Quantum transport through a resonant level coupled to chaotic leads

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We study a resonant level coupled to two leads with the latter being described by random matrices. After taking appropriate thermodynamic limit, we obtain a steady current across the resonant level when the Fermi energies of two leads are different. Both the real-time dynamics of current and the I-V curve show features similar to those in the case of regular leads. We derive a formula for the steady current by using the eigenstate thermalization hypothesis and the distribution of off-diagonal elements in the density matrix. Our formula coincides well with the numerical result obtained by solving the Schrödinger equation and then taking the long-time limit.

I. INTRODUCTION

Transport through a nanostructure or single molecule has been attracting the attention of condensed matter physicists during the last thirty years. The development of techniques made it possible to manufacture a mesoscopic island of electrons inside the semiconductor heterostructure or attach a single molecule to metallic leads\(^1,2\). The movement of electrons through these devices is described by quantum mechanics. The electron’s motion is sensitive to the shape of the scattering region, configuration of disorder, electron-electron interaction and electron-phonon interaction. Theoretical and experimental efforts together lead to the discovery of abundant phenomena, such as the universal conductance fluctuations\(^3\), Coulomb blockade\(^4\), Kondo effect\(^1,2\), universal \(\pi\)-phase lapse\(^5\), to name just a few. On the other hand, quantum chaos theory was built on the study of random matrices by Wigner, Dyson and others\(^6,7\), who expected to explain the observed statistical properties of energy levels of heavy nuclei. The theory was developed quickly and applied to different branches of physics, ranging from nuclear to atomic and solid state physics\(^8,9\). Generic features were found not only in the energy levels but also in the observables and wave functions of a quantum system whose classical counterpart is chaotic\(^10,11\). These features were used to explain the process of thermalization, or the existence of nonequilibrium steady states in recent studies\(^16-18\). The application of quantum chaos theory in modeling the transport through a nanostructure was motivated by the need to explain the universal conductance fluctuations\(^21\). It has become a powerful tool in the study of mesoscopic transport\(^22-24\).

Nonequilibrium steady state (NESS) is the focus of attention in the study of transport. If the scattering region is coupled to two infinite leads at different temperatures or chemical potentials, the initial imbalance between leads cannot be removed within finite period. Instead of thermalizing, the system will evolve into a current-carrying NESSH\(^25\). The NESSH is usually obtained by a time propagation from some simple initial state. This approach sometimes causes difficulties due to the lack of reliable numerical or analytical method to access the long-time evolution. A few alternative approaches were proposed by making use of the generic features of chaotic systems\(^26-28\). Nonequilibrium steady state hypothesis (NESSH) is a hypothesis for the density matrix of a chaotic system\(^25,29\). In the eigenbasis of Hamiltonian, the diagonal elements of the density matrix were known to be a Gaussian function of energy after coarse-graining\(^22\). For imbalanced initial states, the off-diagonal elements are inversely proportional to the energy difference. Together with eigenstate thermalization hypothesis (ETH), NESSH explains the finite value of currents in the long-time limit\(^11\). It was numerically verified in a few models, but the current formula based on it has not been checked.

A transport device is composed of a scattering region and the leads. For simplicity, the leads are usually treated as non-interacting reservoirs with uniform level spacing. The whole system then does not display chaotic features, since the lead is overwhelmingly large compared to the scattering region. In real experiments, the leads indeed have irregular shapes, unavoidable impurities, electron-electron interaction and electron-phonon interaction. But it is generally believed that a simplified model of leads has little effect on the transport properties which experimentalists are interested in. In this paper, we study a model of chaotic leads which are described by random matrices. Our motivation is to check the current formula based on NESSH and ETH, which stands in the presence of chaotic leads. Our results verify the current formula. We also find that the transport properties of our model are similar to those of regular leads.

The rest of the paper is organized as follows. The model is introduced in Sec. II In Sec. III we explain ETH, NESSH and derive the current formula. We then verify the formula numerically, and discuss the real-time dynamics of current and current-voltage curve. Sec. IV summarizes our results.

II. MODEL

The model is composed of a resonant level and two leads. The Hamiltonians of the leads are supposed to be random matrices. We start from two independent random matrices \(A_1\) and \(A_2\), which are for the left and right
leads, respectively. The distribution of $A_i$ ($i = 1, 2$) is that of a Gaussian orthogonal ensemble (GOE)\cite{1} with the probability density $P(A_i) \propto \exp[-(A_i^2)/2\sigma^2]$, where $\sigma$ is related to the level spacing. We diagonalize $A_i$ and obtain a series of eigenvalues $\epsilon_{ik}$. The Hamiltonians of the leads are then expressed in the eigenbasis as

$$H_i = \sum_k \epsilon_{ik} c_i^\dagger c_{ik},$$

(1)

where $\epsilon_{ik}$ denotes the energy levels of the leads and $c_{ik}$ and $c_i^\dagger$ are the fermionic field operators. $\epsilon_{ik}$ satisfies the well-known Wigner-Dyson distribution. The dimension of $A_i$ (denoted as $N_0$) is indeed the lead's size. The averaged level spacing in the lead is proportional to $\sigma$ according to random matrix theory. While the bandwidth should keep invariant as the lead’s size increases. Therefore, we keep $N_0\sigma$ a constant when changing $N_0$. In the numerical simulation, large level spacing appears at the spectrum edge of $A_i$, which is unphysical. We keep only $\epsilon_{ik}$ that lies within an interval $[-\Delta, \Delta]$ where $2\Delta$ denotes the bandwidth. After this truncation, the lead has approximately a uniform density of states.

The Hamiltonian of the resonant level is $H_d = \epsilon_d d^\dagger d$. The coupling between the leads and the resonant level is set to a random number. The corresponding Hamiltonian is $H_c = \sum_{i,k} t_{ik} (c_i^\dagger d + H.c.)$. Here $t_{ik}$ is an independent random number which has a Gaussian distribution, i.e. $P(t_{ik}) = \exp \left(-t_{ik}^2/2\sigma_t^2\right)/\sqrt{2\pi\sigma_t}$, where $\sigma_t$ denotes the coupling strength. The total Hamiltonian is written as

$$H = H_1 + H_2 + H_d + H_c.$$  

(2)

In previous studies, the coupling $t_{ik}$ is usually set to a constant or be the same for the left and right leads ($t_{ik} = t_{2k}$). In that case, the whole system can be decoupled into the resonant level coupled to a single reservoir and the other isolated reservoir, by defining the (anti)symmetric basis $c_{\pm k} = (c_{ik} \pm c_{2k})/\sqrt{2}$. This does not hold for model (2), because the levels in different leads are not degenerate and also the couplings to different leads are independent random numbers. In model (2), the parity symmetry is kept only at the statistical level. $t_{ik}$ being a random number is necessary for ETH and NESSH to hold.

It is worth emphasizing that, in model (2), only the single-particle energy levels or wave functions have chaotic features. When we talk about chaos in this paper, we keep ourselves in the single-particle picture. And in the numerical simulation, we choose $N_0$ to be large enough so that the sampling has little effect on the results. We then do not carry out the sampling average.

Since there is no interaction between particles, we use exact diagonalization (ED) to obtain all the single-particle eigenvectors $\{|\alpha\rangle\}$ and eigenvalues $\{E_\alpha\}$ of Hamiltonian (2). In Fig. $1$ we plot the single-particle density of states $D(E)$. We see that $D(E)$ changes smoothly with $E$ and reaches a maximum at $E = 0$. And the density of states increases with the lead’s size, as we expect.

![Figure 1](image.png)

FIG. 1. (Color online) The density of states for different $N_0$. We set $\epsilon_d = 0$, $\Delta = 3$, $N_0\sigma = 200$ and $\sqrt{\sigma_t} = \sqrt{2}/(SD)$ with $D_l$ being the averaged density of states in the leads. $D(E)$ is obtained by choosing an energy interval of width $\delta E$ centered at $E$ and then counting the eigenenergies falling within it. In this figure we choose $\delta E = 0.4$.

For realizing a current-carrying nonequilibrium state, we employ next protocol. At the time $\tau < 0$, two leads are at zero temperature with the particles occupying the levels up to the Fermi energies. The Fermi energies of the left and right leads are set to $V/2$ and $-V/2$, respectively. The coupling $t_{ik}$ is switched on at the time $\tau = 0$, and the particles then flow from the left (lead 1) to right (lead 2).

The observable that we are interested in is the current $I$, which is defined as

$$I = \frac{1}{2} \left( \frac{dN_2}{d\tau} - \frac{dN_1}{d\tau} \right) = \frac{i}{2} \sum_{j,k} (-1)^j t_{jk} \left( c_{j,k}^\dagger d - d^\dagger c_{j,k} \right),$$

(3)

where $N_j = \sum_k c_{j,k}^\dagger c_{j,k}$ is the number of particles in lead $j$. $\epsilon$ denotes the imaginary unit. In the study of transport, one usually defines the broadening of the resonant level as $\Gamma(E) = \sum_{\epsilon_{ik}} \pi \delta(E - \epsilon_{ik})/\epsilon_{ik}^2$. To obtain a well-defined thermodynamic limit, we keep $\Gamma$ invariant as the lead’s size increases. Therefore, we set $\epsilon_t$ to be inversely proportional to $\sqrt{D_l}$, where $D_l$ is the averaged density of states in the leads. Note that $\sigma_t^2$ is the mean of $\epsilon_{ik}$.

The current contributed by a single particle initially located at the level $k$ of lead $j$ can be expressed as

$$I^k(\tau) = \sum_{\alpha \neq \beta} e^{-i(E_{\alpha} - E_{\beta})\tau} P_{\alpha\beta}^k I_{\beta\alpha},$$

(4)

where $P_{\alpha\beta}^k = \langle \alpha | P^k | \beta \rangle$ and $I_{\beta\alpha} = \langle \beta | I | \alpha \rangle$ are the initial density matrix and current matrix in the single-particle eigenbasis, respectively. Here $P^k$ denotes the density matrix of a single particle occupying the level $\epsilon_{jk}$ of lead $j$. According to the definition of current operator, it is easy
to see that $I_{\alpha\alpha}$ must be zero. This explains why the terms with $\alpha = \beta$ are excluded in Eq. (3).

In the absence of particle-particle interactions, the total current through the resonant level can be obtained by summing up the currents contributed by each particle, i.e. $I(\tau) = \sum_{k} I^k(\tau)$. At $\tau = 0$ the particles occupy the levels of lead 1 and 2 up to the Fermi energies. The current contributed by the particles at the levels lower than $-V/2$ in lead 1 will compensate the current contributed by the particles in lead 2. Therefore, we only need to consider the contribution from the particles in lead 1 at the levels between $-V/2$ and $V/2$. We define a new matrix $\rho_{\alpha\beta} = \sum_k \rho_{\alpha k}^{(k)}$, where the sum is over the energy levels between $-V/2$ and $V/2$ in lead 1. Thus, the total current can be expressed as

$$I(\tau) = \sum_{\alpha \neq \beta} e^{-i(E_\alpha - E_\beta)\tau} \rho_{\alpha\beta} I_{\beta\alpha}. \quad (5)$$

### III. ETH, NESSH and Current Formula

We rewrite Eq. (5) by using ETH and NESSH. According to them, the off-diagonal elements of the current matrix and $\rho_{\alpha\beta}$ can be expressed as

$$I_{\alpha\beta} = D^{-1/2}(\hat{E}) f_{\beta}(\hat{E}, \omega) R_{\alpha\beta}^D,$$
$$\rho_{\alpha\beta} = D^{-3/2}(\hat{E}) f(\hat{E}, \omega) R_{\alpha\beta}, \quad (6)$$

where $\hat{E} = (E_\alpha + E_\beta)/2$ and $\omega = E_\alpha - E_\beta$ are the average energy and energy difference, respectively. $D(\hat{E})$ is the density of states at the average energy. The functions $f_{\beta}$ and $f$ determine the dependence of the energy on the current after coarse-graining, which are critical for calculating the expectation value of current. $R_{\alpha\beta}^D$ and $R_{\alpha\beta}$ are real random numbers with zero mean and unit variance, which reflect the fluctuation of the off-diagonal elements. The hermitianity of $\rho$ and $I$ requires $f_{\beta}(\hat{E}, \omega) = f_{\beta}^{*}(\hat{E}, -\omega)$, $f(\hat{E}, \omega) = f^{*}(\hat{E}, -\omega)$, $R_{\alpha\beta} = R_{\beta\alpha}^D$ and $R_{\alpha\beta} = R_{\beta\alpha}$. Since the elements of the Hamiltonian are real, all its eigenvectors have real components. $\rho_{\alpha\beta}$ is then real but $I_{\alpha\beta}$ is purely imaginary, whereas, $f(\hat{E}, \omega) = f(\hat{E}, -\omega)$ is real but $f_{\beta}(\hat{E}, \omega) = -f_{\beta}(\hat{E}, -\omega)$ is purely imaginary functions.

Note that the first equation of (6) is the eigenstate thermalization hypothesis for the off-diagonal elements of the current operator in the eigenbasis of Hamiltonian. This hypothesis was raised by Srednicki18 and verified in several numerical experiments (see Ref. 17 for a review). The second equation of (6) is the nonequilibrium steady-state hypothesis. It assumes that the off-diagonal elements of density matrix have similar form as those of observable matrix. It was verified in a few models of spins and lattice fermions20,23. $\rho_{\alpha\beta}$ is the sum of single-particle density matrix. We find that NESSH also stands for $\rho_{\alpha\beta}$.

According to NESSH, for an initial state with imbalance between two leads, the dynamical characteristic function $f$ scales as $1/\omega$ in the limit $\omega \to 0$, that is

$$f = \frac{\rho(\hat{E}, \omega)}{\omega} \quad (7)$$

with $\rho(\hat{E}, \omega)$ converging to a finite value in the limit $\omega \to 0$. Substituting Eq. (8) and (9) into Eq. (3), we obtain

$$I(\tau) = \int d\hat{E}d\omega e^{-i\omega\tau} D(\hat{E} + \omega/2) D(\hat{E} - \omega/2) \frac{\rho(\hat{E}, \omega)}{\omega} f_{\beta}(\hat{E}, -\omega) R_{\alpha\beta}^D R_{\beta\alpha}^D \quad (8)$$

where we have used $\sum_\alpha \to \int d\omega D(\omega)$. We are interested in the steady current in the long time limit, denoted as $I = \lim_{\tau \to \infty} I(\tau)$. Noticing that $f_{\beta}$ is not continuous at $\omega = 0$, we use the notation $f_{\beta}(\hat{E}, 0^+) = \lim_{\omega \to 0^+} f_{\beta}(\hat{E}, \omega)$. It is easy to see $f_1(\hat{E}, 0^+) = -f_1(\hat{E}, 0^+)$, because $f_{\beta}$ is an odd function of $\omega$. $R_{\alpha\beta}^D R_{\beta\alpha}^D$ is a random number, and we use $C_{\rho\beta} = R_{\alpha\beta}^D R_{\beta\alpha}^D$ to denote its mean. $C_{\rho\beta}$ is a continuous function of $\hat{E}$ and $\omega$. In the limit $\tau \to \infty$, the integral with respect to $\omega$ in Eq. (8) can be done precisely. And it is not difficult to find

$$I = i\pi \int d\hat{E} \rho(\hat{E}, 0)f_{\beta}(\hat{E}, 0^+)C_{\rho\beta}(\hat{E}, 0). \quad (9)$$

Eq. (9) is the current formula of a steady state, which is based on ETH and NESSH and is expected to stand in general chaotic systems. Next we will check Eq. (9) numerically.

Let us see the properties of the functions $\rho(\hat{E}, 0)$ and $f_{\beta}(\hat{E}, 0^+)$. Fig. 2(a) displays $|f_{\beta}|$ as a function of $\hat{E}$. Note that $f_{\beta}$ is purely imaginary, therefore, we plot its absolute value. It is clear that $f_1$ does not change much with $\hat{E}$. One can approximately take $f_{\beta}(\hat{E}, 0^+) \approx f_{\beta}(0, 0^+)$ as a constant. On the other hand, the function $\rho$ displays a peak structure. In the case of $\epsilon_d = 0$, the peak is centered at $\hat{E} = 0$ (see Fig. 2(b)). The different characteristics between $\rho$ and $f_1$ are due to the fact that $f_1$ comes from the observable operator but $\rho$ is from the density matrix. $f_{\beta}$ is independent of the occupation of particles but $\rho$ depends on it.

At the same time, both $f_{\beta}$ and $\rho$ depend on the lead’s size. The magnitude of $f_{\beta}$ decreases as $N_0$ increases, while that of $\rho$ increases. $f_{\beta}$ and $\rho$ do not have a well-defined limit as $N_0 \to \infty$ (the thermodynamic limit). But the product $\rho f_{\beta} C_{\rho\beta}$ does have a well-defined thermodynamic limit, which leads to a finite steady current. It is worth emphasizing that the steady current is nonzero only in thermodynamic limit. For finite size of leads, the initial imbalance can be removed within finite period, and then the current always decays to zero.

The shape of $\rho(\hat{E}, 0)$ depends both on the initial occupation and the position of the resonant level. Fig. 3(a) shows $\rho$ at different voltage bias. Here an important energy scale is the resonant level broadening $\Gamma$, which defines the region of resonant tunneling. When $V$ is less
than \( \Gamma \), \( \rho \) displays a rectangular peak with a flat top, and the width of the peak is approximately \( 2V \). As \( V \) increases, the peak becomes wider. But as \( V \) goes beyond \( \Gamma \), the peak is not rectangular any more. Instead, \( \rho \) drops quickly to zero as \( |\bar{E}| \) is larger than \( \Gamma \). The width of the peak is determined by \( \Gamma \), being less than \( 2V \). Fig. 2(b) displays \( \rho \) at different \( \epsilon_d \). The center of the peak changes with \( \epsilon_d \). Indeed, the peak is approximately centered at \( \bar{E} = \epsilon_d \). But the shape of \( \rho \) is indifferent to \( \epsilon_d \).

The shape of \( \rho(\bar{E}, 0) \) is reminiscent of the transmission coefficient in the transport through a resonant level. For the single-impurity Anderson model with uniform level-spacing in leads, the steady current is well known to be an integral of the function \( 1/(|E^2 - \epsilon_d| + \Gamma^2) \) in the range \([-V/2, V/2]\). We see that \( \rho(\bar{E}, 0) \) has a similar shape to \( 1V/(|\bar{E}^2 - \epsilon_d| + \Gamma^2) \), where \( 1V \) is the indicator function which equals to 1 in the range \([-V/2, V/2]\) but zero otherwise. As is well known, in the transport through a resonant level, the particle can tunnel from one lead to the other lead if its energy is close to the resonant level, otherwise, the particle is blocked. It is the particles of energy around the resonant level which contribute mainly to the current, while the other particles contribute little. This fact is reflected by the peak structure of \( \rho(\bar{E}, 0) \).

![FIG. 2. (Color online) (a) The function \( f_\beta(E, 0^+) \) with different \( N_0 \). We obtain \( f_\beta(E, 0^+) \) by averaging \( I_{\alpha\beta} \) over the energy interval \( \omega \in (0, \delta_\omega) \). Here we set \( \delta_\omega = 0.1 \). (b) The function \( \rho(\bar{E}, 0) \) with different \( N \). \( \rho(\bar{E}, 0) \) is obtained by averaging \( \rho_{\alpha\beta} \) over the energy interval \( \omega \in (0, \delta_\omega) \). The voltage bias is set to \( V = 1 \). The other parameters are set to be the same as those of Fig. 1. Especially, \( \sigma = \sqrt{2/(5D_f)} \) corresponds to \( \Gamma \sim 0.8\pi \).](image1)

![FIG. 3. (Color online) (a) The three bottom lines (blue) plot the function \( \rho(\bar{E}, 0) \) at different voltage bias, while the three top lines (red) plot the function \( C_{\rho I}(\bar{E}, 0) \). The functions at different \( V \) are distinguished by different linetypes. In this panel, we set \( \Delta = 3, \epsilon_d = 0, N_{\epsilon\sigma}(\bar{E}) = 200, N_0 = 7000 \) and \( \sigma_l = \sqrt{1/(10D_I)} \) (corresponding to \( \Gamma \sim 0.2\pi \)). The functions \( \rho \) and \( C_{\rho I} \) are obtained by averaging \( \rho_{\alpha\beta} \) and \( R_{\alpha\beta} R_{\beta\alpha}^d \) over the energy interval \( \omega \in (0, \delta_\omega) \), respectively. \( \delta_\omega = 0.1 \) is chosen. (b) We fix \( V = 0.7 \) and plot the functions \( \rho \) (three bottom lines) and \( C_{\rho I} \) (three top lines) at different \( \epsilon_d \). \( \epsilon_d = -0.5, 0, 0.5 \) corresponds to the solid, dashed and dotted lines, respectively.](image2)
cialized initial condition, i.e. the particles occupying the levels of lead 1 in the energy range \([-V/2, V/2]\). The current obtained in such a way is a function of time. Fig. 4 plots the evolution of current for different lead’s size. For large enough leads \((N_0 = 7000)\), the current decays quickly to its quasi-stable value and stays there for quite a long time. Indeed, the current displays a clear plateau already for \(N_0 = 4000\). The plateau in the curve \(I(\tau)\) indicates that the imbalanced initial state will evolve into a NESS in the thermodynamic limit \((N_0 \to \infty)\). This is what we expect. The chaotic lead with random coupling is a good model for mesoscopic transport.

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\begin{align*}
\text{FIG. 4. (Color online) The real-time dynamics of current with different sizes of leads. We set } & \Delta = 3, \epsilon_d = 0, N_0 \sigma = 200, \\
& V = 0.5 \text{ and } \sigma_I = \sqrt{1/(10D_I)} \text{ (corresponding to } \Gamma \sim 0.2\pi). \\
\text{The dashed line is } & I = 0.076, \text{ which is obtained by numerically integrating Eq. (9). The inset plots the steady current } I \\
\text{as a function of the voltage bias } & V.
\end{align*}
\]

The plateau of \(I(\tau)\) is compared with the steady current obtained from Eq. (9) for various choice of parameters. Fig. 4 shows an example, in which the result of Eq. (9) \((I = 0.076)\) is marked. We see that the plateau of \(I(\tau)\) goes closer to 0.076 as \(N_0\) increases, and becomes indistinguishable from the straight line \(I = 0.076\) as \(N_0 = 7000\). For the other choice of parameters, we also obtain a good coincidence between the plateau of \(I(\tau)\) and Eq. (9). Therefore, Eq. (9) is a good approximation for the steady current.

Finally, the inset of Fig. 4 plots the I-V curve. The steady current grows linearly with voltage bias at small \(V\), and gradually saturates at large \(V\), which is reminiscent of the inverse tangent function that is the the I-V curve of the single-impurity Anderson model. The leads of random matrices coupled randomly to a resonant level do result in the similar I-V curve as the leads of uniform level spacing coupled uniformly to a resonant level.

IV. SUMMARY

In summary, if the leads are random matrices and the coupling between the resonant level and leads is a random number, the density matrix and current matrix of the system display chaotic features. A generic expression (Eq. (9)) for the steady current in thermodynamic limit is obtained, which is verified by comparison with the numerical results. The steady current is an integral of the product of \(f_I\), \(\rho\) and \(\mathcal{C}_{\rho I}\) with respect to energy. Here, \(f_I\), \(\rho\) and \(\mathcal{C}_{\rho I}\) correspond to the off-diagonal elements of the current operator and initial density matrix after coarse graining and their correlation, respectively. \(\rho\) as a function of energy displays a peak structure, which has a similar shape as the transmission coefficient. Consequently, the I-V curve is similar to that of regular leads and constant coupling (single-impurity Anderson model).

The formula (9) clearly shows that the observable of NESS depends only on the off-diagonal elements with infinitesimal energy difference. According to it, the steady current is determined by the values of \(\rho\), \(f_I\) and \(\mathcal{C}_{\rho I}\) in the limit \(\omega \to 0\), but is indifferent to their values at any finite \(\omega\). The steady current is also indifferent to the diagonal elements at \(\omega = 0\), because the diagonal elements of current matrix are all zero. This is a nonequilibrium version of memory loss. After the system evolves into a NESS, most elements of its initial density matrix have no contribution to observables except the off-diagonal ones with infinitesimal energy difference.

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