Current biasing a multilayered device as a boundary condition for inhomogeneous nonequilibrium dynamical mean-field theory

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Recently, nonequilibrium dynamical mean-field theory was developed as a new technique to solve the bulk nonequilibrium many-body problem. The computational effort needed to solve the nonequilibrium problem in the bulk is similar to the efforts needed to solve the inhomogeneous multilayered problem for current flow perpendicular to the planes. Because the leads provide the appropriate boundary conditions for the open system, one can directly solve for the steady state within a frequency representation, and thereby obtain the current-voltage relation for the device. Here we discuss the problem of determining the boundary condition for the Green's functions, which can be used to determine the so-called self-energy of the leads, which is a critical step needed in this problem.

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INTRODUCTION

Nearly all useful electronic devices rely on nonlinear behavior in the current-voltage relation for the device in order to operate. Examples include semiconductor transistors, tunnel diodes, Josephson junctions, and so on. Recently, motivated by the creation of two-dimensional electron gases at the interfaces of band/Mott-insulating devices [1], interest has focused on devices made from strongly correlated materials because the strong correlation effects have the potential to be more easily tuned than in more conventional devices. To date, these strongly correlated multilayered devices have been described primarily in linear response [2–6], although there has been some work completed in nonequilibrium [7, 8]. But the fundamental problem of determining the current-voltage relation has remained elusive. Here we show how one can use ballistic metal leads and current biasing to determine the appropriate boundary condition for describing the steady-state behavior of these devices.

A schematic picture of such a device is given in Fig. 1. The metallic leads are chosen to be ballistic metals because they can be easily current biased. We imagine the system starts in the infinite past in equlibrium at a temperature T. An electric field is turned on for a finite period of time to generate current flow and then is turned off. We describe the field with the Peierls substitution in the vector-potential-only gauge [9]. After the field is turned off, the vector potential is equal to $-A_0$ for large positive and large negative values of the z coordinate. This generates a constant current flow in the ballistic metal leads. In order to maintain current conservation throughout the device, we need to create local electric fields over a finite number of planes, where the current falls below the value in the ballistic metal (due to scattering or due to proximity to the barrier region). For these planes, we can describe the vector potential with a simple linear function $A_\alpha(t) = -A_0 - E_\alpha t$, which yields an electric field of E_α in the z-direction at the αth plane

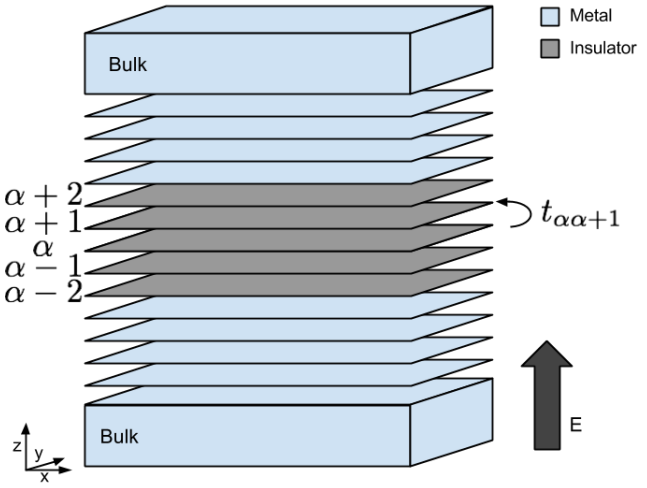

FIG. 1: (Color online) Schematic of the multilayered device. On the top and the bottom, the system is attached to bulk leads which carry current in the longitudinal direction. Each plane is labeled by a Greek index α, while Roman indices are used to describe the planar sites. For an interacting device, the ballistic metal leads are attached to the barrier region in the center, which is where the scattering occurs. In this region, an electric field needs to be applied to guarantee current conservation through the device.

(we choose units such that $\hbar = c = e = a = 1$, with a the lattice spacing). Because the vector potential is linear in time, the system as a whole will satisfy time translation invariance and can be described by taking a Fourier transform from time to frequency and employing a frequency representation for all relevant functions. This provides a huge simplification of the problem, as one can determine the steady state using a similar formalism as is used in equilibrium and thereby calculate the current-phase relation.

The system is an open system since particles and heat

are carried by the current that flows through the leads to the active region of the device and back to the leads. In such systems, the effect of the leads on the transport within the active region of the device can be fully encoded in a term that acts like an extra self-energy for the active region of the device and is called the self-energy of the leads [10]. Since electrons cannot be created or destroyed, we must enforce charge current conservation for the current flow through each longitudinal plane. We assume the current density is uniform on each plane, as the planes are chosen to be homogeneous. Within this formalism, one can very simply modify the algorithm used in equilibrium to calculate the retarded Green's functions and the many-body density of states (DOS). It ends up being identical in form to the equilibrium case except for a shift of the energy by the local electric field for the recurrence relation which determines the self-energy of the leads; in the bulk region of the leads, the electric field vanishes and the DOS in the presence of current flow remains the same as the DOS in equilibrium, as one might expect since the quantum states remain the same, only their occupancy is changed to create current flow. Within this approach, heat current need not be conserved. Indeed, current flow through the active region creates Joule heat which is carried with the particle current, and also transferred to an "effective reservoir" in the regions near the interfaces of the device.

It is the Keldysh or lesser component of the Green's function that determines the occupancy of the states, and since their Dyson equation is homogeneous, one needs an appropriate boundary condition to calculate them in the active region of the device. This boundary condition arises from the behavior of the bulk system under constant current flow, which is a problem that can be solved exactly. In this contribution, we show how to exactly solve the bulk problem and to use it to solve for the self-energy of the leads, which provides this necessary boundary condition.

The remainder of the paper is organized as follows: In Sec. II, we describe the formalism used to determine the lead self-energy, in Sec. III, we present the numerical results, and in Sec. IV, we provide our conclusions.

FORMALISM

There are a few different theoretical methods used to describe a finite open system attached to metallic leads. Probably the most popular method is to assume the left lead and the right are attached to separate reservoirs, one at voltage $V/2$ and the other at voltage $-V/2$. Then the hopping between the leads and the device are slowly turned on and the system is allowed to reach the steady state [11]. One calculates the current flow in this steady state, and uses that with the voltage applied across the device to determine the current-voltage relation. This approach corresponds to a voltage-biased device and it is probably the most commonly used technique in calculations. We propose to use a different method which should yield completely equivalent results, but works in a very different fashion. Here, the device and the leads are connected initially and the system is equilibrated at a temperature T. Next an electric field is turned on for a short period of time to establish a current flow through the device. If the leads are ballistic metals, then the field can be turned off, and the leads will continue to have constant current flow for all time. Additional constant electric fields are then turned on within the finite region of the device, where scattering occurs, in order to maintain particle current conservation. The system is let to evolve to the steady state, which is then used to determine the current-voltage relation by calculating the voltage by integrating the electric field that is required to guarantee current conservation.

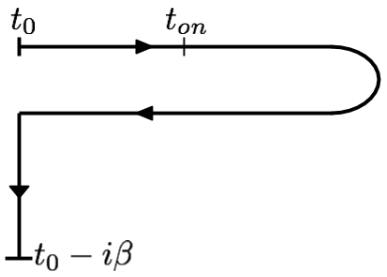

FIG. 2: Kadanoff-Baym-Keldysh contour used to calculate the contour-ordered Green's function. The system starts in equilibrium at time t_0 and $\beta = 1/T$ is the inverse temperature for the initial equilibrium state. The electric field is turned on at time t_{on}, and then the system evolves to the steady state. In the calculational method described here, both t_0 and t_{on} are taken in the limit where they approach $-\infty$. This evolution can be explicitly calculated for the noninteracting leads, which then form the boundary condition for the interacting problem to be solved. In this limit, one can also ignore the imaginary branch of the contour, since the steady state does not maintain any correlations with the intial equilibrium state.

The many-body formalism begins with the so-called contour-ordered Green's function, defined by [12–14]

$$g^c_{\alpha i\beta j}(t,t') = -\frac{i}{\mathcal{Z}}\mathrm{Tr}\left[\mathcal{T}_c e^{-\beta\mathcal{H}(-\infty)} c_{\alpha i}(t) c^\dagger_{\beta j}(t')\right], \quad (1)$$

where $\mathcal{H}(-\infty)$ is the initial equilibrium Hamiltonian, $\mathcal{Z} = \mathrm{Tr}\exp[-\beta\mathcal{H}(-\infty)]$ is the initial equilibrium partition function, $\mathcal{T}_c$ is the contour-ordering operator, which orders the times according to their order along the contour, and $c_{\alpha i}(t)$ $[c^\dagger_{\alpha i}(t)]$ are the annihilation [creation] operators for a spinless electron in the Heisenberg representation with respect to the time-dependent Hamiltonian $\mathcal{H}(t)$ on plane α at planar site i; these operators satisfy

the usual fermionic anticommutation relations when evaluated at the same time. This representation in terms of spatial components only is inconvenient for dealing with multilayered systems, so we perform a partial Fourier transform with respect to the planar indices, since the system is translationally invariant in every plane, to define the mixed-basis Green's function [2]

$$g^c_{\alpha\beta}(k^\parallel;t,t') = -\frac{i}{\mathcal{Z}}\mathrm{Tr}\left[\mathcal{T}_c e^{-\beta\mathcal{H}(-\infty)} c_{\alpha k^\parallel}(t) c^\dagger_{\beta k^\parallel}(t')\right], \tag{2}$$

where $k^\parallel$ is the two-dimensional planar momentum.

We ignore specific details of the Hamiltonian in our current discussion, because the results are general and hold for all Hamiltonians with local interactions. The equilibrium Hamiltonian is, however, assumed to have a nearest-neighbor hopping term determined by hopping integrals $t^\parallel_\alpha$ for hopping within the αth plane and $t^\perp_{\alpha\alpha+1}$ for hopping between the $\alpha+1$st plane and the αth plane. Because the system has either a constant vector potential or a constant electric field applied across it, the nonequilibrium Hamiltonian is described with a longitudinal hopping integral that satisfies

$$t^\perp_{\alpha\alpha+1}(t) = t^\perp_{\alpha\alpha+1} e^{iA_\alpha(t)}, \text{ and } t^\perp_{\alpha+1\alpha}(t) = t^\perp_{\alpha\alpha+1} e^{-iA_\alpha(t)}, \tag{3}$$

since $t^\perp_{\alpha+1\alpha} = t^\perp_{\alpha\alpha+1}$ when the system is in equilibrium. Here, the vector potential always has a constant shift, but also can have a linear term in time when there is an electric field at the αth plane. The two hopping terms are complex conjugates as is required for a Hermitian Hamiltonian. Note that the parallel hopping remains time independent when current only flows perpendicular to the planes. It is convenient to introduce the planar bandstructure $\epsilon^\parallel_\alpha(k^\parallel)$ to describe the band dispersion within each plane ($k^\parallel$ is the two-dimensional planar momentum). We let δ denote the nearest neighbor translation vector within each plane, then $\epsilon^\parallel_\alpha(k^\parallel) = -t^\parallel_\alpha \sum_\delta \exp(ik^\parallel\cdot\delta)$.

It is a straightforward calculation to determine the equation of motion for the contour-ordered Green's function under the assumption of a local self-energy (which is required by nonequilibrium dynamical mean-field theory). Defining the contour-ordered delta function in the standard way such that $\int_c dt' \delta_c(t,t') f(t') = f(t)$, one finds

$$\begin{aligned}\int_c d\bar{t}\Big\{ &\left[\left(-i\frac{\partial}{\partial t} + \mu - \epsilon^\parallel_\alpha(k^\parallel)\right)\delta_c(t,\bar{t}) - \Sigma^c_\alpha(t,\bar{t})\right] \\ &\times g^c_{\alpha\beta}(k^\parallel;\bar{t},t') \\ +\ &\Big[t^\perp_{\alpha\alpha+1} e^{iA_\alpha(t)} g^c_{\alpha+1\beta}(k^\parallel;t,\bar{t}) \\ &+ t^\perp_{\alpha-1\alpha} e^{-iA_{\alpha-1}(t)} g^c_{\alpha-1\beta}(k^\parallel;t,\bar{t})\Big]\delta_c(\bar{t},t')\Big\} \\ &= \delta_c(t,t')\delta_{\alpha\beta}. \end{aligned} \tag{4}$$

Here $\Sigma^c_\alpha(t,t')$ is the local contour-ordered self-energy for the Green's function at the αth plane.

This equation is of the form $g^{-1}g = \mathbb{I}$, which allows us to find g by taking the matrix inverse of g^{-1}, as is usually done when solving the Dyson equation. Here, we must think of the matrix for g^{-1} as a series of double time blocks that are sparsely distributed in a spatial pattern given by α and β that includes a diagonal and the two subdiagonals, and is in the form of a block tridiagonal matrix. The inverse of such a matrix can be found by employing a series of recursion relations [2, 4, 5, 15]. To derive these, we imagine our system as a set of equations for all possible α and β indices, and we work with matrix inverses with respect to the time blocks only. One might ask whether such inverses are well defined. They clearly are in equilibrium, as they are used to solve the problem in frequency space. Here, we show that they also are well defined *a posteriori* after assuming that they are and showing that the results of all of the recursions remain well defined. Hence, we start by multiplying Eq. (4) from the right by the inverse of the block matrix $g^{c-1}_{\alpha\beta}(k^\parallel;t,t')$ where the inverse is only with respect to the time indices of the matrix for a fixed α and β. Next, we let $\beta\to\alpha$ and $\alpha\to\alpha-n$ for $n>0$, to yield

$$\begin{aligned} 0 \ =\ &\left[-i\frac{\partial}{\partial t} + \mu - \epsilon^\parallel(k^\parallel)\right]\delta_c(t,t') - \Sigma^c_{\alpha-n}(t,t') \\ +\ & t^\perp_{\alpha-n\alpha-n+1} e^{iA_{\alpha-n}(t)} \int_c d\bar{t} g^c_{\alpha-n+1\alpha}(k^\parallel;t,\bar{t}) \\ &\times g^{c-1}_{\alpha-n\alpha}(k^\parallel;\bar{t},t') \\ +\ & t^\perp_{\alpha-n-1\alpha-n} e^{-iA_{\alpha-n-1}(t)} \int_c d\bar{t} g^c_{\alpha-n-1\alpha}(k^\parallel;t,\bar{t}) \\ &\times g^{c-1}_{\alpha-n\alpha}(k^\parallel;\bar{t},t'). \end{aligned} \tag{5}$$

Next, we define the contour-ordered left function $L^c_{\alpha-n}$ via

$$\begin{aligned} L^c_{\alpha-n}(k^\parallel;t,t') \ =\ & -t^\perp_{\alpha-n\alpha-n+1} e^{iA_{\alpha-n}(t)} \\ &\times \int_c d\bar{t} g^c_{\alpha-n+1\alpha}(k^\parallel;t,\bar{t}) g^{c-1}_{\alpha-n\alpha}(k^\parallel;\bar{t},t'). \end{aligned} \tag{6}$$

Using this definition, we can rewrite Eq. (5) in terms of the L^c function. To do this, we need the inverse of the L^c function with respect to the time indices. If we recall that $(AB)^{-1} = B^{-1}A^{-1}$, then we find

$$\begin{aligned} L^c_{\alpha-n}(k^\parallel;t,t') = &\left[-i\frac{\partial}{\partial t} + \mu - \epsilon^\parallel_{\alpha-n}(k^\parallel)\right]\delta_c(t,t') \\ &-\Sigma^c_{\alpha-n}(t,t') \\ &-t^{\perp 2}_{\alpha-n-1\alpha-n} e^{-iA_{\alpha-n-1}(t)} L^{c-1}_{\alpha-n-1}(k^\parallel;t,t') e^{iA_{\alpha-n-1}(t')}. \end{aligned} \tag{7}$$

One can perform a similar procedure to determine the contour-ordered right functions. Once again, we start from Eq. (4) and let $\alpha\to\alpha+n$ and $\beta\to\alpha$, with $n>0$.

The contour-ordered right function $R^c_{\alpha+n}$ is defined via

$$R^c_{\alpha+n}(k^\parallel;t,t') = -t^\perp_{\alpha+n-1\alpha+n}e^{-iA_{\alpha+n-1}(t)} \times \int_c d\bar{t} g^c_{\alpha+n-1\alpha}(k^\parallel;t,\bar{t}) g^{c-1}_{\alpha+n\alpha}(k^\parallel;\bar{t},t'). \quad (8)$$

The corresponding recursion relation becomes

$$R^c_{\alpha+n}(k^\parallel;t,t') = \left[-i\frac{\partial}{\partial t} + \mu - \epsilon^\parallel_{\alpha+n}(k^\parallel)\right]\delta_c(t,t') - \Sigma^c_{\alpha+n}(t,t') - t^{\perp 2}_{\alpha+n+1\alpha+n}e^{iA_{\alpha+n}(t)}R^{c-1}_{\alpha+n+1}(k^\parallel;t,t')e^{-iA_{\alpha+n}(t')}. \quad (9)$$

Finally, if one examines the equation of motion in Eq. (4) for $\alpha = \beta$ and uses the definitions for the left and right functions in Eqs. (7) and (8), respectively, one finds

$$\begin{aligned} g^{c-1}_{\alpha\alpha}(k^\parallel;,t,t') &= \left[-i\frac{\partial}{\partial t} + \mu - \epsilon^\parallel_\alpha(k^\parallel)\right]\delta_c(t,t') \\ &- \Sigma^c_\alpha(t,t') \\ &- t^{\perp 2}_{\alpha-1\alpha}e^{-iA_{\alpha-1}(t)}L^{c-1}_{\alpha-1}(k^\parallel;t,t')e^{iA_{\alpha-1}(t')} \\ &- t^{\perp 2}_{\alpha\alpha+1}e^{iA_\alpha(t)}R^{c-1}_{\alpha+1}(k^\parallel;t,t')e^{-iA_\alpha(t')}. \end{aligned} \quad (10)$$

Note that this result is the diagonal time-block element of the full inverse of the contour-ordered Green's function, and not just the inverse of the time block. Clearly, one can see that the sum of the inverses of the left and the right functions can be thought of as an extra contribution to the self-energy for the system, which we call the self-energy of the leads. This formula remains a bit unwieldy, so it is customary to iterate the L and R recursion relations one more time to determine L_α and R_α. Then, the diagonal element of the Green's function becomes

$$\begin{aligned} g^{c-1}_{\alpha\alpha}(k^\parallel;,t,t') &= -\left[-i\frac{\partial}{\partial t} + \mu - \epsilon^\parallel_\alpha(k^\parallel)\right]\delta_c(t,t') \\ &+ \Sigma^c_\alpha(t,t') + L^c_\alpha(k^\parallel;t,t') + R^c_\alpha(k^\parallel;t,t'), \end{aligned} \quad (11)$$

which agrees with the form used in equilibrium calculations.

Now, to see that the system can be solved in a frequency representation, we assume that we have reached a steady state, where the contour-ordered self-energy $\Sigma^c_\alpha(t,t')$ is time-translation invariant, and depends only on the relative time $t-t'$. Since we will derive below the L and R functions in the bulk, and show that they depend only on the relative time when there is constant current flow, then all of the terms in the two recursion relations given in Eqs. (7) and (9) depend on the relative time only, since the vector potential is at most a linear function in time, so the exponential factors combine and become a function only of $t-t'$. Hence, the L and R functions will depend only on the relative time as will the local Green's function.

It is not so simple to use the contour-ordered objects in the full algorithm used to solve the problem, so we now separate out the retarded, advanced, and Keldysh (or lesser) components [13, 14, 16]. Since the retarded and advanced functions are related to each other in a simple way, we really need to solve for only two sets of functions: (i) the retarded ones and (ii) the Keldysh (or lesser) ones. The strategy to do this is straightforward, but quite tedious. To start, we rewrite the contour-ordered Green's function g^c, which is defined for two times on the contour, as a matrix-valued function, with both times on the real axis. We use + and − signs to indicate that the real time lies on the upper (outward) branch or the lower (inward) branch. Hence we perform the transformation [13]

$$g^c \to \bar{g}^c(t,t') = \begin{pmatrix} G^{++}(t,t') & G^{+-}(t,t') \\ G^{-+}(t,t') & G^{--}(t,t') \end{pmatrix} \quad (12)$$

where the overbar indicates the 2×2 matrix representation. These four components are overdetermined, because only three of them are independent. One can transform the Green's function from this 2×2 representation to the so-called Larkin-Ovchinnikov representation, which is a set of matrix transformations which convert $\bar{g}^c$ to the upper triangular form [16]

$$\bar{g}^c \to \underline{G} = \begin{pmatrix} g^R(t,t') & g^K(t,t') \\ 0 & g^A(t,t') \end{pmatrix} \quad (13)$$

where the retarded Green's function satisfies $g^R = G^{++} - G^{+-}$, the advanced Green's function satisfies $g^A = G^{++} - G^{-+}$, and the Keldysh Green's function satisfies $g^K = G^{++} + G^{--}$. Explicitly writing out these definitions yields

$$g^R_{\alpha\beta}(k^\parallel;t,t') = -\frac{i}{\mathcal{Z}}\theta(t-t')\mathrm{Tr}e^{-\beta\mathcal{H}(-\infty)}\{c_{\alpha k^\parallel}(t), c^\dagger_{\beta k^\parallel}(t')\}_+, \quad (14)$$

for the retarded Green's function,

$$g^A_{\alpha\beta}(k^\parallel;t,t') = \frac{i}{\mathcal{Z}}\theta(t'-t)\mathrm{Tr}e^{-\beta\mathcal{H}(-\infty)}\{c_{\alpha k^\parallel}(t), c^\dagger_{\beta k^\parallel}(t')\}_+, \quad (15)$$

for the advanced Green's function, and

$$g^K_{\alpha\beta}(k^\parallel;t,t') = -\frac{i}{\mathcal{Z}}\mathrm{Tr}e^{-\beta\mathcal{H}(-\infty)}[c_{\alpha k^\parallel}(t), c^\dagger_{\beta k^\parallel}(t')]_-, \quad (16)$$

for the Keldysh Green's function. One can immediately see that the following identity

$$g^{R*}_{\alpha\beta}(k^\parallel;t,t') = g^A_{\beta\alpha}(k^\parallel;t',t) \quad (17)$$

holds between retarded and advanced Green's functions, while for the Keldysh Green's function, we have

$$g^{K*}_{\alpha\beta}(k^\parallel;t,t') = -g^K_{\beta\alpha}(k^\parallel;t',t). \quad (18)$$

When we Fourier transform to frequency, we find the identities become

$$g^{R*}_{\alpha\beta}(k^\parallel;\omega) = g^A_{\beta\alpha}(k^\parallel;\omega) \quad (19)$$

and

$$g^{K*}_{\alpha\beta}(k^{\parallel};\omega) = -g^{K}_{\beta\alpha}(k^{\parallel};\omega), \tag{20}$$

which implies that the local Keldysh Green's function is purely imaginary in frequency space.

It sometimes is convenient to use the so-called lesser Green's function to evaluate observables. The lesser Green's function is defined by

$$g^{<}_{\alpha\beta}(k^{\parallel};t,t') = \frac{i}{\mathcal{Z}}\mathrm{Tr}e^{-\beta\mathcal{H}(-\infty)}c^{\dagger}_{\beta k^{\parallel}}(t')c_{\alpha k^{\parallel}}(t). \tag{21}$$

After Fourier transforming to the frequency domain, it can be found from the retarded, advanced, and Keldysh Green's functions via

$$g^{<}_{\alpha\beta}(k^{\parallel};\omega) = \frac{1}{2}\left[g^{K}_{\alpha\beta}(k^{\parallel};\omega) - g^{R}_{\alpha\beta}(k^{\parallel};\omega) + g^{A}_{\alpha\beta}(k^{\parallel};\omega)\right]. \tag{22}$$

Using this upper triangular representation, one can go through some tedious algebra to transform the left and right recurrence relations to this upper triangular form. In addition, one can Fourier transform from the relative time representation to the frequency representation. Reading off the diagonal and off-diagonal components, we find the recursion relations become

$$\begin{aligned} L^{R}_{\alpha-n}(k^{\parallel};\omega) &= \omega+\mu-\epsilon^{\parallel}_{\alpha-n}(k^{\parallel}) - \Sigma^{R}_{\alpha-n}(\omega) \\ &- \frac{t^{\perp 2}_{\alpha-n\alpha-n-1}}{L^{R}_{\alpha-n-1}(k^{\parallel};\omega+E_{\alpha-n-1})}. \end{aligned} \tag{23}$$

Here, E_α is the electric field at plane α. It is easy to see that the advanced function satisfies $L^A = L^{R*}$. The advanced recursion relation has precisely the same form as in Eq. (23) except all R superscripts are replaced by A superscripts. Since the retarded and advanced self-energies are related by complex conjugates, as are the initial (bulk) $L_{-\infty}$ starting values, the two recursions are complex conjugates of each other, and hence so are L^R_α and L^A_α for all α.The Keldysh recursion relation then becomes

$$\begin{aligned} L^{K}_{\alpha-n}(k^{\parallel};\omega) &= -\Sigma^{K}_{\alpha-n}(\omega) \\ &+ \frac{t^{\perp 2}_{\alpha-n\alpha-n-1}L^{K}_{\alpha-n-1}(k^{\parallel};\omega+E_{\alpha-n-1})}{|L^{R}_{\alpha-n-1}(k^{\parallel};\omega+E_{\alpha-n-1})|^2}. \end{aligned} \tag{24}$$

The similar equations for the right functions are as follows: (i) for the retarded right functions we have

$$\begin{aligned} R^{R}_{\alpha+n}(k^{\parallel};\omega) &= \omega+\mu-\epsilon^{\parallel}_{\alpha+n}(k^{\parallel}) - \Sigma^{R}_{\alpha-n}(\omega) \\ &- \frac{t^{\perp 2}_{\alpha+n+1\alpha+n}}{R^{R}_{\alpha+n+1}(k^{\parallel};\omega-E_{\alpha+n})} \end{aligned} \tag{25}$$

(with $R^{R*} = R^A$) and (ii) for the Keldysh right functions we have

$$\begin{aligned} R^{K}_{\alpha+n}(k^{\parallel};\omega) &= -\Sigma^{K}_{\alpha+n}(\omega) \\ &+ \frac{t^{\perp 2}_{\alpha+n+1\alpha+n}R^{K}_{\alpha+n+1}(k^{\parallel};\omega-E_{\alpha+n})}{|R^{R}_{\alpha+n+1}(k^{\parallel};\omega-E_{\alpha+n})|^2}. \end{aligned} \tag{26}$$

One can immediately see that the retarded (and advanced) recursions are independent of the Keldysh functions, so they can be solved separately from the Keldysh case (which depends on all three types of functions). To begin, we must determine $L^R_{-\infty}$ and R^R_∞. The recursion for the left functions starts for negative α and moves up through positive αs and for the right function it is the reverse. The starting point for both recursions is found from the recursion relations for the ballistic metal, where $\Sigma^R_{\pm\infty}(\omega) = 0$, $\epsilon^{\parallel}_{\pm\infty}(k^{\parallel}) = \epsilon^{\parallel}(k^{\parallel})$ and $t^{\perp}_{\alpha\alpha-1} = t^{\perp}$ for $\alpha \to \pm\infty$. Then the equation for $L^R_{-\infty}$ satisfies

$$L^{R2}_{-\infty}(k^{\parallel};\omega) - [\omega+\mu-\epsilon^{\parallel}(k^{\parallel})]L^{R}_{-\infty}(k^{\parallel};\omega) + t^{\perp 2} = 0 \tag{27}$$

with solution

$$\begin{aligned} L^{R}_{-\infty}(k^{\parallel};\omega) &= \frac{\omega+\mu-\epsilon^{\parallel}(k^{\parallel})}{2} \\ &\pm \frac{1}{2}\sqrt{[\omega+\mu-\epsilon^{\parallel}(k^{\parallel})]^2 - 4(t^{\perp})^2}. \end{aligned} \tag{28}$$

When the square root is imaginary, we choose the sign so that the imaginary part of L^R is *greater than zero* (this may seem odd for a retarded object, but it happens because of how the L^R function enters into determining the retarded Green's function). When the square root is real, we choose the sign such that L^R is larger in magnitude than $t^{\perp}$. This solution is identical to what was used in equilibrium, as we anticipated, since the current carrying state has no electric field over it, so the states are unchanged, just their occupancy differs from that in the bulk. Direct calculation also shows that $R^R_\infty(k^{\parallel};\omega) = L^R_{-\infty}(k^{\parallel};\omega)$.

The dynamical mean-field theory proceeds via an iterative solution [4]. One starts with a guess for the self-energies on all of the planes. Then we compute the local Green's functions from Dyson's equation, which requires us to use the L and R functions. Next, one uses the Dyson equation for the impurity problem to extract the effective medium. The impurity problem is solved for this effective medium, and then the self-energy is extracted from the Dyson equation for the impurity problem again. This then produces the new self-energy guess for the next iteration. In this work, we focus on the bulk system, so we do not describe the details for how to solve the impurity problem, which will be done elsewhere.

In a real calculation, we work with a finite number of planes. In equilibrium, this typically was thirty planes on each side of the barrier region plus the number of planes in the barrier. One then sets the L^R functions equal to $L^R_{-\infty}$ up to the first plane that is being simulated in the finite system. From there, we use the recursion relations in Eq. (23) to determine all of the L^R_α functions. The right functions proceed similarly. We fix R^R at the value R^R_∞ until we get to the first simulated plane from the top, and then we use the recursion relations in Eq. (25) to find all of the R^R_α functions. From these two results, we

find the local retarded Green's function for each plane. Taking complex conjugates then gives all of the advanced functions.

Unfortunately, one cannot use the same procedure for the Keldysh functions that we used to find the retarded functions. This is because the recursion relations for the Keldysh case are homogeneous equations when the Keldysh self-energy vanishes, and hence they can be manipulated into an identity that reduces to $0 = 0$ and does not allow one to solve for the L^K or R^K functions in the bulk limit. Instead, we go back to the original definitions of the L and R functions and manipulate them to determine the Keldysh functions in the bulk. To begin, we note that

$$L^R_{\alpha-1}(k^\parallel;\omega) = -t^\perp_\alpha e^{-iA_0}\frac{g^R_{\alpha\alpha}(k^\parallel;\omega)}{g^R_{\alpha-1\alpha}(k^\parallel;\omega)} \tag{29}$$

for the retarded function and

$$\begin{aligned} L^K_{\alpha-1}(k^\parallel;\omega) &= -t^\perp_\alpha e^{-iA_0}\Bigg[-\frac{g^R_{\alpha\alpha}(k^\parallel;\omega)g^K_{\alpha-1\alpha}(k^\parallel;\omega)}{g^R_{\alpha-1\alpha}(k^\parallel;\omega)g^A_{\alpha-1\alpha}(k^\parallel;\omega)} \\ &+ \frac{g^K_{\alpha\alpha}(k^\parallel;\omega)}{g^A_{\alpha-1\alpha}(k^\parallel;\omega)}\Bigg]. \end{aligned} \tag{30}$$

Using Eq. (29), we rewrite Eq. (30) as

$$\begin{aligned} L^K_{\alpha-1}(k^\parallel;\omega) &= -L^R_{\alpha-1}(k^\parallel;\omega)\frac{g^K_{\alpha-1\alpha}(k^\parallel;\omega)}{g^A_{\alpha-1\alpha}(k^\parallel;\omega)} \\ &- t^\perp_\alpha e^{-iA_0}\frac{g^K_{\alpha\alpha}(k^\parallel;\omega)}{g^A_{\alpha-1\alpha}(k^\parallel;\omega)}. \end{aligned} \tag{31}$$

Performing the same type of analysis for the right functions yields

$$\begin{aligned} R^K_{\alpha+1}(k^\parallel;\omega) &= -R^R_{\alpha+1}(k^\parallel;\omega)\frac{g^K_{\alpha+1\alpha}(k^\parallel;\omega)}{g^A_{\alpha+1\alpha}(k^\parallel;\omega)} \\ &- t^\perp_\alpha e^{iA_0}\frac{g^K_{\alpha\alpha}(k^\parallel;\omega)}{g^A_{\alpha+1\alpha}(k^\parallel;\omega)}. \end{aligned} \tag{32}$$

These two relations now provide a pathway to calculate the L^K and R^K functions in the bulk by simply calculating the local and nearest-neighbor Green's functions in the bulk using the mixed basis. This is what we do next.

To begin, we must calculate the retarded Green's function in nonequilibrium. We start the system in equilibrium at time t_0 and turn the field on at time t_{on} and leave it on for one unit of time, where the vector potential decreases from 0 to $-A_0$. We take the limit where both t_0 and t_{on} approach $-\infty$. Since the Hamiltonian commutes with itself at different times, even when the field is on, the Green's function is simple to determine in momentum space [$k = (k^\parallel, k_z)$ is the three-dimensional momentum] [**?**]

$$g^R(k;t,t') = -i\theta(t-t')e^{-i[\epsilon^\parallel(k^\parallel)-2t^\perp\cos(k_z+A_0)-\mu](t-t')} \tag{33}$$

when both t and t' are much larger than $-\infty$ and k_z is the z-component of the momentum. Taking the Fourier transform to the frequency representation yields

$$g^R(k;\omega) = \frac{1}{\omega+\mu-\epsilon^\parallel(k^\parallel)+2t^\perp\cos(k_z+A_0)+i0^+} \tag{34}$$

In order to show that this result yields the same self-energy of the leads as found in Eq. (28), we need to Fourier transform k_z to real space in order to represent the Green's function in the mixed basis. Let z_α denote the z-component of the αth plane. Then the mixed-basis Green's function is found from

$$g^R_{\alpha\beta}(k^\parallel;\omega) = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk_z e^{-i(z_\alpha-z_\beta)k_z}g^R(k;\omega). \tag{35}$$

We substitute Eq. (34) into Eq. (35) and use the notation $\omega+\mu-\epsilon^\parallel(k^\parallel)-i0^+ = 2t^\perp\gamma$ and $k'_z = k_z + A_0$ to get

$$g^R_{\alpha\beta}(k^\parallel;\omega) = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk'_z \frac{e^{-i(z_\alpha-z_\beta)(k'_z-A_0)}}{2t^\perp(\gamma+\cos k'_z)}. \tag{36}$$

This integral can be evaluated via a contour integration and the residue theorem. We convert the integral over k'_z to an integral over the unit circle with $Z = \exp(ik'_z)$. This gives

$$g^R_{\alpha\beta}(k^\parallel;\omega) = \frac{e^{i(z_\alpha-z_\beta)A_0}}{2\pi it^\perp}\oint\frac{dZ}{Z}\frac{Z^{-z_\alpha+z_\beta}}{(2\gamma+Z+1/Z)} \tag{37}$$

with the integral over the unit circle, evaluated in the standard counter clockwise direction. The poles lie at the roots of $Z^2+2\gamma Z+1=0$, or $Z_\pm = -\gamma\pm\sqrt{\gamma^2-1}$. If $|\gamma| > 1$, then the two roots are real, and since their product is one, one root lies outside the unit circle and one root inside. If $|\gamma| < 1$, then the two roots are complex, with opposite signs of their imaginary parts. There also can be a pole at $Z = 0$ if $z_\alpha - z_\beta > 0$. We assume that $z_\alpha - z_\beta < 0$ for now. Then if we let Z_{in} denote the root inside the unit circle and Z_{out} denote the root outside the unit circle, then the integral becomes

$$g^R_{\alpha\beta}(k^\parallel;\omega) = \frac{e^{i(z_\alpha-z_\beta)A_0}}{t^\perp}\frac{Z_{in}^{-z_\alpha+z_\beta}}{Z_{in}-Z_{out}}. \tag{38}$$

In particular, the local Green's function satisfies

$$g^R_{\alpha\alpha}(k^\parallel;\omega) = \frac{1}{\pm\sqrt{[\omega+\mu-\epsilon^\parallel(k^\parallel)-i0^+]^2-4t^{\perp 2}}}, \tag{39}$$

where the plus or minus sign is chosen according to which root lies within the unit circle. One can also choose the sign according to causality *a posteriori*: when the Green's function is complex, it must have a negative imaginary part and analyticity determines how it behaves when it is real. For a fixed $k^\parallel$ this is the local retarded Green's function for a one-dimensional system, as one

expects. Indeed, if we evaluate the frequency representation of Eq. (9) and examine the retarded component, then substituting in the results in the bulk limit, including Eq. (28), yields the result in Eq. (39), which is a good check that this approach works correctly.

Using this result for the local Green's function, we can combine it with the Fourier transform of Eq. (11) to determine what the equilibrium L^K function is. We know the Keldysh component of the diagonal Green's function is $g^K_{\alpha\alpha}(k^\parallel;\omega)$ and the Keldysh component of the inverse local Green's function is schematically given by $(g^{-1})^K = -(g^R)^{-1}g^K(g^A)^{-1}$, so we find, because $L^K = R^K$ in equilibrium, that $L^K = -g^K/(2|g^R|^2)$. But $g^K = -2if^K \mathrm{Im} g^R$, with the equilibrium Keldysh distribution function defined just below Eq. (43). Within the band, which is the only place that K functions are nonzero, g^R is pure imaginary, so we get

$$L^K_{-\infty,\ eq.}(k^\parallel;\omega) = -if^K(\omega)\sqrt{4(t^\perp)^2 - [\omega+\mu-\epsilon^\parallel(k^\parallel)]^2}, \tag{40}$$

where the square root is the positive root.

We also need to evaluate the nearest-neighbor Green's functions in this mixed basis. When $\beta = \alpha+1$, the result simply follows from the above integration, where we find

$$g^R_{\alpha\alpha+1}(k^\parallel;\omega) = e^{-iA_0}\frac{-\frac{\omega+\mu-\epsilon^\parallel(k^\parallel)}{2t^\perp} \pm \sqrt{\frac{[\omega+\mu-\epsilon^\parallel(k^\parallel)]^2}{4t^{\perp 2}} - 1}}{\pm\sqrt{[\omega+\mu-\epsilon^\parallel(k^\parallel) - i0^+]^2 - 4t^{\perp 2}}}, \tag{41}$$

and the plus or minus sign is chosen according to the discussion given above. For the other nearest-neighbor Green's function ($\alpha\alpha-1$), it looks like one has to work harder since there is an extra pole at $Z=0$. But this isn't the case. If $z_\alpha - z_\beta > 0$, then we can factor out the exponential term in Eq. (36) that depends on A_0 and then we let $k'_z \to -k'_z$, which is the equivalent of interchanging α and β in the remaining integral. Hence the integral is independent of the sign of $z_\alpha - z_\beta$ and we find

$$g^R_{\alpha\alpha-1}(k^\parallel;\omega) = e^{iA_0}\frac{-\frac{\omega+\mu-\epsilon^\parallel(k^\parallel)}{2t^\perp} \pm \sqrt{\frac{[\omega+\mu-\epsilon^\parallel(k^\parallel)]^2}{4t^{\perp 2}} - 1}}{\pm\sqrt{[\omega+\mu-\epsilon^\parallel(k^\parallel) - i0^+]^2 - 4t^{\perp 2}}}. \tag{42}$$

For example, using Eqs. (39) and (41) in Eq. (29), then gives the result in Eq. (28), as it must. The general formula for Eq. (38) is then to replace the exponent of Z_{in} in the numerator by $|z_\alpha - z_\beta|$.

Our next step is to calculate the Keldysh (or lesser) Green's functions in the bulk. Both of these functions can be written as

$$\begin{aligned} g^{K,<}(k;t,t') &= if^{K,<}[\epsilon^\parallel(k^\parallel) - 2t^\perp\cos(k_z) - \mu] \\ &\times\ e^{-i[\epsilon^\parallel(k^\parallel) - 2t^\perp\cos(k_z+A_0) - \mu](t-t')}, \end{aligned} \tag{43}$$

in the large-time limit, where the distribution function $f(x)$ satisfies $f^<(x) = 1/[1+\exp(\beta x)]$ and $f^K(x) = 2f^<(x) - 1$. Fourier transforming to frequency space yields

$$\begin{aligned} g^{K,<}(k;\omega) &= 2\pi i f^{K,<}[\epsilon^\parallel(k^\parallel) - 2t^\perp\cos(k_z) - \mu] \\ &\times\ \delta[\omega+\mu-\epsilon^\parallel(k^\parallel) + 2t^\perp\cos(k_z+A_0)]. \end{aligned} \tag{44}$$

Next, we Fourier transform with respect to k_z to get the mixed-basis Green's functions

$$g^{K,<}_{\alpha\beta}(k^\parallel;\omega) = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk_z e^{-i(z_\alpha - z_\beta)k_z} g^{K,<}(k;\omega), \tag{45}$$

which can be immediately done because the integrand is proportional to a delta function. One needs to note that there are two roots where the argument of the delta function vanishes, and that we must divide the integrand by the absolute value of the derivative of the argument of the delta function, evaluated at each root. Note that the Keldysh (lesser) Green's function is nonzero only when we are within the band, implying

$$\left|\frac{\omega+\mu-\epsilon^\parallel(k^\parallel)}{2t^\perp}\right| \le 1. \tag{46}$$

The end result is

$$
\begin{aligned}
g^{K,<}_{\alpha\beta}(k^{\parallel};\omega) &= i\Bigg\{ f^{K,<}\Big[\omega\cos(A_0) - (\mu-\epsilon^{\parallel}(k^{\parallel}))(1-\cos(A_0)) - \sqrt{4(t^{\perp})^2 - (\omega+\mu-\epsilon^{\parallel}(k^{\parallel}))^2}\sin(A_0)\Big] \\
&\times \left[-\frac{\omega+\mu-\epsilon^{\parallel}(k^{\parallel})}{2t^{\perp}} - i\sqrt{1-\left(\frac{\omega+\mu-\epsilon^{\parallel}(k^{\parallel})}{2t^{\perp}}\right)^2}\right]^{z_\alpha - z_\beta} \\
&+ f^{K,<}\Big[\omega\cos(A_0) - (\mu-\epsilon^{\parallel}(k^{\parallel}))(1-\cos(A_0)) + \sqrt{4(t^{\perp})^2 - (\omega+\mu-\epsilon^{\parallel}(k^{\parallel}))^2}\sin(A_0)\Big] \\
&\times \left[-\frac{\omega+\mu-\epsilon^{\parallel}(k^{\parallel})}{2t^{\perp}} + i\sqrt{1-\left(\frac{\omega+\mu-\epsilon^{\parallel}(k^{\parallel})}{2t^{\perp}}\right)^2}\right]^{z_\alpha - z_\beta} \Bigg\} \\
&\times \frac{1}{\sqrt{4(t^{\perp})^2 - (\omega+\mu-\epsilon^{\parallel}(k^{\parallel}))^2}} e^{i(z_\alpha - z_\beta)A_0}. \qquad (47)
\end{aligned}
$$

If we define $\omega^{\pm}$ by

$$
\begin{aligned}
\omega^{\pm}(k^{\parallel};A_0) &= \omega\cos(A_0) - (\mu-\epsilon^{\parallel}(k^{\parallel}))(1-\cos(A_0)) \\
&\pm \sqrt{4(t^{\perp})^2 - (\omega+\mu-\epsilon^{\parallel}(k^{\parallel}))^2}\sin(A_0) \qquad (48)
\end{aligned}
$$

then we have the local Green's function satisfies

$$
g^{K,<}_{\alpha\alpha}(k^{\parallel};\omega) = i\frac{f^{K,<}[\omega^{+}(k^{\parallel};A_0)] + f^{K,<}[\omega^{-}(k^{\parallel};A_0)]}{\sqrt{4(t^{\perp})^2 - (\omega+\mu-\epsilon^{\parallel}(k^{\parallel}))^2}}, \qquad (49)
$$

and the nearest-neighbor Green's functions are

$$
\begin{aligned}
g^{K,<}_{\alpha\alpha+1}(k^{\parallel};\omega) &= i\Bigg\{ f^{K,<}[\omega^{+}(k^{\parallel};A_0)]\left[-\frac{\omega+\mu-\epsilon^{\parallel}(k^{\parallel})}{2t^{\perp}} - i\sqrt{1-\left(\frac{\omega+\mu-\epsilon^{\parallel}(k^{\parallel})}{2t^{\perp}}\right)^2}\right] \qquad (50) \\
&+ f^{K,<}[\omega^{-}(k^{\parallel};A_0)]\left[-\frac{\omega+\mu-\epsilon^{\parallel}(k^{\parallel})}{2t^{\perp}} + i\sqrt{1-\left(\frac{\omega+\mu-\epsilon^{\parallel}(k^{\parallel})}{2t^{\perp}}\right)^2}\right]\Bigg\} \frac{e^{-iA_0}}{\sqrt{4(t^{\perp})^2 - (\omega+\mu-\epsilon^{\parallel}(k^{\parallel}))^2}}
\end{aligned}
$$

and

$$
\begin{aligned}
g^{K,<}_{\alpha+1\alpha}(k^{\parallel};\omega) &= i\Bigg\{ f^{K,<}[\omega^{+}(k^{\parallel};A_0)]\left[-\frac{\omega+\mu-\epsilon^{\parallel}(k^{\parallel})}{2t^{\perp}} + i\sqrt{1-\left(\frac{\omega+\mu-\epsilon^{\parallel}(k^{\parallel})}{2t^{\perp}}\right)^2}\right] \qquad (51) \\
&+ f^{K,<}[\omega^{-}(k^{\parallel};A_0)]\left[-\frac{\omega+\mu-\epsilon^{\parallel}(k^{\parallel})}{2t^{\perp}} - i\sqrt{1-\left(\frac{\omega+\mu-\epsilon^{\parallel}(k^{\parallel})}{2t^{\perp}}\right)^2}\right]\Bigg\} \frac{e^{iA_0}}{\sqrt{4(t^{\perp})^2 - (\omega+\mu-\epsilon^{\parallel}(k^{\parallel}))^2}}
\end{aligned}
$$

where, in all cases, these Green's functions vanish when the argument of the square root becomes negative. When $A_0 = 0$, these results reduce to the known equilibrium result; in particular,

$$
g^{K,<}_{\alpha\alpha}(k^{\parallel};\omega) = \frac{2if^{K,<}(\omega)}{\sqrt{4(t^{\perp})^2 - (\omega+\mu-\epsilon^{\parallel}(k^{\parallel}))^2}}, \qquad (52)
$$

as expected.

Now we have all the information needed to calculate the boundary functions $L^{K}_{-\infty}$ and R^{K}_{∞} in Eqs. (31) and

(32). The result is, after some long algebra,

$$L^{K,<}_{-\infty}(k^{\parallel};\omega) = -if^{K,<}[\omega^{+}(k^{\parallel};A_0)] \times \sqrt{4(t^{\perp})^2-[\omega+\mu-\epsilon^{\parallel}(k^{\parallel})]^2} \quad (53)$$

and

$$R^{K,<}_{\infty}(k^{\parallel};\omega) = -if^{K,<}[\omega^{-}(k^{\parallel};A_0)] \times \sqrt{4(t^{\perp})^2-[\omega+\mu-\epsilon^{\parallel}(k^{\parallel})]^2}. \quad (54)$$

Obviously, both of these results also become the equilibrium result in Eq. (40) when $A_0 = 0$.

The results for the lesser Green's functions are identical to those for the Keldysh Green's functions except for a simple change in the distribution function.

This then concludes the derivation of the formalism. To work out the full results with a strongly correlated active region of the device requires one to also self-consistently determine the electric field to maintain current conservation. We don't discuss these issues further here, as our goal was to determine the boundary conditions which lead to the so-called "self-energy of the leads" and this is now complete.

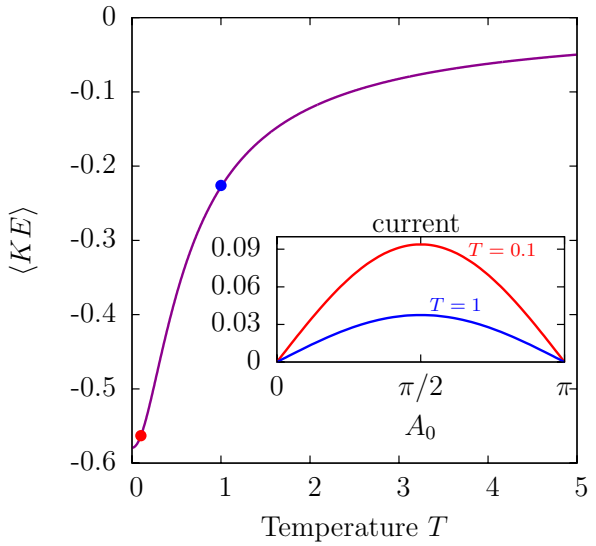

FIG. 3: (Color online) Main panel: average kinetic energy (purple) of noninteracting electrons hopping between nearest neighbors on a simple cubic lattice as a function of the initial equilibrium temperature. Inset: current in the z-direction versus A_0 for two temperatures $T = 0.1t$ (red) and $T = t$ (blue) when the field is applied along one of the cubic axes only.

NUMERICAL RESULTS

The current is easy to calculate within this formalism. For the bulk case, with a constant shift of the vector potential by $-A_0$ in the z-direction, one has

$$J_z(t,A_0) = -i\sum_k v_{k+A_0} g^{<}(k;t,t) \quad (55)$$

where $v_k = d\epsilon(k)/dz = 2t^{\perp}\sin(k)$ is the band velocity. Using, $g^{<}(k;t,t) = if^{<}(\epsilon(k)-\mu)$ gives

$$J_z(t,A_0) = \sum_k 2t^{\perp}\sin(k_z+A_0)f^{<}(\epsilon(k)-\mu). \quad (56)$$

If we work in a homogeneous system, where $t^{\parallel} = t^{\perp} = t$, then we can rewrite the current (which doesn't depend on time once the field is turned off) as

$$J_z(A_0) = -\frac{1}{3}\sum_k \epsilon(k) f^{<}(\epsilon(k)-\mu)\sin(A_0). \quad (57)$$

This shows that the amplitude of the current is proportional to the negative of the average kinetic energy in the initial equilibrium state and has a simple sinusoidal dependence on the amplitude of the vector potential. This result is plotted in Fig. 3.

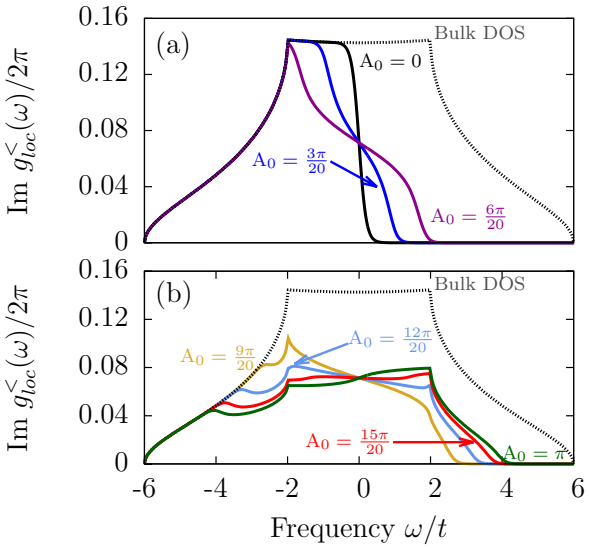

FIG. 4: (Color online) Local lesser Green's function for an initial equilibrium temperature given by $T = 0.1t$ and with perpendicular current flow corresponding to a constant vector potential shift given by A_0 as labeled in the different curves. Panel (a), shows how higher energy states initially increase their occupation versus the equilibrium result. Panel (b) continues increasing A_0 until the current vanishes again at $A_0 = \pi$. Further increasing the vector potential makes the current go negative, and the local lesser Green's function is identical to the result with $A_0 = 2\pi - A_0'$. The bulk density of states is also shown as a reference.

In Figs. 4 and 5, we plot the local lesser Green's function versus the density of states when the system is carrying current for a low and for a high temperature. The

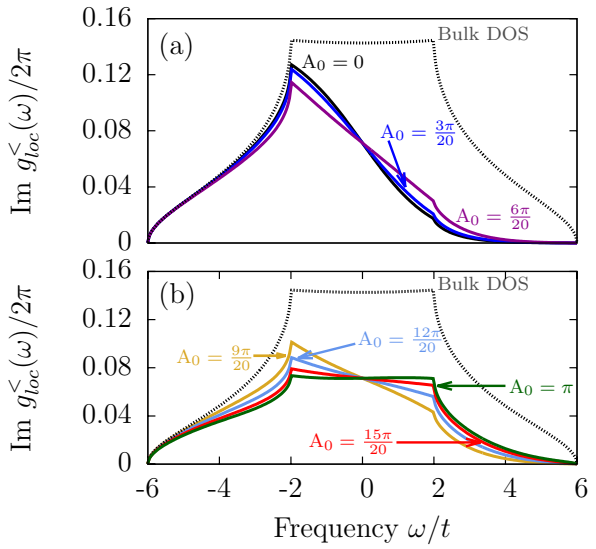

FIG. 5: (Color online) Local lesser Green's function for an initial equilibrium temperature given by $T = t$ and with perpendicular current flow corresponding to a constant vector potential shift given by A_0 as labeled in the different curves. Panel (a), shows how higher energy states initially increase their occupation versus the equilibrium result. Panel (b) continues increasing A_0 until the current vanishes again at $A_0 = \pi$. Further increasing the vector potential makes the current go negative, and the local lesser Green's function is identical to the result with $A_0 = 2\pi - A_0'$. The bulk density of states is also shown as a reference.

lesser Green's function is found from Eq. (22), and the imaginary part divided by 2π corresponds to the local density of states multiplied by a current-dependent effective distribution function. This distribution function has a simple form only for $A_0 = 0$, where it becomes the Fermi-Dirac distribution function $f^<(\omega - \mu)$. In all other cases, the distribution function changes with the parallel momentum and hence one has to perform a weighted average over the two-d momentum, or equivalently one performs an integration over the 2d density of states. The net distribution function ends up looking more like the sum of two effective Fermi-Dirac distributions, but even then, the exact shape is somewhat different. Note that as more current flows through the system, higher energy states are occupied, but the system never gets into a negative temperature situation because the field is applied only in one axial direction rather than along the diagonal. One can also see that for a large A_0, the initial temperature plays a smaller role in determining the distribution function.

These results prepare us to calculate the fully correlated case, where there is an active region. This will be done elsewhere.

SUMMARY

In this work, we have presented the formal groundwork for how to determine the current-voltage relation of a strongly correlated multilayered device with inhomogeneous dynamical mean-field theory. Unlike conventional nonequilibrium dynamical-mean field theory, which requires a formalism in the time domain, the steady state can be solved for in the frequency domain, as long as one can calculate the boundary conditions given by the ballistic leads of the system which are current biased. This is done here, which sets the stage for the solution of the full strongly correlated problem. The only issues that we did not describe in detail are how to solve the relevant impurity problems and how to find the self-consistent electric fields through the device. These results will be presented elsewhwere. We believe that solving the full problem will provide insight into the nonlinear behavior of strongly correlated devices, especially those contructed from Mott insulators.

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