The local temperature and chemical potential inside a mesoscopic device driven out of equilibrium

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Abstract. In this paper we introduce a method for calculating the local temperature and chemical potential inside a mesoscopic device out of equilibrium. We show how to check the conditions of local thermal equilibrium when the whole system is out of equilibrium. In particular, we study the on-site chemical potentials inside a chain coupled to two reservoirs at a finite voltage bias. We observe in the presence of disorder a large fluctuation in on-site chemical potentials, which can be suppressed by the electron–electron interaction. By taking the average with respect to the configurations of the disorder, we recover the classical picture where the voltage drops monotonically through the resistance wire. We prove the existence of local intensive variables in a mesoscopic device which is in equilibrium or not far from equilibrium.

Keywords: disordered systems (theory), mesoscopic systems (theory), quantum transport in one dimension

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1. Introduction

In recent years the thermodynamic properties of a quantum system driven out of equilibrium have attracted more and more attention [1]–[7]. In particular, in mesoscopic transport a standard method of studying nonequilibrium steady states (NESS) has been established by using the evolution approach in the Keldysh formalism [8]–[10]. In mesoscopic transport we study small quantum systems with a few degrees of freedom which must be described by quantum mechanics. The small system is connected to several infinite reservoirs which are in thermal equilibrium, with different temperatures and chemical potentials. The nonequilibrium steady state is approached by an evolution starting from the supposed initial condition. The evolution approach has been widely used to study the transport through quantum point contacts, quantum dots, single molecules and carbon nanotubes. Good agreement between theoretical predictions and experimental results has been obtained.

Now a fundamental question arises as to whether the concepts in equilibrium thermodynamics apply to the mesoscopic system driven out of equilibrium. For example, temperature is an important concept in equilibrium thermodynamics, where it is also called the intensive thermodynamic variable of a system. According to the zeroth law of thermodynamics, it is always possible to assign a temperature to a system in thermal equilibrium. Even if the whole system is out of equilibrium, when the conditions of local equilibrium are fulfilled, we can divide the system into small cells which are in thermal equilibrium to a good approximation. In principle we are then able to define the local

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temperature in each cell. However, up to now the sole way of calculating the temperature according to the density matrix of a system is by using the extremal principle in statistical mechanics. According to Glansdorff and Prigogine [11], for systems away from equilibrium there is no general variational principle. Then temperature, arising from the Lagrangian multiplier in statistical mechanics, loses its meaning. Although many authors have focused their efforts on local extremal principles [11]–[23] which can be used for obtaining local solutions when the system is not far from equilibrium and dissipative processes dominate, there is no consensus as regards whether these principles can be applied to mesoscopic transport [24].

Mesoscopic transport should have been a touchstone of the principles in nonequilibrium statistical mechanics. But this is not the case because of a lack of definitions of local intensive thermodynamic variables, which play central roles in statistical mechanics. In the evolution approach, even if the currents can be easily calculated, up to now there has been no way of calculating the temperature in a local region of the mesoscopic device, because the current and the temperature are two different kinds of physical quantities: the current is calculated as the expectation value of the quantum operator of current with respect to the density matrix of the system, while the temperature is intensive, and in statistical mechanics is introduced ‘by hand’ as a Lagrangian multiplier before one writes down the density matrix. There is no ‘temperature operator’, although in fact temperature is also measurable like all the other physical quantities. Such a discrepancy between temperature and other physical quantities causes trouble in the theory of quantum transport. In fact there is no reason for ignoring the local intensive variables in mesoscopic devices, since in principle we could continuously increase the device size without meeting a point of breakdown of the underlying physical laws, e.g. the Schrödinger equation, until the device is in the macroscopic region where the driving forces are the gradients of intensive variables rather than the differences between reservoir values.

In this paper we get rid of this discrepancy by introducing a method for checking whether the local equilibrium condition is fulfilled in arbitrary nonequilibrium steady states and for calculating the local temperature and chemical potential. We apply our method to a disordered chain subject to a current, and study the on-site chemical potential by attaching an auxiliary site to it. We study the distribution of on-site chemical potentials at different disorder strengths and reservoir voltage biases. In section 2 we discuss how to reach the nonequilibrium steady state in an evolution approach by taking the thermodynamic limit before taking \( t \to \infty \). In section 3, we discuss the condition of local equilibrium and suggest a method for calculating the local intensive variables. In section 4, we introduce the model of a disordered 1D chain and show the distribution of on-site chemical potentials inside it subject to finite voltage bias. Section 5 is a short summary.

2. When will a system evolve into a nonequilibrium steady state?

When we say that a system evolves into a nonequilibrium steady state, we mean that when time goes to infinity the system relaxes toward a stationary state in which some flows are nonzero, but there is no time variation. The NESS should be distinguished from the equilibrium state in which some nonzero flows exist in a ring structure. The
latter can exist in an isolated system with finite number of degrees of freedom, such as the mesoscopic ring in a magnetic field with a persistent current. But an isolated system with finite number of degrees of freedom will never evolve into a NESS, since if there exists a flow in an irreversible process, the flow carries some quantity (mass, energy or charge) from one part of the system to another part, causing a continuous decreasing of the quantity in one part and increasing in the other part due to the conservation law. This contradicts the steady state argument.

To avoid the paradox between irreversibility and stationarity, we embed the system in an environment so that the composite isolated system is infinite. Then the total quantity in the whole system is infinite, so any global conservation law is invalidated. At the same time if we consider the local subsystem, the density of matter and the flow are both time invariant.

In practice, to approach a nonequilibrium steady state we generally begin with a finite model and then increase the number of degrees of freedom to infinity. This process is called taking the thermodynamic limit. One must note that in most cases taking the thermodynamic limit and taking \( t \rightarrow \infty \) are not exchangeable. To get the nonequilibrium steady state one must take the thermodynamic limit before taking \( t \rightarrow \infty \). Next we give two examples, namely the single-impurity Anderson model and an infinite chain.

### 2.1. The single-impurity Anderson model

Let us recall the single-impurity Anderson model which describes a quantum dot coupled to two leads (the left and right leads). This model is exactly solvable without considering electron–electron interaction and has been extensively studied by the condensed matter community. It is well known that a stationary current through the dot will be established if the two leads are at different chemical potentials and the coupling between leads and the dot has been switched on in the infinite past.

The crucial condition for a stationary nonzero current is that the number of levels in the leads must be infinite. Otherwise the current perpetually oscillates with an average value of zero. This is easy to see if we suppose that there is only one level in each lead. Then the Hamiltonian is written as

\[
\hat{H} = \omega (\hat{c}_L \hat{d}_L + \hat{c}_R \hat{d}_R + \hat{d} \hat{d}^\dagger) + g(\hat{c}_L \hat{d}^\dagger + \hat{c}_R \hat{d}^\dagger + \text{h.c.}),
\]

where \( \hat{c}_L, \hat{c}_R \) and \( \hat{d} \) denote the annihilation operators in the left lead, the right lead and the dot respectively. The left lead is occupied by an electron at time \( t = 0 \). After switching on the coupling, we find the current to be

\[
I_L(t) = \frac{\sqrt{2}}{2} |g| \sin(\sqrt{2}|g|t) + \frac{\sqrt{2}}{4} |g| \sin(2\sqrt{2}|g|t),
\]

which satisfies the conservation law

\[
I_L(t) = -\frac{dN_L(t)}{dt}.
\]

Here \( N_L \) is the electron number in the left lead. Whatever finite number of levels there are in leads, the time-averaged current must be zero. Otherwise the current will eventually empty one lead and make the other overflow. In thermodynamic limit, however, the term...
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in the right-hand side of equation (3) is nonsense since $N_L$ is infinite. So the conservation law no longer prohibits a nonzero current.

One should notice that the stationary current in a NESS is not carried by the eigenstates of the Hamiltonian. The invariant term of the current operator in the Anderson model is zero. In other words, the expectation value of $\hat{I}_L$ is zero with respect to arbitrary eigenstates, because the current operator is $\hat{I}_L \sim [\hat{H}, \hat{N}_L]$. The fact that the eigenstates carry no current distinguishes NESS with equilibrium states carrying nonzero current.

2.2. An infinite chain

In the single-impurity Anderson model we employ open boundary conditions, while the NESS can also be approached in an infinite chain with periodic boundary conditions.

The Hamiltonian of a chain of length $2N$ with periodic boundary conditions is written as

$$\hat{H} = -g \sum_{i=1}^{2N-1} (\hat{c}_i^\dagger \hat{c}_{i+1} + \text{h.c.}) - g(\hat{c}_{2N}^\dagger \hat{c}_1 + \text{h.c.}).$$

In the momentum basis it is diagonal, with $\hat{H} = \sum_{k=0}^{2N-1} \epsilon_k \hat{c}_k^\dagger \hat{c}_k$ where $\epsilon_k = -2g \cos(2\pi k/2N)$. The operator at site $j$ is expressed in the momentum basis as

$$\hat{c}_j = \sum_{k=0}^{2N-1} e^{i2\pi jk/2N} \sqrt{2N} \hat{c}_k.$$ (5)

Then we immediately have

$$\hat{c}_j(t) = \sum_{j'=1}^{2N} W_{jj'} \hat{c}_{j'},$$

where $W_{jj'} = \sum_{k=0}^{2N-1} (1/2N)e^{i(\pi k(j-j')/N-\epsilon_k t)}$ is the propagator.

Now we suppose that the sites from $j = 1$ to $N$ are all occupied by electrons and sites from $j = N + 1$ to $2N$ are empty at the initial time $t = 0$. Then the hopping interaction in equation (4) is switched on. The local current and electron density at arbitrary time are worked out easily, given the current operator, from site $j$ to $(j + 1)$:

$$\hat{I}_{j\rightarrow j+1} = -ig(\hat{c}_j^\dagger \hat{c}_{j+1} - \hat{c}_{j+1}^\dagger \hat{c}_j).$$

(6)

Obviously this definition satisfies the local conservation law $\frac{dn_j}{dt} = I_{j-1\rightarrow j} - I_{j\rightarrow j+1}$.

The current is evaluated as

$$I_{j\rightarrow j+1}(t) = 2g \sum_{j'=1}^{N} \text{Im} W_{jj'}^* W_{j+1,j'},$$

and the electron density at site $j$ as

$$n_j(t) = \sum_{j'=1}^{N} |W_{jj'}|^2.$$ (8)

According to the behavior of the scaled parameter $g$ as $N \rightarrow \infty$, the system will evolve into either a NESS with nonzero local current or a steady state with zero current everywhere.
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Figure 1. The evolution of current from site $N$ to $N+1$ for different chain lengths when $g/N$ is a constant. Here we set $g = N/800$. The $y$-axis is the ratio of the current to $g$ and $x$-axis the time. One should note that the unit of time is not shown in the figure. But it is in fact $800N/g$. The function $I_{N\to N+1}(t)/g$ can converge when $N$ is as large as 800.

If $g/N$ remains constant, the electron density $n_j(t)$ and the ratio $I_{j\to j+1}(t)/g$ oscillate around certain values with a period which does not vary with $N$ (see figure 1). As $N \to \infty$, $n_j(t)$ and $I_{j\to j+1}(t)/g$ both have well defined thermodynamic limits. For arbitrary $j$, the oscillation amplitudes of $n_j(t)$ and $I_{j\to j+1}(t)/g$ decay in the course of time. When time goes to infinity the electron density approaches 0.5 and the current goes to zero everywhere.

If $g$ remains constant, however, as $N$ increases, the period of the functions $n_j(t)$ and $I_{j\to j+1}(t)$ increase accordingly. For any finite $N$, the current eventually decays toward zero. But if we take the thermodynamic limit first, the period of oscillations goes to infinity. The current at some sites will approach a nonzero value when we take $t \to \infty$ thereafter.

Let us first study the currents at sites $j = (1 + x)N$ when $0 < x < 1$ is a constant. One should note that $j$ will vary with $N$. In the thermodynamic limit these sites are infinitely far away from the electron reservoir (the sites from 1 to $N$), so the current $I_{j\to j+1}$ and the electron density $n_j$ both approach zero. On the other hand, at a site $j = (1 + x)N$ with $-1 < x < 0$, which is in the reservoir, the current approaches 0 and the electron density approaches 1.

The site $N + n$ where $n$ is an arbitrary integer is in the boundary between the reservoir and the vacuum. There the current approaches approximately 0.636 (see figure 2), a nonzero value. At the same time the electron density approaches 0.5. Here $n$ can be arbitrarily large or small since in the thermodynamic limit we always have $|n| \ll N$ whatever $n$ is. Then in the system consisting of sites $N + n$, which can even be macroscopic in size, there exists a well defined nonequilibrium steady state.

As shown above, solving the equations of motion and taking the thermodynamic limit before taking $t \to \infty$ supplies a platform for studying the NESS. In section 3 we will discuss how to define the thermodynamic intensive variables, such as the temperature and
Figure 2. The evolution of the current for different $N$ when $g$ is a constant. Here we set $g = 1$. With increasing $N$ the period of the current will go to infinity. If one takes $N \to \infty$ before taking $t \to \infty$, the steady limit of the current will be around 0.636.

chemical potential, in the NESS obtained by this approach. The definition of intensive variables is important both in experiments where they can be measured and in the theory of nonequilibrium thermodynamics where they must be given beforehand.

3. How do we calculate the local temperature and chemical potential in a system in nonequilibrium steady states?

Today, quantum mechanics is believed to be the universal theory describing the evolution of both microscopic and macroscopic systems. In quantum mechanics the observables are represented by linear operators acting on the Hilbert space. On the other hand the concepts in thermodynamics, such as the temperature $T$ and chemical potential $\mu$, have been widely used to describe the macroscopic systems in everyday life. But unfortunately these intensive variables in thermodynamics cannot be directly related to quantum operators. Instead, in statistical mechanics, $T$ and $\mu$ are introduced ‘by hand’ as the Lagrangian multipliers for the energy $\hat{H}$ and the particle number $\hat{N}$ respectively. The lack of interpretations for $T$ and $\mu$ at the microscopic level causes problems in nonequilibrium thermodynamics, where there is no generally accepted variational principle, and then the temperature and chemical potential (or more strictly the local temperature and local chemical potential) cannot be determined from the density matrix of the system. In other words, there is no way of calculating $T$ and $\mu$ in a NESS which is not the result of a variational principle but the steady limit of the state evolving according to the Schrödinger equation. We contribute to solving this problem by providing a method for calculating the local temperature and chemical potential in a system according to its density matrix.

To avoid ambiguity, we would like to emphasize that we do not define the local temperature and chemical potential in arbitrary NESS. In fact the definitions of $T$ and $\mu$ make sense only in systems where the local thermodynamic equilibrium conditions are
fulfilled. In other words, if we divide the system into small cells, each cell must look like it is in an equilibrium state, even if the whole system undergoes an irreversible process. In systems violating the local equilibrium arguments, one would get arbitrary $T$ and $\mu$ by employing different measurement schemes which give a unique result in an equilibrium system. As will be shown, an approach examining whether the local equilibrium conditions are fulfilled naturally arises from our method.

Let us recall the process of using a mercury thermometer to measure the temperature of an object. We attach the thermometer closely to the target and wait for long enough for the temperatures of the target and the thermometer to become the same. If the target is much larger than the thermometer, its temperature will not be changed during the equilibration process. Then we read out the temperature according to the volume of mercury. This procedure suggests a general scheme for measuring local $T$ and $\mu$ of a system either in equilibrium or out of equilibrium, by attaching an auxiliary apparatus to the region for which we want to take a measurement. After waiting for a period longer than the equilibration time, the auxiliary apparatus will equilibrate if the conditions of local equilibrium are satisfied even if the whole system may be still out of equilibrium. Then $T$ and $\mu$ are read out in the auxiliary apparatus according to their orthodox definitions in equilibrium. The auxiliary apparatus (the ‘thermometer’) should satisfy the following conditions: it must be very small so that it has almost no effect on the original state of the system; and there must be a simple relation between its temperature and some measurable property. Obviously a single site is a suitable candidate for being such an auxiliary apparatus, since it is the smallest apparatus and its occupation number for fermions can be expressed as

$$n_d = \frac{1}{e^{\beta(\epsilon_d - \mu)} + 1},$$

where $\epsilon_d$, $\beta$ and $\mu$ are the energy level, the inverse of temperature and the chemical potential respectively.

Our method is based on the ambitious assumption that a single site will equilibrate after being attached to a large system. This is true only under special conditions, i.e., the coupling between the site and the system must be infinitesimal. Consider an impurity site coupled to a Fermi sea with chemical potential $\mu$ and temperature $T$. This is just the single-impurity Anderson model without interaction. We switch on the coupling at time $t = 0$. Given the energy level $\epsilon_d$ and the level width $\Gamma$ at the impurity site, in the steady limit when time goes to infinity we find the occupation number to be

$$n_d = \frac{\Gamma}{\pi} \int_{-\infty}^{\infty} \frac{1}{e^{\beta(\epsilon - \mu)} + 1} \frac{1}{(\epsilon - \epsilon_d)^2 + \Gamma^2}. \quad (10)$$

Only in the weak coupling limit $\Gamma \rightarrow 0$ does we have $(\Gamma/\pi)/(\epsilon - \epsilon_d)^2 + \Gamma^2 \rightarrow \delta(\epsilon - \epsilon_d)$ and then we recover equation (9). We rewrite equation (9) as

$$\ln\left(\frac{1}{n_d} - 1\right) = \beta \epsilon_d - \beta \mu. \quad (11)$$

Then $\beta$ and $\mu$ can be easily determined by plotting $\ln(1/n_d - 1)$ with respect to $\epsilon_d$.

If the condition of local thermodynamic equilibrium is satisfied, according to the definition, the auxiliary site attached to the system must be in equilibrium and then
equation (11) must be satisfied. Conversely, if the linear relation in equation (11) is satisfied at the attached site, we would make sure that the condition of local equilibrium is fulfilled.

In summary, we let a system evolve into a nonequilibrium steady state. Then we couple an auxiliary site to a local region of the system. The coupling strength should be infinitesimal. We switch on the coupling and calculate the occupation number \( n_d \) at the site in the steady limit. We adjust the energy level \( \epsilon_d \) at the auxiliary site to obtain a series of pairs \((\epsilon_d, n_d)\). If we cannot fit equation (11) to the series of data points, we conclude that the local region is not in equilibrium. If we succeed, we then determine the local temperature and chemical potential from the fitting parameters. This is our method for using one auxiliary site to calculate the local intensive thermodynamic parameters in a NESS.

Next we give some comments on the possible applications of this. Up to now, solving the equation of motion has been the only generally accepted way of reaching a NESS in mesoscopic transport. In this approach we usually assume a central conductor connected to at least two infinite reservoirs which are in equilibrium at the initial time. The boundary conditions of the central conductor are given by the temperatures and chemical potentials of the reservoirs, which are assumed not to vary with time. The steady current through the central conductor can be calculated. The curve of current versus voltage bias is plotted and compared with experimental results. However, sometimes we are more interested in the distribution of local chemical potentials inside the central scattering region, which cannot be resolved from boundary conditions. Our method provides a way to calculate the local \( T \) and \( \mu \) in the central conductor. The results can be compared with experiments. The local \( T \) and \( \mu \) are more important than the reservoir temperature and chemical potential in the theory of nonequilibrium thermodynamics, where the gradients of intensive variables are called thermodynamic forces and are the reasons for flows.

4. The distribution of chemical potentials inside a disordered chain

A chain connected to two reservoirs has been widely used to model the quantum point contact and the quantum wire fabricated in semiconductor heterostructures. If the two reservoirs are in different chemical potentials, a current will be driven through the wire. This is the Landauer–Büttiker picture for mesoscopic transport. In the ballistic transport regime when the wire is clean, there is only contact resistance in the device. In other words, there are sharp voltage drops at the interface between the reservoirs and the wire, while the voltage is equal everywhere inside the wire.

What is more interesting is the case of a dirty wire, where we would expect the intrinsic resistance and a gradual drop of voltage through the wire. As in a macroscopic circuit, in a dirty wire the current can be treated as the result of the gradient of the voltage inside the wire instead of the voltage bias of the reservoirs. The reservoirs are no more than the simulation of the voltage source in a circuit, while they are necessary for preparing the NESS.

A disordered chain is obtained by proposing random on-site potentials \( \epsilon_j \), where \( j \) denotes the chain site. For simplicity we suppose that there is no correlation between \( \epsilon_j \) at different sites. The average of \( \epsilon_j \) is denoted as \( \bar{\epsilon} \). We suppose that \( \epsilon_j \) has a uniform distribution in the interval \([\bar{\epsilon} - \Delta/2, \bar{\epsilon} + \Delta/2]\), where \( \Delta \) denotes the disorder strength.
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Then the total Hamiltonian including the two reservoirs is written as

$$\hat{H} = \sum_{k,\alpha=L,R,\sigma} \epsilon_k \hat{c}_{k}\sigma \hat{c}_{k}\sigma + g_l \sum_{k} (\hat{c}_{kL}\sigma \hat{c}_{1}\sigma + \hat{c}_{kR}\sigma \hat{c}_{n}\sigma + \text{h.c.})$$

$$+ \sum_{\sigma,j=1}^{n} \epsilon_j \hat{c}_{j}\sigma \hat{c}_{j}\sigma + g \sum_{j=1}^{n-1} (\hat{c}_{j}\sigma \hat{c}_{j+1}\sigma + \text{h.c.}) + U \sum_{j=1}^{n} \hat{c}_{j}\sigma \hat{c}_{j}\sigma (\text{h.c.}) + n \sum_{j=1}^{n} \epsilon_j \hat{c}_{j}\sigma \hat{c}_{j}\sigma + g_{n-1} \sum_{j=1}^{n-1} (\hat{c}_{j}\sigma \hat{c}_{j+1}\sigma + 1 + \text{h.c.}) + \text{h.c.}.$$  \hfill (12)

where $\hat{c}_{k}\sigma$ is the annihilation operator of the electron in the lead, $\sigma = \uparrow, \downarrow$ denotes the spin and $\alpha = L, R$ denotes the left and right leads. The leads are in thermal equilibrium at temperatures $T_L$ and $T_R$, and at chemical potentials $\mu_L$ and $\mu_R$ respectively. The operator $\hat{c}_{j}\sigma$ with $j = 1, 2, \ldots, n$ denotes the annihilation operator at site $j$ in the chain. The strength of coupling between nearby sites in the chain is set to be $g$, and that between the leads and the chain is set to be $g_l$.

For general parameters, the above Hamiltonian is non-integrable due to the existence of Coulomb interaction. Several complicated numerical methods and approximation schemes have been developed for solving this model. For simplicity, in this paper we will first solve the model without considering interaction by setting $U = 0$. Then we consider the effect of the interaction in the self-consistent mean field approximation. Without interaction the electrons in different spin channels will transport independently and the spin index can be neglected. The simplified Hamiltonian becomes

$$\hat{H} = \sum_{k,\alpha=L,R,\sigma} \epsilon_k \hat{c}_{k}\alpha \hat{c}_{k}\alpha + g_l \sum_{k} (\hat{c}_{kL}\alpha \hat{c}_{1}\alpha + \hat{c}_{kR}\alpha \hat{c}_{n}\alpha + \text{h.c.}) + \sum_{j=1}^{n} \epsilon_j \hat{c}_{j}\alpha \hat{c}_{j}\alpha + g \sum_{j=1}^{n-1} (\hat{c}_{j}\alpha \hat{c}_{j+1}\alpha + \text{h.c.}).$$  \hfill (13)

We employ in the left and right electron reservoirs the momentum basis and assume a constant density of states denoted by $\rho$. At the same time the reservoirs can also be simulated by the semi-infinite chains. In this sense the Hamiltonian of equation (13) describes an infinite chain with emphasized central sites, similar to the Hamiltonian of equation (4). If we define $\Gamma = \rho \pi g_l^2$ as the energy unit (like what we do in the single-impurity Anderson model) and set $g = \Gamma$, the strength of coupling between central sites has the same amplitude as that between nearby sites in reservoirs. This corresponds to a comparatively strong coupling between central sites. In the following we always set $g = \Gamma$. One could also take different values of $g$. But when $g \ll \Gamma$, the transmission spectrum has very sharp peaks, and one should be very careful when performing numerical integration routines.

4.1. The electron density and the current at site $m$

The steady current and electron density at an arbitrary site $m$ in the disordered chain are obtained by the Keldysh technique, in which an adiabatic evolution is proposed with $g$ and $g_l$ switched on little by little. In this model, adiabatically switching on the coupling makes no difference with a quench of coupling for the physical quantities in the steady limit. In detail, we define the retarded Green functions as

$$G_{i,j}(t, t') = -i \theta(t - t') \langle \{ \hat{c}_{i}(t), \hat{c}_{j}^{\dagger}(t') \} \rangle ,$$  \hfill (14)
and the lesser Green functions as
\[ G_{i,j}^{<}(t, t') = i\langle \hat{c}_i^\dagger(t')\hat{c}_i(t) \rangle, \]  
where \( i, j = 1, 2, \ldots, n \) denote the sites in the chain. The electron density and current at arbitrary sites in the chain can be related to the simultaneous lesser Green functions.

The frequency representation of the Green functions is defined as
\[ G^r_{i,j}(\omega) = \int d(t - t') \ e^{i\omega(t-t')} G^r_{i,j}(t, t'), \]  
\[(16)\]

In the frequency representations the retarded Green function satisfies the Dyson equation, i.e.
\[ G^r(\omega) = G^{0r}(\omega) + G^{0r}(\omega)\Sigma^r(\omega)G^r(\omega), \]  
\[(17)\]
where \( G^r(\omega) \) is a \( n \times n \) matrix whose elements are \( G^r_{i,j}(\omega) \). \( G^{0r}(\omega) \) is the free Green function matrix when \( g = g_l = 0 \), and its elements are
\[ G^{0r}_{i,j}(\omega) = \frac{1}{\omega - \epsilon_i + i\eta}. \]  
\[(18)\]
where \( \eta > 0 \) is infinitesimal. \( \Sigma^r(\omega) \) is the self-energy matrix, which comes from two sources. The first is the energy of hopping between nearby sites in the chain, i.e.
\[ \Sigma_{j,j+1}^r = g. \]  
\[(19)\]
The second is the broadening of levels at the edge sites due to the coupling to leads, i.e.
\[ \Sigma_{1,1}^r(\omega) = \Sigma_{n,n}^r(\omega) \]
\[ = g^2 \sum_k \frac{1}{\omega - \epsilon_k + i\eta} \]
\[ = -i\Gamma, \]  
\[(20)\]
where \( \Gamma = \rho \pi g^2 \). The other elements of the self-energy matrix are all zero. By solving equation (17) we can express the retarded Green function as
\[ G^r(\omega) = (G^{0r}(\omega)^{-1} - \Sigma^r(\omega))^{-1}. \]  
\[(21)\]
Here we need to calculate the inverse of a \( n \times n \) matrix, which can be finished by computer.

The lesser Green function in the frequency representation is related to the retarded one in the Keldysh formalism, i.e.
\[ G_{i,j}^{<} = g_l^2 \left( G_{i,1}^{\pi} \sum_k G_{kL}^{0<} G_{1,j}^a + G_{i,n}^{\pi} \sum_k G_{kR}^{0<} G_{n,j}^a \right), \]  
\[(22)\]
where \( G_{k\alpha}^{0<}(\omega) = 2\pi i(1/e^{\beta_\alpha(\omega-\mu_\alpha)} + 1)\delta(\omega - \epsilon_k) \) with \( \alpha = L, R \) are the lesser Green functions in the left and right leads respectively. Here \( \beta_\alpha = 1/(k_B T_\alpha) \) and \( \mu_\alpha \) are the inverse of temperature and the chemical potential in lead \( \alpha \) respectively, and \( G_{i,j}^a \) denotes the advanced Green function, which is the complex conjugate of the corresponding retarded Green function, i.e. \( G_{i,j}^a = (G_{j,i}^r)^* \). Equation (22) takes the form
\[ G_{i,j}^{<} = 2i\Gamma \left( G_{i,1}^r G_{1,j}^a f_L + G_{i,n}^r G_{n,j}^a f_R \right), \]  
\[(23)\]
where \( f_\alpha(\omega) = 1/(e^{\beta_\alpha(\omega-\mu_\alpha)} + 1) \) is the Fermi function in lead \( \alpha \).

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Finally we perform inverse Fourier transformation and get the lesser Green function in the time representation, i.e.,

\[
G_{i,j}^< (t, t') = \int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega(t-t')}}{2\pi} G_{i,j}^<(\omega).
\] (24)

The electron density at site \(m\) is defined as \(n_m = \langle \hat{c}_m^\dagger \hat{c}_m \rangle\), which can be expressed as \(n_m = -iG_{m,m}^<(0,0)\) according to the definition of the lesser Green function. Substituting equation (24) in, we have

\[
n_m = \frac{1}{2\pi i} \int d\omega G_{m,m}^<(\omega).
\] (25)

The current from site \(m\) to \((m+1)\) is expressed as \(I_{m\rightarrow m+1} = (g/\hbar) \langle \hat{c}_m^\dagger \hat{c}_{m+1} - \text{h.c.} \rangle\), which satisfies the electron number conservation law \(dn_m/dt = I_{m\rightarrow m-1} - I_{m\rightarrow m+1}\). Similarly it is related to the lesser Green function as follows:

\[
I_{m\rightarrow m+1} = -\frac{2g}{\hbar} \text{Re} \int d\omega G_{m,m+1}^<(\omega).
\] (26)

Equations (21), (23), (25) and (26) together give the complete procedure for calculating the electron density and current at an arbitrary site.

In the numerical approach, we first use a random number generator to generate a group of on-site potentials \(\epsilon_j\). One should note that the distribution of \(\epsilon_j\) is uniform in the interval \([\bar{\epsilon} - \Delta/2, \bar{\epsilon} + \Delta/2]\). Then the electron density and current are calculated subject to this group of \(\epsilon_j\). Obviously repeating the calculation will not produce the same result, since \(\epsilon_j\) is randomly generated. We are more interested in the average value of the current, which is obtained by repeating the calculation many times. At each time a new group of \(\epsilon_j\) is generated. We repeat this procedure until the averaged current is convergent.

4.2. The on-site temperature and chemical potential

We calculate the temperature and chemical potential at an arbitrary site in the chain. This is done by attaching an auxiliary site to the site at which we want to measure. For example, if we want to measure the temperature \(T_m\) and the chemical potential \(\mu_m\) at site \(m\), we will modify the Hamiltonian of equation (13) by including the extra terms

\[
\hat{H}_{\text{mea}} = g'(\hat{d}^\dagger \hat{c}_m + \text{h.c.}) + \epsilon_d \hat{d}^\dagger \hat{d},
\] (27)

where \(\hat{c}_m\) and \(\hat{d}\) denote the annihilation operators at site \(m\) and the auxiliary site respectively. Here \(\epsilon_d\) denotes the energy level at the auxiliary site and is adjustable, and \(g'\) denotes the auxiliary coupling strength which should be infinitesimal. The whole system consisting of the chain coupled to two leads and the auxiliary site is described by the Hamiltonian \(\hat{H} + \hat{H}_{\text{mea}}\), where \(\hat{H}\) is defined in equation (13).

Again the Keldysh technique is employed to calculate the occupation number at the auxiliary site \(n_d = \langle \hat{d}^\dagger \hat{d} \rangle\) corresponding to different \(\epsilon_d\). This should be done by adiabatically switching on \(g'\) after the chain described by \(\hat{H}\) has been in a nonequilibrium steady state. Due to the lack of initial correlation, this is equivalent to switching on \(g_l\), \(g_i\) and \(g'\) simultaneously when we are only interested in the steady limit of the local quantity \(n_d\).
Now the chain and the auxiliary site together are treated as the central conductor, which in total contains \((n + 1)\) sites. We define the retarded Green function relating to the auxiliary site as

\[
G_{i,n+1}(t, t') = -i\theta(t - t')\langle \hat{c}_i(t), \hat{d}^\dagger(t') \rangle, \quad G_{n+1,j,n+1}'(t, t') = -i\theta(t - t')\langle \hat{d}(t), \hat{c}^\dagger_j(t') \rangle, \quad G_{n+1,n+1}'(t, t') = -i\theta(t - t')\langle \hat{d}(t), \hat{d}^\dagger(t') \rangle,
\]

where \(i, j = 1, 2, \ldots, n\). Combining this with the Green functions defined in equation (14) we get an \((n + 1)\times (n + 1)\) matrix. It can be expressed in a form similar to equation (21), as

\[
G^r(\omega) = (G^{0r}(\omega)^{-1} - \tilde{\Sigma}^r(\omega))^{-1},
\]

where \(G^{0r}(\omega)\) is the \((n + 1) \times (n + 1)\) diagonal matrix. The elements of \(G^{0r}\) are defined in equation (18) except for the one concerning the auxiliary site \(G_{n+1,n+1}^{0r} = 1/(\omega - \epsilon_d + i\eta)\).

Now the self-energy matrix comes from three sources: the energy of hopping between nearby sites in the chain; the energy of coupling between the edge sites and the leads; and the energy of coupling between the \(m\) site and the auxiliary site. The corresponding elements are

\[
\tilde{\Sigma}_{j,j+1}^r = \tilde{\Sigma}_{j+1,j}^r = g
\]

with \(j = 1, 2, \ldots, n - 1\),

\[
\tilde{\Sigma}_{1,1}^r = \tilde{\Sigma}_{n,n}^r = -i\Gamma,
\]

and

\[
\tilde{\Sigma}_{m,n+1}^r = \tilde{\Sigma}_{n+1,m}^r = g'.
\]

The expression for the lesser Green function in equation (23) remains invariant because the auxiliary site is not directly coupled to the leads. In particular, we have

\[
G_{n+1,n+1}^<( = 2i\Gamma(|G_{n+1,1}^r|^2 f_L + |G_{n+1,n}^r|^2 f_R).
\]

The occupation number at the auxiliary site is expressed as

\[
n_d = \frac{1}{2\pi i} \int d\omega \ G_{n+1,n+1}^<(\omega).
\]

We know that \(g' \to 0\) is the necessary condition of local equilibrium at the auxiliary site. In the numerical approach, the weak coupling limit is realized by the self-adaptation algorithm. We begin with a finite \(g'\), and reduce it by half in each loop until the final result \(n_d\) converges to a desired precision.

At beginning of the numerical approach, we generate a group of on-site potentials \(\epsilon_j\). Then we calculate in turn the current through the chain and the occupation number at the auxiliary site with respect to different \(\epsilon_d\) and \(m\). When calculating the current, we turn off the coupling to the auxiliary site. One should note that the destiny of an auxiliary site is to measure the temperature and the chemical potential at sites in the chain. One does not measure at different sites simultaneously but rather at one after another. We finally get a series of functions \(n_d(\epsilon_d)\) with \(m\) varying from 1 to \(n\). We then calculate the average of the temperature and chemical potential at site \(m\) with respect to different configurations of disorder.

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Figure 3. The transmission spectrum $-2g \text{Re} G^<_{m,m+1}(\omega)$ at different disorder strengths. In this figure the chain length is set to 50. We set $V = \mu_L - \mu_R = 0.5 \Gamma$ and $T_L = T_R = 0.01 \Gamma$.

4.3. The transition from delocalization to localization as the disorder strength $\Delta$ increases

What we are studying is the transport through a mesoscopic chain. At particle–hole symmetry we set the average of the Fermi energies in the left and right leads equal to the average of the on-site potentials in the chain, i.e. $(\mu_L + \mu_R)/2 = \bar{\epsilon} = 0$. The linear conductance of the chain in the absence of disorder ($\Delta = 0$) reaches the unitary limit $e^2/h$. In the absence of disorder the transport through the chain is well understood under the framework of ballistic transport.

In the presence of disorder, however, we observe the gradual transition from delocalization to localization as the disorder strength increases. This transition should be attributed to the Anderson localization, while the transition in our model is a ‘smooth’ one, unlike the phase transition in the thermodynamic limit, since the chain consists of only a few sites. Strictly speaking, there is no disorder-induced phase transition in an infinite one-dimensional system, where an infinitesimal concentration of impurities will cause the exponential decay in the extension of the wavefunction. For a chain with a few sites, we see the gradual transition from a continuous band to sharp peaks and wide forbidden regimes between peaks in the transmission spectrum as the disorder strength $\Delta$ increases (see figure 3). This is understood as the transition from ballistic transport in the clean limit to the transport shuttled by the localized levels weakly coupled to the reservoirs.

The feature of Anderson localization is clearly observed in the figure showing averaged current (see the bottom figure of figure 4), in which the current shows an exponential decay as the length of the chain increases. When we calculate the current, the on-site potentials are randomly generated according to $\bar{\epsilon}$ and $\Delta$. For each generation of on-site potentials we obtain a different current. The averaged current is expressed as

$$\bar{I} = \frac{\sum_{j=1}^{M} I_j}{M},$$

(35)
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Figure 4. The top figure shows the averaged current $\bar{I}$ and the standard deviation of the current $\sigma_I$ as a function of disorder strength $\Delta$. The voltage bias between the two leads is $V = \mu_L - \mu_R = 0.05\Gamma$, and the temperature in the leads is $T_L = T_R = 0.1\Gamma$. The length of the chain is set to 10. We observe the localization–delocalization transition in the regime of intermediate disorder strength, where the deviation of the current reaches its maximum. A large value of $\sigma_I$ indicates a strong fluctuation of the current, which often happens near the critical point of a phase transition. The bottom figure shows the averaged current as a function of the chain length. The voltage bias is $V = 0.2\Gamma$.

and the standard deviation of current is expressed as

$$\sigma_I = \sqrt{\frac{\sum_{j=1}^{M} (I_j - \bar{I})^2}{M}},$$

where $I_j$ is the result for current corresponding to the $j$th generation of on-site potentials and $M$ is the total number of generations.

The top figure of figure 4 shows the average and the standard deviation of current varying with the disorder strength. In the clean limit as $\Delta = 0$, the current approximately approaches $(e^2/h)V$ and the standard deviation is exactly zero. As the disorder strength $\Delta$ increases, the averaged current drops monotonically, while the standard deviation first increases until its maximum is reached and then drops toward zero. At an intermediate disorder strength, $\sigma_I$ reaches its maximum. The strong fluctuation of the current in this regime indicates the transition from delocalization to localization.
4.4. The local equilibrium condition and the on-site temperature and chemical potential

Local thermodynamic equilibrium is an important concept in the study of nonequilibrium thermodynamics. Generally the local equilibrium condition is only fulfilled in systems not far from equilibrium. In the case of a chain connected to two leads, it is required that the temperature difference and the voltage bias of the two leads are small. We have explained how to use an auxiliary site to check whether the local equilibrium condition at an arbitrary site in the chain is fulfilled by calculating the occupation number at the auxiliary site as a function of the energy level. In figure 5 we plot \( \ln(1/n_d - 1) \) as a function of \( \epsilon_d \) under different voltage biases, defined as \( V = \mu_L - \mu_R \). According to equation (11), the local equilibrium condition is fulfilled if this function is a straight line. As shown in figure 5, when \( V \) is exactly zero or very small the function of \( \ln(1/n_d - 1) \) remains an approximately linear function and thus the condition of local equilibrium is still fulfilled. But as the voltage bias increases, the function \( \ln(1/n_d - 1) \) obviously deviates from a linear function, as shown by the curve labeled \( V = 0.5\Gamma \).
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Figure 6. The value of $\ln(1/n_d - 1)$ is plotted with respect to $\epsilon_d$ at different sites in a disordered chain of length 10. The left and right lead temperatures are $T_L = T_R = 0.1\Gamma$. The voltage bias is set to $V = 0.05\Gamma$. The disorder strength is $\Delta = \Gamma$.

An interesting question arises, as to whether the local equilibrium condition is less stringent if the auxiliary site is simultaneously coupled to a large number of sites in the chain (and not only to a given site). We study a model in which the auxiliary site is coupled to up to 100 sites in a chain of length 200. Under finite voltage bias, the deviation of the function $\ln(1/n_d(\epsilon_d) - 1)$ from a straight line is found to be independent of the number of sites where measurements are made simultaneously, in contrast to the results observed for an equilibrium system [25].

At small voltage bias, the function $\ln(1/n_d - 1)$ is linear at an arbitrary site inside the chain. The slope of the function is explained as the inverse of local temperature, and its value at $\epsilon_d = 0$ as $(-\beta\mu)$ where $\mu$ is the local chemical potential. Then we can extract the local temperature $T_m = 1/\beta_m$ and the local chemical potential $\mu_m$ at each site $m$. One may have doubts as to the validity of this method, since what we are interested in is the distribution of on-site temperatures and chemical potentials in nonequilibrium, when they are different from the reservoir ones. However at finite voltage bias, the condition of local equilibrium is only fulfilled approximately. Strictly speaking, the function $\ln(1/n_d - 1)$ deviates from a linear function a little bit even at small voltage bias. Then how do we know that the discrepancy between on-site chemical potentials and reservoir ones, if there is any, is not the result of the deviation of $\ln(1/n_d - 1)$ from a linear function? This suspicion is quashed by plotting the function $\ln(1/n_d - 1)$ at different sites simultaneously (see figure 6). In figure 6, we see that subject to a finite voltage bias and disorder strength, the functions $\ln(1/n_d - 1)$ at different sites are parallel to each other. They obviously have different intercepts with the axes and at the same time the same slope, which is just the inverse of the reservoir temperature. This is strong evidence that the deviation of $\ln(1/n_d - 1)$ from a linear function is very small compared to the difference between on-site potentials. Thus our method resolves the on-site chemical potentials to a good extent.

We study the distribution of on-site chemical potentials at different voltage biases and disorder strengths. Even if the result depends on the configuration of on-site potentials

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Figure 7. The distribution of on-site chemical potentials inside a chain of length 10 at different voltage biases $V$ and disorder strengths $\Delta$. Strong fluctuation of on-site chemical potentials is observed at finite voltage bias in the presence of disorder.

and is not repeatable when $\Delta \neq 0$, it shows some features which can be attributed to $V$ and $\Delta$ (see figure 7). In equilibrium with $V = 0$, the on-site chemical potential is zero throughout the chain whether there is disorder or not, coinciding with the fact that the chemical potentials in an equilibrium system should be equal everywhere. When there is no disorder, the on-site chemical potential remains zero everywhere even at finite voltage bias, because without disorder the resistance of the device comes only from contact resistance, and there is no drop of voltage inside the chain. In the presence of both voltage bias and disorder, we see strong fluctuation of the on-site chemical potentials. As the disorder strength increases, the fluctuation becomes stronger. This is in contrast to the familiar phenomena in macroscopic circuits where we expect a monotonic drop of voltage through the resistance wire. This can be explained by the mesoscopic nature of the chain, where the movement of electrons must be described by quantum mechanics. In a localization regime with intermediate $\Delta$, the position of the electron in the chain is constrained to lie in a small region; thus its kinetic energy has strong fluctuation due to the uncertainty principle, leading to the strong fluctuation in the on-site chemical potentials.

The abnormal fluctuation of the on-site chemical potentials is then canceled out by taking the average with respect to configurations of disorder. Using a form similar to that for the averaged current in equation (35), we define the averaged chemical potential as

$$\bar{\mu}_m = \frac{\sum_{j=1}^{M} \mu_{jm}^j}{M},$$

(37)

where $\mu_{jm}^j$ denotes the chemical potential at site $m$ in the $j$th generation. In a real mesoscopic wire, the configuration of disorder is generally not controllable, and is unknown to the simulators. By taking the average with respect to the disorder configurations, one could obtain some universal features of the distribution of on-site chemical potentials. This is a well-established method in studying disordered systems. As shown in figure 8,
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Figure 8. The distribution of averaged on-site chemical potentials. Here we set the voltage bias to \( V = 0.05 \Gamma \) and the disorder strength to \( \Delta = \Gamma \). On taking the average with respect to configurations of disorder, we observe the regular distribution replacing strong fluctuations.

the averaged chemical potential drops monotonically through the chain, recovering the features of macroscopic resistance wires.

4.5. The effect of interaction

We have studied the distribution of on-site chemical potentials in a non-interacting disordered chain. A natural question arises as to what is the influence of electron–electron interaction on our results. Next we consider the complete Hamiltonian in equation (12) consisting of the on-site Coulomb interaction. We combine it with the measuring term

\[
\hat{H}_{\text{mea}} = g' \sum_{\sigma} (\hat{d}_\sigma^\dagger \hat{c}_{m\sigma} + \text{h.c.}) + \epsilon_d \sum_{\sigma} \hat{d}_\sigma^\dagger \hat{d}_\sigma.
\]

(38)

The two spin channels are considered at the auxiliary site, while the on-site interaction is not, because if we consider the Coulomb energy, there will be four states with different energies at the auxiliary site. This increases the difficulty in deciding the local temperature and chemical potential.

Again the Keldysh techniques are employed to calculate the occupation number at the auxiliary site as a function of \( \epsilon_d \) in NESS. The Green function can be expressed as a perturbative expansion of \( U \). The Green functions of zeroth order in \( U \) have been given in the above calculations, i.e., in equations (21) and (23). We take the self-consistent mean field approximation by summing up all the diagrams in the perturbative expansion in which Hartree type self-energies are inserted. This is finished by replacing the on-site potentials \( \epsilon_j \) by \( \epsilon_j + Un_j \) in the expression for \( G^{\text{br}}(\omega) \) in equation (18), and hence in the expressions for \( G^<(\omega) \) and \( G^>(\omega) \) in equations (21) and (23). Here \( n_j \) is the occupation number at site \( j \) and satisfies the self-consistent equation

\[
n_j = \frac{1}{2\pi i} \int d\omega G^<_{j,j}(\omega).
\]

(39)
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![Figure 9](image)

**Figure 9.** The distribution of on-site chemical potentials at different interaction strengths $U$ and disorder strengths $\Delta$. The chain is set to be at particle–hole symmetry with $\bar{\epsilon} = -U/2$. The voltage bias is $V = 0.05\Gamma$, and the left and right lead temperatures are both $0.1\Gamma$. Without disorder the interaction has no effect on the on-site chemical potentials (see the two curves labeled $\Delta = 0$).

In the presence of disorder, the electron–electron interaction will suppress the fluctuation of on-site chemical potentials caused by the localization of electrons.

The above self-consistent equations can be solved using an iterative method, as the interaction strength $U$ is small.

We plot the distribution of the on-site chemical potentials at the particle–hole symmetric point where $\bar{\epsilon} = -U/2$ (see figure 9). We find that the interaction will suppress the fluctuation of on-site chemical potentials in the presence of disorder. This is similar to the phenomenon where in a closed system the interaction will cause equilibration of the system from arbitrary initial states.

### 5. Conclusions

In summary, we study a chain coupled to two semi-infinite leads. Such a chain will evolve into a nonequilibrium steady state after a quench of the coupling between the leads and the chain if the two leads are at different chemical potentials. We then demonstrate the central idea of this paper of attaching an auxiliary site to the chain to measure the local temperature and chemical potential at each site inside the chain. We find that our method will work if and only if the voltage biases between the two leads are small when the conditions of local thermodynamic equilibrium are fulfilled. We then consider a disordered chain by introducing random on-site potentials. The localization–delocalization transition is observed as the disorder strength increases. More importantly, we observe that the local on-site chemical potential inside the chain is everywhere zero if either the voltage bias or the disorder is absent. We observe in the presence of both voltage bias and disorder a large fluctuation in the on-site chemical potentials, instead of the monotonic drop of voltage usually observed in a macroscopic resistance wire. The fluctuation can be suppressed by the electron–electron interaction. This is attributed to the mesoscopic

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nature of the chain. By taking the average with respect to different configurations of disorder, we recover the monotonic drop of the chemical potential. We believe that our method can be generalized to arbitrary nonequilibrium steady states to check whether the conditions of local equilibrium are fulfilled and, if they are fulfilled, to calculate the local intensive thermodynamic parameters.

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