barrier model is illustrated in Fig. 2. The length of the ring is L, with periodic boundary conditions on $-(L/2) < r < (L/2)$. A dot region $|Q| < a/2$ is defined by the potential

$$U(r; c_1, c_2) = \frac{1}{c_1} \delta\left(r + \frac{a}{2}\right) + \frac{1}{c_2} \delta\left(r - \frac{a}{2}\right). \qquad (51)$$

It is assumed that c_1 and c_2 are small enough so one can classify the ring eigenstates into two categories: wire states and dot states. The latter are those states that are localized in the dot region $|Q| < a/2$ in the limit of infinitely high barriers. We define the Fermi energy as the energy of the last occupied wire level in the limit of infinitely high barriers.

The three parameters that we can control are the flux $x_3 = \Phi = \hbar\phi$, the bias $x_1 = c_1 - c_2$, and the dot potential $x_2 = E_{\text{dot}}$ which is related to $c_1 + c_2$. The energy E_{dot} correspond to the dot state which is closest to the Fermi energy E_F from above. We assume that the other dot levels are much further away from the Fermi energy, and can be ignored. Note that another possible way to control the dot potential, is simply by changing a gate voltage: That means to assume that there is a control over the potential floor in the region $|Q| < a/2$.

The pumping cycle is assumed to be in the $\Phi = 0$ plane, so there is no issue of conservative persistent current contribution. The pumping cycle is defined as follows: We start with a positive bias ($x_1 > 0$) and lower the dot potential from a large $x_2 > E_F$ value to a small $x_2 < E_F$ value. As a result, one electron is transfered via the *left* barrier into the dot region. Then we invert the bias ($x_1 < 0$) and raise back x_2. As a result the electron is transferred back into the wire via the *right* barrier.

A closer look at the above scenario [Fig. 2(b)] reveals the following: As we lower the dot potential across a wire level, an electron is adiabatically transferred once from left to right and then from right to left. As long as the bias is positive ($x_1 > 0$) the net charge being pumped is very small ($|Q| \ll 1$). Only the lowest wire level that participate in the pumping cycle carries $Q = \mathcal{O}(1)$ net charge: It takes an electron from the left side, and after the bias reversal it emits it into the right side. Thus the pumping process in this model can be regarded as a particular example[14] of an adiabatic transfer scheme: The electrons are adiabatically transferred from state to state, one by one, as in "musical chair game."

For a single occupied level the net Q is the sum of charge transfer events that take place in four avoided crossings (two avoided crossings in case of the lowest level). For many particle occupation the total Q is the sum over the net Q's which are carried by individual levels. For a dense zero temperature Fermi occupation the summation over all the net Q's is a telescopic sum, leaving noncanceling contributions only from the first and the last adiabatic crossings. The latter involve the last occupied level at the Fermi energy.

XIV. THE THREE SITE LATTICE HAMILTONIAN

Rather than analyzing the two-delta-barriers version of the double barrier model, we consider below a simplified version that still contains the *same* essential ingredients. This is obtained by considering a three site lattice Hamiltonian. The advantage is obviously the possibility to make an exact analytical treatment that does not involve approximations.

The middle site in the three site lattice Hamiltonian supports a single dot state, while the two other sites support two wire states. The Hamiltonian is

$$\mathcal{H} \mapsto \begin{pmatrix} 0 & c_1 & e^{i\phi} \\ c_1 & u & c_2 \\ e^{-i\phi} & c_2 & 0 \end{pmatrix}. \qquad (52)$$

The three parameters are the bias $x_1 = c_1 - c_2$, the dot energy $x_2 = u$, and the flux $x_3 = \Phi = \hbar\phi$. For presentation purpose we assume that $0 < c_1, c_2 \ll 1$, and characterize the wire-dot coupling by the parameter $c = \sqrt{c_1 c_2}$.

The eigenstates are E_n. Disregarding the interaction with the dot ($c = 0$) we have two wire states with $E = \pm 1$. This implies degeneracies for $x_2 = u = \mp 1$. Once we switch on the coupling ($c > 0$), the only possible degeneracies are between the even dot state and the odd wire state of the mirror symmetric Hamiltonian ($x_1 = 0$). The flux should be either integer (for degeneracy of the dot level with the lower wire level), or half integer (for degeneracy of the dot level with the upper wire level). Thus we have two vertical chains of degeneracies:

the negative chain $= (0, -1 + c^2, 2\pi\hbar \times \text{integer})$,

the positive chain $= (0, +1 - c^2, \pi + 2\pi\hbar \times \text{integer})$.

In order to calculate the $\vec{B}$ field and pumped charge Q, we have to find the eigenvalues and the eigenvectors of the Hamiltonian matrix. The secular equation for the eigenvalues is

$$E^3 - uE^2 - (1 + c_1^2 + c_2^2)E + u - 2c_1c_2\cos(\phi) = 0.$$

Using the notations

$$Q = \frac{1}{9}u^2 + \frac{1}{3}(1 + c_1^2 + c_2^2),$$

$$R = \frac{1}{27}u^3 + \frac{1}{6}(1 + c_1^2 + c_2^2)u - \frac{1}{2}u + c_1c_2\cos(\phi)\cos(\theta)$$

$$= \frac{R}{\sqrt{Q^3}}$$

the roots of the above cubic equation are

$$E_n = \frac{1}{3}u + 2\sqrt{Q}\cos\left(\frac{1}{3}\theta + n\frac{2\pi}{3}\right), \tag{53}$$

where $n = 0, \pm 1$. The corresponding eigenstates are

$$|n(x)\rangle \mapsto \frac{1}{\sqrt{S}}\begin{pmatrix} c_2 e^{i\phi} + c_1 E_n \\ 1 - E_n^2 \\ c_1 e^{-i\phi} + c_2 E_n \end{pmatrix}, \tag{54}$$

where S is the normalization, namely,

$$S = (1 - E_n^2)^2 + (c_1 + c_2 E_n)^2 + (c_2 + c_1 E_n)^2. \tag{55}$$

For the calculation of the pumped charge in the next paragraph it is useful to notice that for $E = \pm 1$ the normalization is $S = 2(c_1 \pm c_2)^2$, while for $E = 0$ the normalization is $S \approx 1$.

After some algebra we find that the first component of the $\vec{B}$ field in the $\Phi = 0$ plane is

$$B^1 = -2\,\mathrm{Im}\left\langle \frac{\partial}{\partial u}n(x) \middle| \frac{\partial}{\partial\phi}n(x) \right\rangle \tag{56}$$

$$= -(c_1^2 - c_2^2)\frac{1}{S^2}\frac{\partial S}{\partial u}, \tag{57}$$

which is illustrated in Fig. 3. From here it follow that if we keep constant bias, and change only $x_2 = u$, then the pumped charge is

$$Q = -\int B^1 dx_2 = -(c_1^2 - c_2^2)\frac{1}{S}\bigg|_{\mathrm{initial}}^{\mathrm{final}}. \tag{58}$$

For a planar ($\Phi = 0$) pumping cycle around the negative vertical chain the main contribution to Q comes from the two crossings of the $x_2 \approx -1$ line. Hence we get

$$Q = \frac{c_1 + c_2}{c_1 - c_2} = \sqrt{1 + 2g_T}, \tag{59}$$

where the Thouless conductance in this context refers to the avoided crossing, and is defined as

$$g_T \equiv \frac{1}{\Delta}\frac{\partial^2\Delta}{\partial\phi^2}\bigg|_{\phi=0} = \frac{2c_1c_2}{(c_1 - c_2)^2}. \tag{60}$$
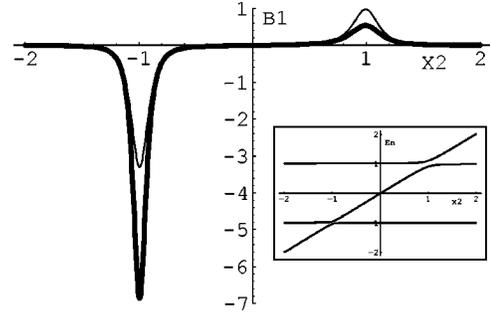

FIG. 3. The first component of the $\vec{B}$ field for a particle in the middle level of the three site lattice model. It is plotted as a function of the dot potential $x_2 = u$. The other parameters are $\phi = 0$, and $c_1 = 0.1$, while $c_2 = 0.04$ for the thick line and $c_2 = 0.02$ for the thin line. In the limit $c_2 \to 0$, all the charge that is transferred from the left side into the dot during the first avoided crossing, is emitted back into the left side during the second avoided crossing. Inset: The eigenenergies $E_n(x)$ for the $c_2 = 0.04$ calculation.

A similar calculation of the pumped charge for a planar cycle around the positive chain leads to

$$Q = -\frac{c_1 - c_2}{c_1 + c_2} = -\sqrt{1 - 2g_T} \tag{61}$$

with $g_T = 2c_1c_2/(c_1 + c_2)^2$. In both cases we have approximate quantization $Q = \pm 1 + \mathcal{O}(g_T)$ for $g_T \ll 1$, while for a tight cycle either $Q \to \infty$ or $Q \to 0$ depending on which line of degeneracies is being encircled. If the pumping cycle encircles both chains then we get $Q = 4c_1c_2/(c_1^2 - c_2^2)$. In the latter case $Q = \mathcal{O}(g_T)$ for $g_T \ll 1$, with no indication for quantization.

XV. SUMMARY AND DISCUSSION

We have shown how the Kubo formalism can be used in order to derive both classical and quantum-mechanical results for the pumped charge Q in a closed system. In this formulation the distinction between dissipative and nondissipative contributions is manifest.

Within the framework of the Kubo formalism (disregarding nonlinear corrections) we have made a distinction between the following levels of treatment: strict adiabaticity (outcome of zero order treatment), adiabatic transport (outcome of stationary first order treatment), and dissipation (the result of first order transitions).

In the adiabatic regime one can assume a *stationary* solution to the adiabatic equation, which implies no dissipation effect. This leads to the picture of adiabatic transport, where the Berry phase is the outcome of a zero order treatment, while the "geometric magnetism" of Eq. (26) is the outcome of a first order treatment of the interlevel couplings.

In some very special cases (translations, rotations and dilations) this assumption (of having a stationary solution) is in fact exact, but in generic circumstance this assumption is an approximation. Outside of the adiabatic regime the stationary solution cannot be trusted.

Assuming quantized *chaotic dynamics* one argues that Fermi-golden-rule transitions between levels lead to (slow)

diffusion in energy [Eq. (E1)]. This leads to the emergence of the dissipative part in the Kubo formula. We have obtained an expression [Eq. (35)] for the energy scale $\Gamma \propto |\dot{x}|^{2/3}$ that controls the dissipative effect. We have explained that the dissipative contribution to the Kubo formula is valid only in the regime $\Delta < \Gamma \ll \Delta_b$. Otherwise the dynamics is either of adiabatic nature ($\Gamma \ll \Delta$) or nonperturbative ($\Gamma > \Delta$).

In order to calculate the pumped charge Q we have to perform a closed line integral over the conductance [Eq. (39)]. This may have in general both adiabatic and dissipative contributions. For the common pumping cycle in the $\Phi = 0$ plane, only the adiabatic contribution exists. This follows from the reciprocity relations (Sec. IX). Still we have emphasized (without any contradiction) that in the same circumstances a dissipation effect typically accompanies the pumping process.

The quantum adiabatic contribution to the pumping is determined by a line integral over a $\vec{B}$ field which is created by *monopoles*. The monopoles, which are related to the degeneracies of the Hamiltonian, are located along vertical chains in x space [Eq. (46)]. The three site model provides the simplest example for such vertical chains: By calculating the $\vec{B}$ field which is created (so to say) by these chains, we were able to determine the charge which is pumped during a cycle [e.g., Eq. (59)].

The (monopoles of the) vertical chains have *near field* regions [Eq. (48)]. If the chains are well isolated in x space, then there are also *far field* regions. The far field regions are defined as those where the Thouless conductance is very small ($g_T \ll 1$). Pumping cycles that are contained in the far field region of a given chain lead to an approximately quantized pumping $Q = \text{integer} + \mathcal{O}(g_T)$. It is important to realize that the existence of far field regions in x space is associated with having a low dimensional system far away from the classical limit. In a quantized chaotic system it is unlikely to have $g_T \ll 1$ along a pumping cycle. As we take the $\hbar \to 0$ limit the vertical chains become very dense, and the far field regions disappear.

In the subtle limiting case of open geometry we expect to get agreement with the S-matrix formula of Büttiker, Prétre, and Thomas (BPT).[6] Using the notations of the present Paper the BPT formula for the current that comes out of (say) the right lead can be written as

$$G^{3j} = \frac{e}{2\pi i} \text{trace} \left(P \frac{\partial S}{\partial x_j} S^\dagger \right), \tag{62}$$

where P is the projector on the right lead channels. For G^{33} the above reduces to the Landauer formula. The details regarding the relation between the Kubo formula and the BPT formula will be published in a separate paper.[10] Here we just note that the derivation is based on a generalization of the Fisher-Lee approach.[3,25,26]

Finally it is important to remember that the theory of driven systems is the corner stone for the analysis of interaction between "slow" and "fast" degrees of freedom. Assume that the x_j are in fact dynamical variable, and that the conjugate momenta are p_j. The standard textbook example

is the study of diatomic molecules. In such a case x_j are the locations of the nuclei. The total Hamiltonian is assumed to be of the general form

$$\mathcal{H}_{\text{total}} = \frac{1}{2M} \sum_j p_j^2 + \mathcal{H}(\boldsymbol{x}), \tag{63}$$

where $\mathcal{H}$ is the Hamiltonian of the "fast" degrees of freedom (in the context of molecular physics these are the electrons). Rather than using the standard basis, one can use the Born-Oppenheimer basis $|x, n(\boldsymbol{x})\rangle = |x\rangle \otimes |n(\boldsymbol{x})\rangle$. Then the Hamiltonian can be written as

$$\mathcal{H}_{\text{total}} = \frac{1}{2M} \sum_j [p_j - A_{nm}^j(\boldsymbol{x})]^2 + \delta_{nm} E_n(\boldsymbol{x}),$$

where the interaction term is consistent with Eq. (19). Thus it is evident that the theory of driven systems is a special limit of this problem, which is obtained if we treat the x_j as classical variables.

APPENDIX A: THE KUBO FORMULA: STANDARD DERIVATION

In this appendix we present an elementary textbook-style derivation of the Kubo formula. For notational simplicity we write the Hamiltonian as $\mathcal{H} = \mathbf{H}_0 - f(t)\mathbf{V}$. It is assumed that the system, in the absence of driving, is prepared in a stationary state ρ_0. In the presence of driving we look for a first order solution $\rho(t) = \rho_0 + \tilde{\rho}(t)$. The equation for $\tilde{\rho}(t)$ is

$$\frac{\partial \tilde{\rho}(t)}{\partial t} \approx -i[\mathbf{H}_0, \tilde{\rho}(t)] + if(t)[\mathbf{V}, \rho_0]. \tag{A1}$$

This equation can be rewritten as

$$\frac{\partial}{\partial t}[\mathbf{U}_0(t)^{-1}\tilde{\rho}(t)\mathbf{U}_0(t)] \approx if(t)[\mathbf{U}_0(t)^{-1}\mathbf{V}\cdot\mathbf{U}_0(t), \rho_0],$$

where $\mathbf{U}_0(t)$ is the evolution operator which is generated by $\mathbf{H}_0$. The solution of the latter equation is

$$\tilde{\rho}(t) \approx \int^t i\{\mathbf{V}[-(t-t')], \rho_0\} f(t') dt', \tag{A2}$$

where we use the usual definition of the "interaction picture" operator $\mathbf{V}(\tau) = \mathbf{U}_0(\tau)^{-1}\mathbf{V}\cdot\mathbf{U}_0(\tau)$.

Consider now the time dependence of the expectation value $\langle\mathbf{F}\rangle_t = \text{tr}[\mathbf{F}\rho(t)]$ of an observable. Disregarding the zero order contribution, the first order expression is

$$\langle \mathbf{F}\rangle_t \approx \int^t i\,\mathrm{tr}\{\mathbf{F}[\mathbf{V}(-(t-t')),\rho_0]\}f(t')dt'$$

$$= \int^t \alpha(t-t')f(t')dt',$$

where the response kernel $\alpha(\tau)$ is defined for $\tau > 0$ as

$$\alpha(\tau) = i\,\mathrm{tr}\{\mathbf{F}[\mathbf{V}(-\tau),\rho_0]\} = i\,\mathrm{tr}\{[\mathbf{F},\mathbf{V}(-\tau)]\rho_0\}$$

$$= i\langle[\mathbf{F},\mathbf{V}(-\tau)]\rangle = i\langle[\mathbf{F}(\tau),\mathbf{V}]\rangle. \tag{A3}$$

We have used above the cyclic property of the trace operation; the stationarity $\mathbf{U}_0\rho_0\mathbf{U}_0^{-1} = \rho_0$ of the unperturbed state; and the definition $\mathbf{F}(\tau) = \mathbf{U}_0(\tau)^{-1}\mathbf{F}\cdot\mathbf{U}_0(\tau)$.

APPENDIX B: REMARKS REGARDING THE GENERALIZED SUSCEPTIBILITY

In this appendix we would like to further illuminate the relation between the generalized susceptibility and the conductance matrix. The generalized susceptibility $\chi^{kj}(\omega)$ is the Fourier transform of the causal response kernel $\alpha^{kj}(\tau)$. Therefore it is an analytic function in the upper half of the complex ω plan, whose real and imaginary parts are related by Hilbert transforms (Kramers-Kronig relations)

$$\chi_0^{kj}(\omega) \equiv \mathrm{Re}[\chi^{kj}(\omega)] = \int_{-\infty}^{\infty} \frac{\mathrm{Im}[\chi^{kj}(\omega')]}{\omega' - \omega}\frac{d\omega'}{\pi}. \tag{B1}$$

The imaginary part of $\chi^{kj}(\omega)$ is the sine transforms of $\alpha^{kj}(\tau)$, and therefore it is proportional to ω for small frequencies. Consequently it is convenient to write the Fourier transformed version of Eq. (3) as

$$[\langle F^k\rangle]_\omega = \sum_j \chi_0^{kj}(\omega)[x_j]_\omega - \mu^{kj}(\omega)[\dot{x}_j]_\omega, \tag{B2}$$

where the dissipation coefficient is defined as

$$\mu^{kj}(\omega) = \frac{\mathrm{Im}[\chi^{kj}(\omega)]}{\omega} = \int_0^\infty \alpha^{kj}(\tau)\frac{\sin(\omega\tau)}{\omega}d\tau. \tag{B3}$$

In this paper we ignore the first term in Eq. (B2) which signify the nondissipative in-phase response. Rather we put the emphasis on the "dc limit" ($\omega \to 0$) of the second term. Thus the conductance matrix $G^{kj} = \mu^{kj}(\omega \to 0)$ is just a synonym for the term "dissipation coefficient." However, "conductance" is a better (less misleading) terminology: it does not have the (wrong) connotation of being specifically associated with dissipation, and consequently it is less confusing to say that it contains a (nondissipative) adiabatic component.

For systems where time reversal symmetry is broken due to the presence of a magnetic field $\mathcal{B}$, the response kernel, and consequently the generalized susceptibility and the conductance matrix satisfies the Onsager reciprocity relations

$$\alpha^{ij}(\tau, -\mathcal{B}) = [\pm]\alpha^{ji}(\tau, \mathcal{B}), \tag{B4}$$

$$\chi^{ij}(\omega, -\mathcal{B}) = [\pm]\chi^{ji}(\omega, \mathcal{B}), \tag{B5}$$

$$G^{ij}(-\mathcal{B}) = [\pm]G^{ji}(\mathcal{B}), \tag{B6}$$

where the plus (minus) applies if the signs of F^i and F^j transform (not) in the same way under time reversal. These reciprocity relations follow from the Kubo formula [Eq. (28)], using $K^{ij}(-\tau, -\mathcal{B}) = -[\pm]K^{ij}(\tau, \mathcal{B})$, together with the trivial identity $K^{ij}(-\tau, \mathcal{B}) = -K^{ji}(\tau, \mathcal{B})$. In Sec. IX we discuss the implications of the reciprocity relations in the context of pumping.

APPENDIX C: EXPRESSIONS FOR B AND G

The functions $C^{ij}(\tau)$ and $K^{ij}(\tau)$ are the expectation values of hermitian operators. Therefore they are real functions. It follows that the real part of their Fourier transform is a symmetric function with respect to ω, while the imaginary part of their Fourier transform is anti symmetric with respect to ω. By definition they satisfy $C^{ij}(\tau) = C^{ji}(-\tau)$ and $K^{ij}(\tau) = -K^{ji}(-\tau)$. It is convenient to regard them as the real and imaginary parts of one complex function $\Phi^{ij}(\tau)$. Namely,

$$\Phi^{ij}(\tau) = \langle F^i(\tau)F^j(0)\rangle = C^{ij}(\tau) - i\frac{\hbar}{2}K^{ij}(\tau), \tag{C1}$$

$$C^{ij}(\tau) = \frac{1}{2}[\Phi^{ij}(\tau) + \Phi^{ji}(-\tau)], \tag{C2}$$

$$K^{ij}(\tau) = \frac{i}{\hbar}[\Phi^{ij}(\tau) - \Phi^{ji}(-\tau)]. \tag{C3}$$

It is possible to express the decomposition $G^{ij} = \eta^{ij} + B^{ij}$ in terms of $\tilde{K}^{ij}(\omega)$. Using the definition (29) we get

$$G^{ij} = \int_0^\infty K^{ij}(\tau)\tau d\tau$$

$$= -\int_{-\infty}^{\infty} \frac{\mathrm{Re}[\tilde{K}^{ij}(\omega)]}{\omega^2}\frac{d\omega}{2\pi} + \left[\frac{1}{2}\frac{\mathrm{Im}[\tilde{K}^{ij}(\omega)]}{\omega}\right]_{\omega=0}. \tag{C4}$$

The first term is antisymmetric with respect to its indexes, and is identified as B^{ij}. The second term is symmetric with respect to its indexes, and is identified as η^{ij}. The last step in the above derivation involves the following identity that hold for any real function $f(\tau)$

$$\int_0^\infty f(\tau)\tau d\tau = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\tilde{f}(\omega)\int_0^\infty e^{-i\omega\tau}\tau d\tau$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\tilde{f}(\omega)\left(-\frac{1}{\omega^2} + i\pi\delta'(\omega)\right)$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\left(-\frac{\mathrm{Re}[\tilde{f}(\omega)]}{\omega^2} - \pi\,\mathrm{Im}[\tilde{f}(\omega)]\delta'(\omega)\right)$$

$$= -\int_{-\infty}^{\infty} \frac{\mathrm{Re}[\tilde{f}(\omega)]}{\omega^2}\frac{d\omega}{2\pi} + \left[\frac{1}{2}\frac{\mathrm{Im}[\tilde{f}(\omega)]}{\omega}\right]_{\omega=0}. \tag{C5}$$

Note that $\mathrm{Im}[\tilde{f}(\omega)]$ is the sine transform of $f(\tau)$, and therefore it is proportional to ω is the limit of small frequencies.

It is of practical value to rederive Eq. (C4) by writing $\Phi^{ij}(\tau)$ using the energies E_n and the matrix elements F^i_{nm}. Then we can get from it straightforwardly (using the definitions) all the other expressions. Namely,

$$\Phi^{ij}(\tau) = \sum_n f(E_n) \sum_m F^i_{nm} F^j_{mn} \exp\left(-i \frac{E_m - E_n}{\hbar} t \right),$$

(C6)

$$\tilde{\Phi}^{ij}(\omega) = \sum_n f(E_n) \sum_m F^i_{nm} F^j_{mn} 2\pi \delta\left(\omega - \frac{E_m - E_n}{\hbar} \right),$$

(C7)

$$\chi^{ij}(\omega) = \sum_{n,m} f(E_n) \left(\frac{-F^i_{nm} F^j_{mn}}{\hbar\omega - (E_m - E_n) + i0} + \frac{F^j_{nm} F^i_{mn}}{\hbar\omega + (E_m - E_n) + i0} \right),$$

(C8)

$$\eta^{ij} = -2\pi\hbar \sum_n f(E_n) \sum_{m(\neq n)} \mathrm{Re}[F^i_{nm} F^j_{mn}] \delta'(E_m - E_n),$$

(C9)

$$B^{ij} = 2\hbar \sum_n f(E_n) \sum_{m(\neq n)} \frac{\mathrm{Im}[F^i_{nm} F^j_{mn}]}{(E_m - E_n)^2}.$$

(C10)

One observes that the expression for B^{ij} coincides with the adiabatic transport result Eq. (26). Alternatively this identification can be obtained by expressing the sum in Eq. (C10) as an integral, getting form it the first term in Eq. (C4):

$$B^{ij} = \frac{2}{\hbar} \int_{-\infty}^{\infty} \frac{\mathrm{Im}[\tilde{\Phi}^{ij}(\omega)]}{\omega^2} \frac{d\omega}{2\pi}$$

$$= \frac{2}{\hbar} \int_{-\infty}^{\infty} \frac{\mathrm{Im}[\tilde{C}^{ij}(\omega)] - \frac{\hbar}{2} \mathrm{Re}[\tilde{K}^{ij}(\omega)]}{\omega^2} \frac{d\omega}{2\pi}$$

$$= -\int_{-\infty}^{\infty} \frac{\mathrm{Re}[\tilde{K}^{ij}(\omega)]}{\omega^2} \frac{d\omega}{2\pi}.$$

(C11)

APPENDIX D: EXPRESSING $\tilde{K}(\omega)$ USING $\tilde{C}(\omega)$

We can use the following manipulation in order to relate $\tilde{K}^{ij}(\omega)$ to $\tilde{C}^{ij}(\omega)$:

$$\tilde{K}^{ij}(\omega) = \sum_n f(E_n) \tilde{K}^{ij}_n(\omega) = \frac{i}{\hbar} 2\pi \sum_{nm} f(E_n) [F^i_{nm} F^j_{mn} \delta(\omega + \omega_{nm}) - F^j_{nm} F^i_{mn} \delta(\omega - \omega_{nm})]$$

$$= \frac{i}{\hbar} 2\pi \sum_{nm} f(E_m) [-F^i_{nm} F^j_{mn} \delta(\omega + \omega_{nm}) + F^j_{nm} F^i_{mn} \delta(\omega - \omega_{nm})]$$

$$= \frac{i}{\hbar} 2\pi \sum_{nm} \frac{f(E_n) - f(E_m)}{2} [F^i_{nm} F^j_{mn} \delta(\omega + \omega_{nm}) - F^j_{nm} F^i_{mn} \delta(\omega - \omega_{nm})]$$

$$= -i\omega\pi \sum_{nm} \frac{f(E_n) - f(E_m)}{E_n - E_m} [F^i_{nm} F^j_{mn} \delta(\omega + \omega_{nm}) + F^j_{nm} F^i_{mn} \delta(\omega - \omega_{nm})] = -i\omega \sum_n f'(E_n) C^{ij}_n(\omega), \quad (D1)$$

where we use the notation $\omega_{nm} = (E_n - E_m)/\hbar$. The third line differs from the second line by permutation of the dummy summation indexes, while the fourth line is the sum of the second and the third lines divided by 2. In the last equality we assume small ω. If the levels are very dense, then we can replace the summation by integration, leading to the relation

$$\int g(E) dE f(E) \tilde{K}^{ij}_E(\omega) = -i\omega \int g(E) dE f'(E) \tilde{C}^{ij}_E(\omega),$$

(D2)

where $\tilde{K}^{ij}_E(\omega)$ and $\tilde{C}^{ij}_E(\omega)$ are microcanonically smoothed functions. Since this equality hold for any smoothed $f(E)$, it follows that the following relation holds (in the limit $\omega \to 0$):

$$\tilde{K}^{ij}_E(\omega) = i\omega \frac{1}{g(E)} \frac{d}{dE} [g(E) C^{ij}_E(\omega)].$$

(D3)

If we do not assume small ω, but instead assume canonical state, then a variation on the last steps in Eq. (D1), using the fact that $[f(E_n) - f(E_m)]/[f(E_n) + f(E_m)] = \tanh[(E_n - E_m)/(2T)]$ is an odd function, leads to the relation

$$\tilde{K}^{ij}_T(\omega) = i\omega \times \frac{1}{\hbar\omega} \tanh\left(\frac{\hbar\omega}{2T} \right) C^{ij}_T(\omega).$$

(D4)

Upon substitution of the above expressions in the Kubo formula for η^{ij}, one obtains the fluctuation-dissipation relation.

APPENDIX E: THE KUBO FORMULA AND THE DIFFUSION IN ENERGY SPACE

The illuminating derivation of Eq. (33) is based on the observation that energy absorption is related to having diffusion in energy space. Let us assume that the probability distribution $\rho(E) = g(E) f(E)$ of the energy satisfies the diffusion equation

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial E}\left[g(E)D_E\frac{\partial}{\partial E}\left(\frac{1}{g(E)}\rho\right)\right]. \tag{E1}$$

The energy of the system is $\langle\mathcal{H}\rangle = \int E\rho(E)dE$. It follows that the rate of energy absorption is

$$\frac{d}{dt}\langle\mathcal{H}\rangle = -\int_0^\infty dE\, g(E)D_E\frac{\partial}{\partial E}\left(\frac{\rho(E)}{g(E)}\right). \tag{E2}$$

For a microcanonical preparation we get

$$\frac{d}{dt}\langle\mathcal{H}\rangle = \frac{1}{g(E)}\frac{d}{dE}[g(E)D_E]. \tag{E3}$$

This diffusion-dissipation relation reduces immediately to the fluctuation-dissipation relation if we assume that the diffusion in energy space due to the driving is given by

$$D_E = \frac{1}{2}\sum_{ij}\tilde{C}_E^{ij}(\omega\to 0)\dot{x}_i\dot{x}_j. \tag{E4}$$

Thus it is clear that a theory for linear response should establish that there is a diffusion process in energy space due to the driving, and that the diffusion coefficient is given by Eq. (E4). More importantly, this approach also allows treating cases where the expression for D_E is nonperturbative, while the diffusion-dissipation relation Eq. (E3) still holds.

A full exposition (and further reference) for this route of derivation can be found in Refs. 16–19. Here we shall give just the classical derivation of Eq. (E4), which is extremely simple. We start with the identity

$$\frac{d}{dt}\langle\mathcal{H}\rangle = \left\langle\frac{\partial\mathcal{H}}{\partial t}\right\rangle = -\sum_k \dot{x}_k F^k(t). \tag{E5}$$

Assuming (for presentation purpose) that the rates $\dot{x}_k$ are constant numbers, it follows that energy changes are related to the fluctuating $F^k(t)$ as

$$\delta E = \langle\mathcal{H}\rangle_t - \langle\mathcal{H}\rangle_0 = -\sum_k \dot{x}_k\int_0^t F^k(t')dt'. \tag{E6}$$

Squaring this expression, and performing microcanonical averaging over initial conditions we obtain

$$\delta E^2(t) = \sum_{ij}\dot{x}_i\dot{x}_j\int_0^t\int_0^t C_E^{ij}(t''-t')dt'\,dt'', \tag{E7}$$

where $C_E^{ij}(t''-t') = \langle F^i(t')F^j(t'')\rangle$ is the correlation function. For very short times this equation implies "ballistic" spreading ($\delta E^2 \propto t^2$) while on *intermediate time scales* it leads to diffusive spreading $\delta E^2(t) = 2D_E t$, where

$$D_E = \frac{1}{2}\sum_{ij}\dot{x}_i\dot{x}_j\int_{-\infty}^\infty C_E^{ij}(\tau)d\tau. \tag{E8}$$

The latter result assumes a short correlation time. This is also the reason that the integration over τ can be extended form $-\infty$ to $+\infty$. Hence we get Eq. (E4). We note that for long times the systems deviates significantly from the initial microcanonical preparation. Hence, for long times, one should justify the use of the diffusion equation (E1). This leads to the classical slowness condition which is discussed in Ref. 19.

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