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Steady-state nonequilibrium dynamical mean-field theory and the quantum Boltzmann equation

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Abstract. We derive the formalism for steady state nonequilibrium dynamical mean-field theory in a real-time formalism along the Keldysh-Kadanoff-Baym contour [1]. The resulting equations of motion are first transformed to Wigner coordinates (average and relative time), and then re-expressed in terms of differential operators. Finally, we perform a Fourier transform with respect to the relative time, and take the first-order limit in the electric field to produce the quantum Boltzmann equation for dynamical mean-field theory. We next discuss the structure of the equations and their solutions, describing how these equations reduce to the Drude result in the limit of a constant relaxation time. We also explicitly demonstrate the equivalence between the Kubo and nonequilibrium approaches to linear response. There are a number of interesting modifications of the conventional quantum Boltzmann equation that arise due to the underlying bandstructure of the lattice.

1. Introduction

Dynamical mean-field theory was introduced in 1989 by Metzner and Vollhardt [2] as a particular limit where the spatial dimension approaches infinity. They showed that the self-energy is local in this case, so the many-body problem simplifies to that of an impurity in a time-dependent field plus a self-consistency relation [3]. Since then, nearly all of the classic problems of many-body physics have been solved (see [4] for a review). The generalization of the formalism to the nonequilibrium case is straightforward, but involves a number of technical complications. In this chapter, we describe the steady-state limit, where we start our system in equilibrium as $t_0 \to -\infty$, then we turn on an external field at a later time t_0' ($t_0' > t_0$) and take the limit where $t_0' \to -\infty$. We consider only a spatially uniform (but possibly time-dependent) electric field here, and ignore all magnetic-field effects. The Hamiltonian is written as the sum of two terms: (i) a time-independent Hamiltonian $\mathcal{H}$ which describes the field-independent piece, and (ii) the time-dependent piece $\mathcal{H}'(t)$ arising from the field dependence. We adjust the electron density with a chemical potential, by subtracting the term $\mu\mathcal{N}$ from the Hamiltonian. The work presented here is a natural extension of the discussion in Mahan's review article [5] to the case of dynamical mean-field theory.

The nonequilibrium formalism works with the so-called contour-ordered Green's function, which is defined for t and t' on the Keldysh-Kadanoff-Baym contour [1, 6] (see Fig. 1) in terms of the electron creation ($c_{\mathbf{r}}^\dagger$) and annihilation ($c_{\mathbf{r}}$) operators at lattice site $\mathbf{r}$:

$$G^c_{\mathbf{r},\mathbf{r}'}(t,t') = -i\mathrm{Tr}\,\mathcal{T}_c e^{-\beta(\mathcal{H}-\mu\mathcal{N})} S_c(\mathcal{H}') c_{\mathbf{r}}(t) c^\dagger_{\mathbf{r}'}(t')/\mathcal{Z}, \tag{1}$$

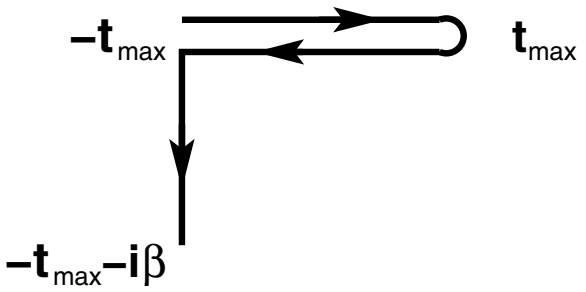

Figure 1. *Keldysh-Kadanoff-Baym contour [1] for the time variables. The time-domain cutoffs are symmetric at* $\pm t_{\max}$ *and we take the limit* $t_{\max} \to \infty$*. The arrows indicate the direction to take along the contour for the time-ordering operation.*

with $S_c(\mathcal{H}') = \exp[-i\int_c dt''\mathcal{H}'_I(t'')]$ the evolution operator for the time-dependent piece of the Hamiltonian in the interaction representation, $\mathcal{O}(t) = \exp[i(\mathcal{H}-\mu\mathcal{N})t]\mathcal{O}\exp[-i(\mathcal{H}-\mu\mathcal{N})t]$ the time-dependent operator for any operator $\mathcal{O}$, $\mathcal{Z} = \mathrm{Tr}\exp[-\beta(\mathcal{H}-\mu\mathcal{N})]$, β is the inverse temperature, and $\mathcal{T}_c$ is the time-ordering operator along the contour ("earlier" times ordered along the contour are moved to the right in the operator expressions). We work in units where $\hbar = c = a = 1$ (a is the lattice spacing).

The contour-ordered Green's function satisfies the Dyson equation (which can be thought of as the definition of the contour-ordered self-energy Σ^c)

$$G^c_{\mathbf{r},\mathbf{r}'}(t,t') = G^{c0}_{\mathbf{r},\mathbf{r}'}(t,t') + \int d\mathbf{r}'' \int_c dt'' \int_c dt''' G^{c0}_{\mathbf{r},\mathbf{r}''}(t,t'')\Sigma^c(t'',t''')G^c_{\mathbf{r}'',\mathbf{r}'}(t''',t') \tag{2}$$

with each time integral being performed over the contour. The Green's function G^{c0} is the noniteracting contour-ordered Green's function in the presence of the field. Combining the nonequilibrium perturbation theory rules described by Langreth [7] with the perturbation theory expansion of Metzner [8], shows that the contour-ordered self-energy is local in infinite dimensions, and hence nonzero only when $\mathbf{r} = \mathbf{r}'$. This is why the self-energy has no spatial label in Eq. (2). Since our field is spatially uniform, all Green's functions are translationally invariant, so transforming to momentum space diagonalizes the spatial part of the Dyson equation (note, we work in the Hamiltonian or temporal gauge with a spatially uniform vector potential before making the theory gauge-invariant).

Keldysh [9] was the first to note that if we are interested in the steady-state limit, as described above, then the contour extends from $-\infty$ to ∞, and we do not need to consider the matrix structure associated with the piece of the branch that extends along the imaginary axis; instead, we take it into account by incorporating the term $\exp[-\beta(\mathcal{H}-\mu\mathcal{N})]/\mathcal{Z}$ into the operator averages to represent the initial equilibrium distribution of the system for times in the distant past. Next, we can re-express the Dyson equation, which involves an integral over the Keldysh contour, into an integral over the real-time axis, but at the price of making the Green's function and self-energy into a 2×2 matrix with the corresponding Dyson equation [5]:

$$\begin{aligned}
\begin{pmatrix} G^R_{\mathbf{k}} & G^K_{\mathbf{k}} \\ 0 & G^A_{\mathbf{k}} \end{pmatrix}(t,t') &= \begin{pmatrix} G^{R0}_{\mathbf{k}} & G^{K0}_{\mathbf{k}} \\ 0 & G^{A0}_{\mathbf{k}} \end{pmatrix}(t,t') \\
&+ \int dt'' \int dt''' \begin{pmatrix} G^{R0}_{\mathbf{k}} & G^{K0}_{\mathbf{k}} \\ 0 & G^{A0}_{\mathbf{k}} \end{pmatrix}(t,t'') \\
&\times \begin{pmatrix} \Sigma^R & \Sigma^K \\ 0 & \Sigma^A \end{pmatrix}(t'',t''') \times \begin{pmatrix} G^R_{\mathbf{k}} & G^K_{\mathbf{k}} \\ 0 & G^A_{\mathbf{k}} \end{pmatrix}(t''',t'),
\end{aligned} \tag{3}$$

where matrix multiplication is understood amongst the 2×2 matrices and we have Fourier transformed from real space to momentum space (the momentum for the Green's functions is $\mathbf{k}$). The three labels (R, K, and A) on the Green's functions and self-energies refer to the names retarded, Keldysh, and advanced, respectively; these objects are formed via specific linear combinations of the contour-ordered Green's function [9]. In order to describe these linear combinations, we must first define four Green's functions from natural choices of the time variables. The time-ordered Green's function is the contour-ordered Green's function with both t and t' on the upper real-time branch; the anti-time-ordered Green's function has both t and t' on the lower real-time branch; the lesser Green's function has t on the upper and t' on the lower real-time branches; and the greater Green's function has t on the lower and t' on the upper real-time branches. Then the retarded Green's function is one-half the time-ordered minus the anti-time-ordered plus the greater minus the lesser Green's functions. The advanced Green's function is one-half the time-ordered minus the anti-time-ordered minus the greater plus the lesser Green's functions. The Keldysh Green's function is the greater plus the lesser Green's functions. There is a conjugate Dyson equation as well, which looks similar to Eq. (3), but with the order of the $G^0 \Sigma G$ term switched to $G \Sigma G^0$.

2. Retarded Green's function

In this section, we will develop the formalism for the retarded Green's function. To start, we examine the equation of motion (EOM) for the noninteracting retarded Green's function in the presence of a uniform electric field. The field is described with a time-dependent vector potential $\mathbf{A}(t)$ and a vanishing scalar potential in the Hamiltonian gauge, where $\mathbf{E} = -\partial_t \mathbf{A}(t)$. This is carried out with a Peierls substitution [10, 11]: $\mathbf{k} \to \mathbf{k} - e\mathbf{A}(t)$ to yield

$$\begin{aligned} \left[i\partial_t + \mu - \epsilon_{\mathbf{k}-e\mathbf{A}(t)} \right] G^{R0}_{\mathbf{k}}(t,t') &= \delta(t-t'), \\ \left[-i\partial_{t'} + \mu - \epsilon_{\mathbf{k}-e\mathbf{A}(t')} \right] G^{R0}_{\mathbf{k}}(t,t') &= \delta(t-t'), \end{aligned} \tag{4}$$

with $\epsilon_{\mathbf{k}} = -t^* \lim_{d\to\infty} \sum_{i=1}^{d} \cos \mathbf{k}_i / \sqrt{d}$; the hopping matrix element between nearest neighbors satisfies $t = t^*/2\sqrt{d}$ in the infinite-dimensional limit [2]. The next step is to take each differential operator in the square brackets in Eq. (4) and operate each on $G^R_{\mathbf{k}}(t,t')$ using the relevant Dyson equation. The equation that involves a derivative with respect to t uses the Dyson equation in Eq. (3), while the one with respect to t' uses the "conjugate" equation. We then take the sum and the difference of the two equations, and transform from the time variables t and t' to the Wigner coordinates [12] that involve the average and relative times: $T = (t+t')/2$ and $t_{\rm rel} = t - t'$. The Green's functions are now expressed in terms of the Wigner coordinates, for example, $G^R_{\mathbf{k}}(T, t_{\rm rel})$. Finally, we make the assumption that the retarded self-energy is a function of the relative time only (which will be argued to be true *a posteriori* for the Falicov-Kimball model [13] below). The two differential equations become

$$\begin{aligned} &\left[i\partial_{t_{\rm rel}} + \mu - \frac{1}{2}\epsilon_{\mathbf{k}+e\mathbf{E}(T+t_{\rm rel}/2)} - \frac{1}{2}\epsilon_{\mathbf{k}+e\mathbf{E}(T-t_{\rm rel}/2)} \right] G^R_{\mathbf{k}}(T, t_{\rm rel}) = \delta(t_{\rm rel}) \\ &+ \frac{1}{2}\int d\bar{t} \left[\Sigma^R(T + \frac{t_{\rm rel}}{2} - \bar{t}) G^R_{\mathbf{k}}(\frac{T}{2} - \frac{t_{\rm rel}}{4} + \frac{\bar{t}}{2}, \bar{t} - T + \frac{t_{\rm rel}}{2}) \right. \\ &\left. + G^R_{\mathbf{k}}(\frac{T}{2} + \frac{t_{\rm rel}}{4} + \frac{\bar{t}}{2}, T + \frac{t_{\rm rel}}{2} - \bar{t}) \Sigma^R(\bar{t} - T + \frac{t_{\rm rel}}{2}) \right], \\ &\left[i\partial_T - \epsilon_{\mathbf{k}+e\mathbf{E}(T+t_{\rm rel}/2)} + \epsilon_{\mathbf{k}+e\mathbf{E}(T-t_{\rm rel}/2)} \right] G^R_{\mathbf{k}}(T, t_{\rm rel}) = \\ &\int d\bar{t} \left[\Sigma^R(T + \frac{t_{\rm rel}}{2} - \bar{t}) G^R_{\mathbf{k}}(\frac{T}{2} - \frac{t_{\rm rel}}{4} + \frac{\bar{t}}{2}, \bar{t} - T + \frac{t_{\rm rel}}{2}) \right. \end{aligned}$$

$$-G^R_{\mathbf{k}}(\frac{T}{2}+\frac{t_{\rm rel}}{4}+\frac{\bar{t}}{2},T+\frac{t_{\rm rel}}{2}-\bar{t})\Sigma^R(\bar{t}-T+\frac{t_{\rm rel}}{2})\Big], \tag{5}$$

where we have assumed a constant uniform electric field, so $\mathbf{A}(t) = -\mathbf{E}t$; the electric field points along the diagonal $(1, 1, 1, ...)$ of the infinite-dimensional hypercube. We need to perform some simple manipulations to get these equations into their final differential form. First we shift $\bar{t} \to \bar{t} + T - t_{\rm rel}/2$ in each integral, and then we let $\bar{t} \to t_{\rm rel} - \bar{t}$ in the first integral of both equations. Finally, we use the fact that any infinitely differentiable function of time $F(T)$ satisfies the Taylor series operator identity $\exp[\bar{t}\partial_T]F(T) = F(T + \bar{t})$ to produce the final time-dependent equations in the Hamiltonian gauge:

$$\begin{aligned}
&\Big[i\partial_{t_{\rm rel}} + \mu - \frac{1}{2}\epsilon_{\mathbf{k}+e\mathbf{E}(T+t_{\rm rel}/2)} - \frac{1}{2}\epsilon_{\mathbf{k}+e\mathbf{E}(T-t_{\rm rel}/2)}\Big]\, G^R_{\mathbf{k}}(T, t_{\rm rel}) = \\
&\delta(t_{\rm rel}) + \int d\bar{t}\Sigma^R(\bar{t}) \cosh\left(\frac{\bar{t}}{2}\partial_T\right) G^R_{\mathbf{k}}(T, t_{\rm rel} - \bar{t}), \\
&\Big[i\partial_T - \epsilon_{\mathbf{k}+e\mathbf{E}(T+t_{\rm rel}/2)} + \epsilon_{\mathbf{k}+e\mathbf{E}(T-t_{\rm rel}/2)}\Big]\, G^R_{\mathbf{k}}(T, t_{\rm rel}) = \\
&-2\int d\bar{t}\Sigma^R(\bar{t}) \sinh\left(\frac{\bar{t}}{2}\partial_T\right) G^R_{\mathbf{k}}(T, t_{\rm rel} - \bar{t}).
\end{aligned} \tag{6}$$

The result in Eq. (6), is an exact equation of motion satisfied by the steady-state Green's function. It is complicated because it has many orders of the differential operators due to the cosh and sinh terms. It is also not yet in the form that we can take the linear limit needed for the quantum Boltzmann equation. The next step is to introduce a Fourier transform with respect to the $t_{\rm rel}$ coordinate:

$$\Sigma^R(t_{\rm rel}) = \frac{1}{2\pi}\int d\omega e^{-i\omega t_{\rm rel}}\Sigma^R(\omega),\ G^R_{\mathbf{k}}(T, t_{\rm rel}) = \frac{1}{2\pi}\int d\omega e^{-i\omega t_{\rm rel}} G^R_{\mathbf{k}}(T, \omega). \tag{7}$$

When this is substituted in, we replace $\bar{t}$ terms by $i\partial_\omega$ (this is accomplished by acting the differential operator on the $\exp[-i\omega t_{\rm rel}]$ term in the Fourier transform and then integrating by parts to move the differential operator from the exponential factor onto the self-energy factor), and we note that $\cosh(i\alpha) = \cos(\alpha)$ and $\sinh(i\alpha) = i\sin(\alpha)$. Finally, we make the equations gauge invariant. For our choice of field, this process is straightforward, and we simply make the coordinate change $\mathbf{k} \to \bar{\mathbf{k}} - e\mathbf{E}T$ [14]. This requires us to modify the derivative with respect to T via $\partial_T \to \partial_T + e\mathbf{E}\cdot\nabla_{\bar{\mathbf{k}}}$ [5]. Note that the gauge transformation operation is simply an average-time-dependent shift of the momentum, so the (local) self-energy is unchanged. Furthermore, the gauge-invariant Green's function $\tilde{G}^R_{\mathbf{k}}(T, \omega) = G^R_{\mathbf{k}-e\mathbf{E}T}(T, \omega)$ turns out to be independent of T; we use the tilde symbol to denote gauge-invariant Green's functions. This last step follows from the fact that the self-energy has no T dependence, and the (steady-state) noninteracting gauge-invariant Green's function (for the simple cosine band), expressed as [15, 16]

$$\tilde{G}^{R0}_{\mathbf{k}}(\omega) = \sum_n \frac{J_n\left(\frac{2\epsilon_{\mathbf{k}}}{eE}\right)}{\omega + \mu - \frac{n}{2}\omega_{\rm Bloch} + i\delta}, \tag{8}$$

has no T dependence either. In Eq. (8), $J_n(z)$ is the Bessel function of the first kind with integer order n, E is the magnitude of each component of the electric field along the hypercube diagonal, and $\omega_{\rm Bloch} = eE$ is the Bloch oscillation frequency; note that this choice for the electric field produces the natural Bloch frequency, even though the norm of the field grows like $\sqrt{d}$. Since both $\tilde{G}^{R0}$ and Σ^R are independent of T, it is a simple exercise to show that the gauge-invariant version of Eq. (3), found by making the gauge transformation explicitly on the equation, leads

to a gauge-invariant retarded Green's function $\tilde{G}^R$ that is also independent of T. The final EOM becomes

$$\begin{aligned}
&(\omega+\mu)\tilde{G}^R_{\mathbf{k}}(\omega) - \frac{\epsilon_{\mathbf{k}}}{2}\tilde{G}^R_{\mathbf{k}}(\omega+\frac{\omega_{\rm Bloch}}{2}) - \frac{\epsilon_{\mathbf{k}}}{2}\tilde{G}^R_{\mathbf{k}}(\omega-\frac{\omega_{\rm Bloch}}{2}) \\
&= 1 + \cos(\frac{1}{2}\partial_{\omega'} e\mathbf{E}\cdot\nabla_{\mathbf{k}})\Sigma^R(\omega')\tilde{G}^R_{\mathbf{k}}(\omega)\Big|_{\omega'=\omega}, \\
&e\mathbf{E}\cdot\nabla_{\mathbf{k}}\tilde{G}^R_{\mathbf{k}}(\omega) - \bar{\epsilon}_{\mathbf{k}}\tilde{G}^R_{\mathbf{k}}(\omega+\frac{\omega_{\rm Bloch}}{2}) + \bar{\epsilon}_{\mathbf{k}}\tilde{G}^R_{\mathbf{k}}(\omega-\frac{\omega_{\rm Bloch}}{2}) \\
&= 2\sin(\frac{1}{2}\partial_{\omega'} e\mathbf{E}\cdot\nabla_{\mathbf{k}})\Sigma^R(\omega')\tilde{G}^R_{\mathbf{k}}(\omega)\Big|_{\omega'=\omega},
\end{aligned} \tag{9}$$

with $\bar{\epsilon}_{\mathbf{k}} = -t^* \lim_{d\to\infty}\sum_{i=1}^{d}\sin(\mathbf{k}_i)/\sqrt{d}$.

The equations in Eq. (9) are exact for dynamical mean-field theory. One can easily verify that the gauge-invariant noninteracting Green's function in Eq. (8) satisfies the first equation of motion after using the identity $\alpha J_{n+1}(\alpha) + \alpha J_{n-1}(\alpha) = 2nJ_n(\alpha)$. Furthermore, if the field vanishes, so $E = 0$, one can see that the first equation is satisfied by $\tilde{G}^R_{\mathbf{k}} = 1/[\omega+\mu-\Sigma^R(\omega)-\epsilon_{\mathbf{k}}]$. The second equation also holds trivially in equilibrium, because $E = 0$. We linearize Eq. (9) in order to find the first nontrivial parts which are needed for the quantum Boltzmann equation. The first equation is the same as in equilibrium ($E = 0$), with the same solution [5], that is, the retarded Green's function is unchanged by the presence of the field to first order in E. The linearized form of the second equation is

$$e\mathbf{E}\cdot\left[\left(1-\frac{\partial\Sigma^R(\omega)}{\partial\omega}\right)\nabla_{\mathbf{k}} + \mathbf{v}_{\mathbf{k}}\frac{\partial}{\partial\omega}\right]\tilde{G}^R_{\mathbf{k}}(\omega) = 0, \tag{10}$$

with $\mathbf{v}_{\mathbf{k}} = \nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}$ the velocity operator. It is a simple exercise to show that the equilibrium form of the Green's function also satisfies this equation [just note that $G^{Req}_{\mathbf{k}}(\omega)$ depends on $\mathbf{k}$ only through $\epsilon_{\mathbf{k}}$, so that $\nabla_{\mathbf{k}}G^{Req}_{\mathbf{k}}(\omega) = \mathbf{v}_{\mathbf{k}}\times\partial G^{Req}_{\mathbf{k}}(\omega)/\partial\epsilon_{\mathbf{k}}$].

The final issue that needs to be resolved is that the retarded self-energy has no average time dependence. This is straightforward to show for the Falicov-Kimball model [13], but requires too many steps to include the full derivation here. The basic idea is that the dynamical mean field for the impurity (which we map onto in the infinite-dimensional limit) is average time independent if the retarded Green's function and initial self-energy are both average time independent. Extracting the new self-energy from the impurity problem in the dynamical mean field does not introduce any average time dependence because all equations and fields are time-translation invariant for the steady-state, so the new self-energy is also average time independent. Since we can start the algorithm with $\Sigma^R = 0$, which has no average time dependence, the iterative algorithm to solve for the retarded self-energy and Green's function never generates any average time-dependence, so those functions will depend only on ω. It is not clear at this point whether this holds for other models, because it is possible that the procedure to determine the retarded self-energy from the impurity problem in the dynamical mean field may introduce some average time dependence into the functions. Such a complication is straightforward to handle, but for simplicity, we have not considered it here.

3. Keldysh Green's function

The derivation for the Keldysh Green's function is similar, but it is complicated by the fact that the gauge-invariant Keldysh Green's function may still have average time dependence in the steady state. This possibility is related to the phenomenon of Bloch oscillations [17], where the steady state in the absence of scattering is an alternating current, oscillating at the Bloch frequency, which clearly is a state that has residual time dependence even in the steady state.

This result arises because we are on a lattice and have restricted ourselves to a single band. In the continuum, the Keldysh Green's function is independent of the average time in the steady state. On the lattice, if we consider multiple bands, then if there is tunneling between bands, mediated by the field, then the Bloch oscillations may also be quenched and the system may evolve into an average time independent system.

Since we have translational invariance, the spatial part of our problem diagonalizes when we work in momentum space, which we do here. We begin with the Dyson equation for the Keldysh Green's function, which follows from taking the Keldysh component of the full Dyson equation in Eq. (3). We can do the same with the "conjugate" equation as well. Finally, we can eliminate the Keldysh Green's function on the right-hand side by careful manipulation of the retarded or advanced Green's function Dyson equations. Hence, there are three forms for the Dyson equation of the Keldysh Green's function. We write each down schematically, with the notation that two time-dependent objects adjacent to one another imply a time integration over the real axis (not the Keldysh-Kadanoff-Baym contour):

$$\begin{aligned} G^K_{\mathbf{k}} &= G^{K0}_{\mathbf{k}} + G^{R0}_{\mathbf{k}}\Sigma^R G^K_{\mathbf{k}} + G^{R0}_{\mathbf{k}}\Sigma^K G^A_{\mathbf{k}} + G^{K0}_{\mathbf{k}}\Sigma^A G^A_{\mathbf{k}}, \\ &= G^{K0}_{\mathbf{k}} + G^{R}_{\mathbf{k}}\Sigma^R G^{K0}_{\mathbf{k}} + G^{R}_{\mathbf{k}}\Sigma^K G^{A0}_{\mathbf{k}} + G^{K}_{\mathbf{k}}\Sigma^A G^{A0}_{\mathbf{k}}, \\ &= (1 + G^R_{\mathbf{k}}\Sigma^R) G^{K0}_{\mathbf{k}} (1 + \Sigma^A G^A_{\mathbf{k}}) + G^R_{\mathbf{k}}\Sigma^K G^A_{\mathbf{k}}. \end{aligned} \tag{11}$$

The noninteracting Keldysh Green's function satisfies a simple differential equation, because it has no discontinuity when $t = t'$ like the advanced and retarded Green's functions. The equations of motion are

$$\left[i\partial_t + \mu - \epsilon_{\mathbf{k}+e\mathbf{E}t}\right] G^{K0}_{\mathbf{k}}(t,t') = 0, \quad \left[-i\partial_{t'} + \mu - \epsilon_{\mathbf{k}+e\mathbf{E}t'}\right] G^{K0}_{\mathbf{k}}(t,t') = 0. \tag{12}$$

Now the derivation proceeds exactly like it did for the retarded Green's function. We operate each of the differential operators in brackets onto the Keldysh Green's function, and use the relevant Dyson equations, and the EOM of the noninteracting retarded, advanced, and Keldysh Green's functions to simplify the equations (the advanced Green's function is equal to the complex conjugate of the retarded Green's function with the time coordinates interchanged). Then we go to Wigner coordinates and change variables in the integrals. The only difference from the derivation for the retarded case is that the Keldysh self-energy generically depends on the average time. After some long algebra, we arrive at

$$\begin{aligned} &\left[i\partial_{t_{\rm rel}} + \mu - \frac{1}{2}\epsilon_{\mathbf{k}+e\mathbf{E}(T+t_{\rm rel}/2)} - \frac{1}{2}\epsilon_{\mathbf{k}+e\mathbf{E}(T-t_{\rm rel}/2)}\right] G^K_{\mathbf{k}}(T,t_{\rm rel}) = \frac{1}{2}\int d\bar{t} \\ &\Big\{ e^{-\frac{\bar{t}}{2}\partial_T} G^K_{\mathbf{k}}(T, t_{\rm rel}-\bar{t})\Sigma^R(\bar{t}) + \left[e^{-\frac{\bar{t}}{2}\partial_T} G^A_{\mathbf{k}}(T,t_{\rm rel}-\bar{t})\right]\left[e^{\frac{t_{\rm rel}-\bar{t}}{2}\partial_T}\Sigma^K(T,\bar{t})\right] \\ &+ \left[e^{\frac{\bar{t}}{2}\partial_T} G^R_{\mathbf{k}}(T,t_{\rm rel}-\bar{t})\right]\left[e^{-\frac{t_{\rm rel}-\bar{t}}{2}\partial_T}\Sigma^K(T,\bar{t})\right] + e^{\frac{\bar{t}}{2}\partial_T} G^K_{\mathbf{k}}(T,t_{\rm rel}-\bar{t})\Sigma^A(\bar{t})\Big\}, \\ &\left[i\partial_T - \epsilon_{\mathbf{k}+e\mathbf{E}(T+t_{\rm rel}/2)} + \epsilon_{\mathbf{k}+e\mathbf{E}(T-t_{\rm rel}/2)}\right] G^K_{\mathbf{k}}(T,t_{\rm rel}) = \int d\bar{t} \\ &\Big\{ e^{-\frac{\bar{t}}{2}\partial_T} G^K_{\mathbf{k}}(T, t_{\rm rel}-\bar{t})\Sigma^R(\bar{t}) + \left[e^{-\frac{\bar{t}}{2}\partial_T} G^A_{\mathbf{k}}(T,t_{\rm rel}-\bar{t})\right]\left[e^{\frac{t_{\rm rel}-\bar{t}}{2}\partial_T}\Sigma^K(T,\bar{t})\right] \\ &- \left[e^{\frac{\bar{t}}{2}\partial_T} G^R_{\mathbf{k}}(T,t_{\rm rel}-\bar{t})\right]\left[e^{-\frac{t_{\rm rel}-\bar{t}}{2}\partial_T}\Sigma^K(T,\bar{t})\right] - e^{\frac{\bar{t}}{2}\partial_T} G^K_{\mathbf{k}}(T,t_{\rm rel}-\bar{t})\Sigma^A(\bar{t})\Big\}, \end{aligned} \tag{13}$$

which are exact equations satisfied by the Keldysh Green's function.

Next, we introduce the Fourier transform of the functions of $\bar{t}$ and $t_{\rm rel} - \bar{t}$, and replace any remaining factors by derivatives with respect to the corresponding frequencies, and then

integrating by parts as necessary to move the derivatives off of the exponential terms and onto the Green's functions or self-energies. Finally, we perform the gauge-invariance transformation by shifting the momentum vector with respect to the average time. We use the tilde to denote gauge-invariant Green's functions; the self-energies are unaffected by the transformation. The final exact equations of motion for the Keldysh Green's function are

$$\begin{aligned}
&(\omega+\mu)\tilde{G}^K_{\mathbf{k}}(T,\omega)-\frac{1}{2}\epsilon_{\mathbf{k}}\tilde{G}^K_{\mathbf{k}}(T,\omega+\frac{1}{2}\omega_{\rm Bloch})-\frac{1}{2}\epsilon_{\mathbf{k}}\tilde{G}^K_{\mathbf{k}}(T,\omega-\frac{1}{2}\omega_{\rm Bloch})=\\
&\frac{1}{2}\Big[e^{\frac{i}{2}\partial_{\omega'}(\partial_T+e\mathbf{E}\cdot\nabla_{\mathbf{k}})}\tilde{G}^K_{\mathbf{k}}(T,\omega)\Sigma^R(\omega')+e^{\frac{i}{2}(\partial_{\omega'}e\mathbf{E}\cdot\nabla_{\mathbf{k}}-\partial_\omega\partial_T)}\tilde{G}^A_{\mathbf{k}}(\omega)\Sigma^K(T,\omega')\\
&+e^{-\frac{i}{2}(\partial_{\omega'}e\mathbf{E}\cdot\nabla_{\mathbf{k}}-\partial_\omega\partial_T)}\tilde{G}^R_{\mathbf{k}}(\omega)\Sigma^K(T,\omega')+e^{-\frac{i}{2}\partial_{\omega'}(\partial_T+e\mathbf{E}\cdot\nabla_{\mathbf{k}})}\tilde{G}^K_{\mathbf{k}}(T,\omega)\Sigma^A(\omega')\Big],\\
&i\partial_T\tilde{G}^K_{\mathbf{k}}(T,\omega)+ie\mathbf{E}\cdot\nabla_{\mathbf{k}}\tilde{G}^K_{\mathbf{k}}(T,\omega)\\
&-i\bar{\epsilon}_{\mathbf{k}}\tilde{G}^K_{\mathbf{k}}(T,\omega+\frac{1}{2}\omega_{\rm Bloch})+i\bar{\epsilon}_{\mathbf{k}}\tilde{G}^K_{\mathbf{k}}(T,\omega-\frac{1}{2}\omega_{\rm Bloch})=\\
&e^{\frac{i}{2}\partial_{\omega'}(\partial_T+e\mathbf{E}\cdot\nabla_{\mathbf{k}})}\tilde{G}^K_{\mathbf{k}}(T,\omega)\Sigma^R(\omega')+e^{\frac{i}{2}(\partial_{\omega'}e\mathbf{E}\cdot\nabla_{\mathbf{k}}-\partial_\omega\partial_T)}\tilde{G}^A_{\mathbf{k}}(\omega)\Sigma^K(T,\omega')\\
&-e^{-\frac{i}{2}(\partial_{\omega'}e\mathbf{E}\cdot\nabla_{\mathbf{k}}-\partial_\omega\partial_T)}\tilde{G}^R_{\mathbf{k}}(\omega)\Sigma^K(T,\omega')-e^{-\frac{i}{2}\partial_{\omega'}(\partial_T+e\mathbf{E}\cdot\nabla_{\mathbf{k}})}\tilde{G}^K_{\mathbf{k}}(T,\omega)\Sigma^A(\omega'),
\end{aligned}\tag{14}$$

where, in both cases, we must take the limit $\omega'\to\omega$. In Eq. (14), we used the facts that the gauge-invariant retarded and advanced Green's functions and the local retarded and advanced self-energies are all independent of the average time T.

Note that in equilibrium, with $E=0$, the equilibrium forms for the Keldysh Green's function and self-energy

$$G^{Keq}_{\mathbf{k}}(\omega)=-2i[2f(\omega)-1]{\rm Im}G^R_{\mathbf{k}}(\omega),\ \Sigma^{Keq}(\omega)=-2i[2f(\omega)-1]{\rm Im}\Sigma^R(\omega),\tag{15}$$

do satisfy Eq. (14). Since the EOM for the Keldysh Green's function is a homogeneous equation, the distribution-function factor $[2f(\omega)-1]$ comes from the initial conditions (or equivalently from the bare Keldysh Green's function) and can be viewed as a boundary condition for the differential equations.

The easiest way to see that the Keldysh Green's function and self-energy may generically have average time dependence, is to start with the gauge-invariant noninteracting Keldysh Green's function in a field (for the simple cosine band):

$$\tilde{G}^{K0}_{\mathbf{k}}(T,\omega)=2\pi i[2f(\epsilon_{\mathbf{k}-e\mathbf{E}T}-\mu)-1]\sum_n J_n\left(\frac{2\epsilon_{\mathbf{k}}}{eE}\right)\delta\left(\omega+\mu-\frac{1}{2}eEn\right).\tag{16}$$

The gauge-invariance transformation, which shifts the momentum wavevector, makes the Bessel-function and delta-function pieces independent of T, but the Fermi-factor piece $[f(\epsilon)=1/\{\exp(\beta\epsilon)+1\}]$ now picks up average time dependence. [One might be surprised by the fact that the noninteracting Keldysh Green's function has the Fermi-Dirac distribution that depends on $\epsilon_{\mathbf{k}}$ in it, since the equilibrium Green's function described above had the factor $f(\omega)$ in it—this occurs because when the field vanishes, either form is correct since the noninteracting Keldysh Green's function has a $\delta(\omega+\mu-\epsilon_{\mathbf{k}})$ term in it, but when a field is present, the noninteracting Keldysh Green's function has an infinite number of δ functions coming from the Wannier-Stark ladder, and the initial equilibrium condition explicitly requires the Fermi-Dirac distribution as a function of $\epsilon_{\mathbf{k}}-\mu$ not ω.] This T-dependence is simple though: the band structure is a periodic function of momentum, which implies that the average time dependence must also be periodic in T; so the idea of a steady state that periodically repeats is possible [indeed, one only gets the

correct Bloch oscillations for the noninteracting system if the form in Eq. (16) is used]. We need to show that both the Keldysh self-energy and the gauge-invariant Keldysh Green's functions are also periodic with the same period. If so, then the T-dependence can be treated in a Fourier series. It is straightforward to show from the full Dyson equation, that if the noninteracting Keldysh Green's function is periodic in T, and the Keldysh self-energy is also periodic in T, then the full Keldysh Green's function is periodic in T. Examining the impurity algorithm, shows that the Keldysh dynamical mean field is periodic in T. If the resulting impurity Green's function and self-energy are also periodic in time, then the impurity solver maintains the periodicity. This clearly holds for the Falicov-Kimball model [13], and likely holds for many other models as well. Note that this analysis says the most general steady state must be periodic with the Bloch period. Such functions also include the constant function, since a constant is periodic with the Bloch period.

Since the average time dependence is periodic, with a period $2\pi/\omega_{\rm Bloch}$, we can expand the Keldysh Green's function and self-energy in a Fourier series as

$$\begin{aligned}\tilde{G}^K_{\mathbf{k}}(T,\omega) &= \sum_n e^{-in\omega_{\rm Bloch}T}\tilde{G}^K_{\mathbf{k}}(n,\omega),\\ \Sigma^K(T,\omega) &= \sum_n e^{-in\omega_{\rm Bloch}T}\Sigma^K(n,\omega).\end{aligned} \tag{17}$$

Substituting these expansions into Eq. (14) produces essentially the same equations except the Keldysh functions depend on the Fourier index n and frequency ω, and the derivatives with respect to T are replaced by $\partial_T \to -in\omega_{\rm Bloch}$. Finally, we take this equation and linearize it to obtain the final two expressions for the quantum Boltzman equation in dynamical mean field theory:

$$\begin{aligned}&(\omega+\mu-\epsilon_{\mathbf{k}})\tilde{G}^K_{\mathbf{k}}(n,\omega) = \tilde{G}^K_{\mathbf{k}}(n,\omega){\rm Re}\Sigma^R(\omega) + {\rm Re}\tilde{G}^R_{\mathbf{k}}(\omega)\Sigma^K(n,\omega)\\
&+\frac{i}{2}n\omega_{\rm Bloch}\tilde{G}^K_{\mathbf{k}}(n,\omega)\partial_\omega{\rm Im}\Sigma^R(\omega) - \frac{1}{2}e\mathbf{E}\cdot\nabla_{\mathbf{k}}\tilde{G}^K_{\mathbf{k}}(n,\omega)\partial_\omega{\rm Im}\Sigma^R(\omega)\\
&+\frac{i}{2}n\omega_{\rm Bloch}\partial_\omega{\rm Im}\tilde{G}^R_{\mathbf{k}}(\omega)\Sigma^K(n,\omega) + \frac{1}{2}e\mathbf{E}\cdot\nabla_{\mathbf{k}}{\rm Im}\tilde{G}^R_{\mathbf{k}}(\omega)\partial_\omega\Sigma^K(n,\omega),\\
&n\omega_{\rm Bloch}\tilde{G}^K_{\mathbf{k}}(n,\omega) + ie\mathbf{E}\cdot\nabla_{\mathbf{k}}\tilde{G}^K_{\mathbf{k}}(n,\omega) - i\bar{\epsilon}_{\mathbf{k}}\omega_{\rm Bloch}\partial_\omega\tilde{G}^K_{\mathbf{k}}(n,\omega) =\\
&2i\tilde{G}^K_{\mathbf{k}}(n,\omega){\rm Im}\Sigma^R(\omega) - 2i{\rm Im}\tilde{G}^R_{\mathbf{k}}(\omega)\Sigma^K(n,\omega)\\
&+n\omega_{\rm Bloch}\tilde{G}^K_{\mathbf{k}}(n,\omega)\partial_\omega{\rm Re}\Sigma^R(\omega) + ie\mathbf{E}\cdot\nabla_{\mathbf{k}}\tilde{G}^K_{\mathbf{k}}(n,\omega)\partial_\omega{\rm Re}\Sigma^R(\omega)\\
&-n\omega_{\rm Bloch}\partial_\omega{\rm Re}\tilde{G}^R_{\mathbf{k}}(\omega)\Sigma^K(n,\omega) + ie\mathbf{E}\cdot\nabla_{\mathbf{k}}{\rm Re}\tilde{G}^R_{\mathbf{k}}(\omega)\partial_\omega\Sigma^K(n,\omega).\end{aligned} \tag{18}$$

These equations are obviously quite complex; the second equation is the one most closely related to the Blotzmann equation, and is the most important one for determining transport.

As a first check, however, we evaluate these equations in equilibrium, with $E=0$; in this case there is no average time dependence, so we are only interested in the $n=0$ equations. Taking the second equation, solving for G^K, and substituting into the first equation for the G^K term that appears on the right hand side, produces the relationship

$$(\omega+\mu-\epsilon_{\mathbf{k}})G^K_{\mathbf{k}}(\omega) = (\omega+\mu-\epsilon_{\mathbf{k}})\frac{\Sigma^K(\omega)}{[\omega+\mu-{\rm Re}\Sigma^R(\omega)-\epsilon_{\mathbf{k}}]^2+[{\rm Im}\Sigma^R(\omega)]^2}, \tag{19}$$

where the factor in the parenthesis cancels on both sides. After the cancellation, we are left with an expression that is consistent with the relation between the Keldysh self-energy and Green's function in equilibrium, but it does not explicitly produce the Fermi-Dirac distribution terms, as discussed above. The quantum Boltzmann equation typically is employed to obtain a relation between the self-energies and the Keldysh Green's function; it is expected that the

self-energies will be determined by solving some kind of many-body theory that describes the system of interest (see the next section).

Because the retarded and advanced Green's functions are unchanged to linear order in the field, and because we are only interested in the terms that are zeroth or first order in E for the quantum Boltzmann equation, we can replace the full Green's functions and self-energies by their equilibrium values when they are multiplied by either E or $\omega_{\rm Bloch}$ [5]. This procedure produces a significant simplification of the results. For example, since the equilibrium Keldysh Green's function and self-energy are both independent of T, only the $n = 0$ component survives, so all $n\omega_{\rm Bloch}$ terms vanish.

We perform the substitution of the equilibrium terms into their respective places, and then undergo some signficant algebra to end up at the final expression for the quantum Boltzmann equations:

$$\begin{aligned}
&(\omega+\mu-\epsilon_{\mathbf{k}})\tilde{G}^K_{\mathbf{k}}(n,\omega) = \tilde{G}^K_{\mathbf{k}}(n,\omega){\rm Re}\Sigma^{Req}(\omega) + {\rm Re}G^{Req}_{\mathbf{k}}(\omega)\Sigma^K(n,\omega)\\
&-4ie\mathbf{E}\cdot\mathbf{v}_{\mathbf{k}}\partial_\omega f(\omega)[{\rm Im}G^{Req}_{\mathbf{k}}(\omega)]^2[\omega+\mu-{\rm Re}\Sigma^{Req}(\omega)-\epsilon_{\mathbf{k}}]\delta_{n0},\\
&\tilde{G}^K_{\mathbf{k}}(n,\omega) = \frac{\Sigma^K(n,\omega)}{[\omega+\mu-{\rm Re}\Sigma^{Req}(\omega)-\epsilon_{\mathbf{k}}]^2+[{\rm Im}\Sigma^{Req}(\omega)]^2}\\
&-4ie\mathbf{E}\cdot\mathbf{v}_{\mathbf{k}}[{\rm Im}G^{Req}_{\mathbf{k}}(\omega)]^2\partial_\omega f(\omega)\delta_{n0}.
\end{aligned} \tag{20}$$

Note that the $\tilde{G}^K_{\mathbf{k}}$ and Σ^K terms are not the equilibrium functions, but contain the equilibrium part plus the first-order shift in E; hence the first-order shift in the Keldysh Green's function arises from two sources—(i) the term coming from the electric-field dependence of the Keldysh self-energy and (ii) the explicit term given at the end of the second equation above (when $n = 0$).

The first equation is identical to the second multiplied by $[\omega+\mu-{\rm Re}\Sigma^{Req}(\omega)-\epsilon_{\mathbf{k}}]$, so there is only one independent quantum Boltzmann equation. We use the second equation in Eq. (20), because that is the equation most closely related to the Boltzmann equation (for a discussion of this issue, see [5]). Note further, that if the Keldysh self-energy has no average time dependence to first-order in E, then neither does the Keldysh Green's function.

4. Linear-response conductivity in dynamical mean field theory

The current operator is determined by the commutator of the polarization operator with the Hamiltonian, and can be expressed by

$$\mathbf{J} = e\sum_{\mathbf{k}}\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}c^\dagger_{\mathbf{k}}c_{\mathbf{k}}, \tag{21}$$

with $c^\dagger_{\mathbf{k}}$ ($c_{\mathbf{k}}$) the electron creation (annihilation) operators for electrons with momentum $\mathbf{k}$; this is the current per spin, since we are considering spinless electrons throughout this manuscript—adding spin increases the current by a trivial factor of 2. The term $\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}} = \mathbf{v}_{\mathbf{k}}$ is the electron velocity. We can calculate the expectation value of the current operator by employing the lesser Green's function $G^< = (G^K - G^R + G^A)/2$ as

$$\langle\mathbf{J}(T)\rangle = -\frac{i}{2}e\int\frac{d\omega}{2\pi}\sum_{\mathbf{k}}\mathbf{v}_{\mathbf{k}}G^<_{\mathbf{k}}(T,\omega). \tag{22}$$

Using the equilibrium forms for the retarded and advanced Green's functions (valid through first-order in E) and the quantum Boltzmann equation in Eq. (20) allows us to solve for the linear-response current

$$\langle\mathbf{J}(T)\rangle = e^2\sum_{\mathbf{k}}(\mathbf{E}\cdot\mathbf{v}_{\mathbf{k}})\mathbf{v}_{\mathbf{k}}\int\frac{d\omega}{2\pi}[-\partial_\omega f(\omega)][{\rm Im}G^{Req}_{\mathbf{k}}(\omega)]^2, \tag{23}$$

and then the conductivity $\sum_\beta \sigma_{\alpha\beta}\mathbf{E}_\beta = \mathbf{J}_\alpha$ becomes

$$\sigma_{\alpha\beta} = \delta_{\alpha\beta}e^2 \sum_{\mathbf{k}} \mathbf{v}_{\mathbf{k}\alpha}^2 \int \frac{d\omega}{2\pi}[-\partial_\omega f(\omega)][\mathrm{Im}G_{\mathbf{k}}^{Req}(\omega)]^2, \tag{24}$$

which is the dynamical mean field theory *dc* conductivity [18]. Note that in our derivation, we used the fact that the Keldysh self-energy is local and has no momentum dependence, so it vanishes when multiplied by the velocity and integrated over momentum, and only the term explicitly proportional to **E** in Eq. (20) survives the summation over momentum. We did not need to assume that there was no average time dependence to the Keldysh Green's function, but if there is average time dependence, it arises from the Keldysh self-energy and cannot have any momentum dependence. This derivation is much simpler than that given in Mahan's review article [5] because the vertex corrections vanish in infinite dimensions [19], so there is no Bethe-Salpeter equation to solve for the current; it simply follows directly from the quantum Boltzmann equation. Note that the full proof of the equivalence between the Kubo formula and the quantum Boltzmann equation was originally proved by Chen and Su [20], who found an additional term neglected by Mahan, that is required for establishing the equivalence.

5. Recovering the Drude-Sommerfeld model for transport

The well-known expression for the Drude conductivity is:

$$\sigma_{dc} = \frac{J}{E} = \frac{ne^2\tau}{m}, \tag{25}$$

where n is the electron density, m is the effective electron mass, and τ is the (constant) relaxation time, introduced phenomenologically by Drude.

Here we concentrate on the conductivity of a strongly correlated system at finite temperature; all scattering is due to the electron-electron interaction. Determining the *dc* conductivity in this case is nontrivial (see, for example [21]). We analyze the behavior of the *dc* conductivity in the Falicov-Kimball model for spinless electrons on the infinite-dimensional hypercubic lattice. The Hamiltonian can be written in the following form [13]:

$$\mathcal{H} = -\frac{t^*}{2\sqrt{d}} \sum_{\langle ij \rangle} c_i^\dagger c_j + U \sum_i w_i c_i^\dagger c_i, \tag{26}$$

where $c_i^\dagger$ and c_i are creation and annihilation operators for an itinerant electron at site i; $t^* = 1$ is the scaled nearest-neighbor hopping [2] that we use for our energy unit; w_i is the localized electron number operator (equal to 0 or 1); and U is the local Coulomb repulsion between localized and itinerant electrons. All electrons are spinless in this example. We also assume that the system is at half-filling, *i.e.*, the particle density for the localized and itinerant electrons is equal to 1/2.

In the limit of vanishing electron-electron interaction on the hypercubic lattice, an arbitrary constant electric field directed along the lattice diagonal $(1, 1, 1, ...)$, produces the current $J(T)$ that can be calculated analytically from Eq. (22). This current displays the expected Bloch oscillations [17]:

$$J(T) = \frac{e}{4\pi\sqrt{d}} \sin(\omega_{\mathrm{Bloch}}T) \int d\epsilon \frac{-\partial f(\epsilon)}{\partial \epsilon} \rho(\epsilon), \tag{27}$$

where $\rho(\epsilon) = \exp(-\epsilon^2)/\sqrt{\pi}$ is the free-particle density of states, and the frequency of the oscillations is exactly the Bloch frequency ω_{Bloch}. It is interesting to discover whether these oscillations survive in the presence of electron-electron scattering, as U is turned on. It is

difficult to observe this effect experimentally, since the period of oscillations for realistic fields is much larger than the typical scattering time, so the electron wavevector is randomized by scattering before it can undergo a Bloch oscillation. In the linear-response regime, the free-electron conductivity grows with the average time, since it is proportional to ET. The Bloch oscillations are absent because the period (proportional to $1/E$) diverges as $E \to 0$.

To calculate the expression for the *dc* conductivity from Eq. (24), one needs to find the equilibrium retarded Green's function for the interacting system. The case of the Falicov-Kimball model in the dynamical mean-field theory limit can be solved exactly [3, 22]. This involves solving the set of the equations for the local Green's function $G_{\rm loc}^{Req}(\omega)$, the local self-energy $\Sigma^{Req}(\omega)$, and the dynamical mean-field $\lambda^{Req}(\omega)$:

$$G_{\rm loc}^{Req}(\omega) = \int d\epsilon \rho(\epsilon) \frac{1}{\omega + \mu - \epsilon - \Sigma^{Req}(\omega)}, \tag{28}$$

$$\lambda^{Req}(\omega) = \omega + \mu - [G_{\rm loc}^{Req}(\omega)]^{-1} - \Sigma^{Req}(\omega), \tag{29}$$

$$G_{\rm loc}^{Req}(\omega) = \frac{1 - w_1}{\omega + \mu - \lambda^{Req}(\omega)} + \frac{w_1}{\omega + \mu - U - \lambda^{Req}(\omega)}, \tag{30}$$

where w_1 is the average particle number for the localized electrons. In the case of half-filling we have $w_1 = 0.5$ and $\mu = 0.5U$.

Once the retarded Green's function is found, the *dc* conductivity can be calculated from Eq. (24) by introducing a joint density of states

$$\rho_2(\epsilon, \bar{\epsilon}) = \frac{1}{\pi} \exp\left(-\epsilon^2 - \bar{\epsilon}^2\right). \tag{31}$$

for the two energy functions $\epsilon_{\mathbf{k}}$ and $\bar{\epsilon}_{\mathbf{k}}$ on the infinite-dimensional hypercubic lattice [23, 16] and integrating over ϵ and $\bar{\epsilon}$.

The integration over $\bar{\epsilon}$ in Eq. (24) is straightforward and it gives the following general expression for the conductivity [18]:

$$\sigma_{dc} = \sigma_0 \int d\omega [-\partial_\omega f(\omega)] \tau(\omega), \tag{32}$$

where $\sigma_0 = e^2\pi/2d$ and the relaxation time satisfies

$$\tau(\omega) = \int d\epsilon \rho(\epsilon) \frac{[{\rm Im}\Sigma^{Req}(\omega)]^2/2\pi^2}{\{[\omega + \mu - {\rm Re}\Sigma^{Req}(\omega) - \epsilon]^2 + [{\rm Im}\Sigma^{Req}(\omega)]^2\}^2}. \tag{33}$$

It is possible to analyze the expression for σ_{dc} analytically in the limit of low temperatures [24]. In this case the derivative $-\partial_\omega f(\omega)$ is a function with a sharp maximum around $\omega = 0$, and it is enough to approximate the relaxation time $\tau(\omega)$ by its low-frequency expansion. In the metallic case when $U < U_c = \sqrt{2}$ it is sufficient to use just the lowest-order expansion $\tau(\omega) = \tau(0)$, yielding

$$\sigma_{dc} = \sigma_0 \tau(0) \tag{34}$$

which is the Drude form. The relaxation time is determined by the zero-frequency imaginary part of the retarded self-energy ${\rm Im}\Sigma^{Req}(0)$, since the real part vanishes ${\rm Re}\Sigma^{Req}(\omega) = (1 - Z)\omega \to 0$ as $\omega \to 0$ (note that $Z < 0$ for the Falicov-Kimball model because it is not a fermi liquid). In this case, the zero-frequency relaxation time can be evaluated as:

$$\tau(0) \simeq \rho(\mu) \int d\epsilon \frac{[{\rm Im}\Sigma^{Req}(0)]^2/2\pi^2}{\{[\mu - \epsilon]^2 + [{\rm Im}\Sigma^{Req}(0)]^2\}^2} = \frac{\rho(\mu)}{4\pi} \frac{1}{{\rm Im}\Sigma^{Req}(0)}. \tag{35}$$

Therefore, the *dc* conductivity is inversely proportional to the imaginary part of the retarded self-energy in the metallic phase; this is the standard Drude picture.

The situation is more complicated in the insulating case with $U > \sqrt{2}$. The interacting density of states $\rho_{int}(\omega) = -(1/\pi)G^{Req}_{\rm loc}(\omega)$ develops a pseudogap at $\omega = 0$. The real part of the self-energy is large for small $|\omega|$, since ${\rm Re}\Sigma^{Req}(\omega)$ has a pole at $\omega = 0$. The imaginary part of the self-energy is small in this case except at $\omega = 0$ where it diverges. In order to analyze the dependence of the *dc* conductivity on the model parameters in this case, we expand the local Green's function in powers of $1/{\rm Re}\Sigma^{Req}(\omega)$ and ${\rm Im}\Sigma^{Req}(\omega)$ in Eq. (28). The solution of the system of equations (28)-(30) for the self-energy to lowest order is [24]:

$$ {\rm Re}\Sigma^{Req}(\omega) = \frac{U^2-2}{4\omega}, \tag{36} $$

$$ {\rm Im}\Sigma^{Req}(\omega) = -\pi\frac{[U^2-2]^3}{64\omega^4}\rho\left[\frac{U^2-2}{4\omega}\right] - \frac{1}{4}\pi[U^2-2]\delta(\omega). \tag{37} $$

The lowest-order approximation gives the following expression for the relaxation time [24]:

$$ \tau(\omega) = \frac{16\omega^4}{\pi^2[U^2-2]^3}. \tag{38} $$

Substituting this expression into Eq. (32) yields ($T = 1/\beta$ is the temperature here):

$$ \sigma_{dc} = \sigma_0\frac{T^4}{[U^2-2]^3}\frac{4}{\pi^2}\int_{-\infty}^{\infty}dx\frac{x^4}{\cosh^2(x)} = \sigma_0\frac{T^4}{[U^2-2]^3}\frac{7\pi^2}{30}. \tag{39} $$

The conductivity in the insulating phase goes to zero as T^4, not exponentially, as expected for a conventional insulator with a true gap. This arises from the fact that there are a small number of states at low energy, but they have an exceedingly long lifetime, so they can carry a significant amount of current.

6. Nonlinear response

We have derived a series of exact differential equations that are satisfied by the nonequilibrium Green's functions in the steady state when a uniform constant electric field is applied [Eqs. (9) and (13)]. These equations appear to be intractable for a direct solution, because they involve differential operators to infinite order, and one needs to solve them with alternative strategies. Instead, we examined the linear-response regime, and found that we obtain the exact *dc* conductivity for dynamical mean field theory that was derived independently from the Kubo formula [18]. One can ask, what happens when we go beyond the linear-response regime and examine nonlinear response? In the noninteracting case, the system will develop Bloch oscillations, so the presence of a *dc* field creates an *ac* current response. As the scattering is turned on, a classical Boltzmann equation analysis predicts that the oscillations will survive for a while, and then ultimately decay due to the scattering. Is it possible that in the steady state there are still oscillations, just with a reduced amplitude, or does the steady state always produce a constant current response? The answer to this question lies at the heart of whether or not the Keldysh Green's functions pick up average time dependence proportional to $\mathbf{v_k}$ (in a periodic fashion) for the steady state, or whether they have no average time dependence proportional to $\mathbf{v_k}$ (as in our linear-response example). There does not appear to be any simple way to resolve this question, but it seems possible to us that the Bloch oscillations can survive with a reduced amplitude, until the scattering gets to be too strong, and the system is forced into a constant, linear-response regime, due to the extremely short lifetimes. If this happens, it would be a

truly quantum effect, since it does not seem to occur in the semiclassical Boltzmann equation. We intend to work further on this problem by directly investigating the solution of the Green's functions and self-energies in the steady state using techniques other than those derived from the equations of motion that have infinite-order differential operators in them.

7. Conclusion

In this work we have generalized the quantum Boltzmann equation approach of Mahan [5] to the case of dynamical mean field theory in a single-band model. This approach provides us with many simplifications, such as the fact that the self-energy has no momentum dependence, hence all momentum derivatives vanish. But it is complicated by some additional nonlinear effects brought on by the presence of the periodic band structure, which ultimately relate to the question of whether or not the system has Bloch oscillations, and how they evolve as the scattering is made stronger. Since we examined a linear-response limit to derive and use the quantum Boltzmann equation, we are not able to directly answer such questions here, instead we will do so in future publications.

We were able to show that taking the linear limit of the nonequilibrium equations of motion, coupled with a simple theory for scattering by static charge defects, produced a quantum generalization of the semiclassical theory for transport with similar results to those of the Drude-Sommerfeld model. Along the way, we derived a series of exact differential equations that the nonequilibrium Green's functions satisfy, we showed how to incorporate periodic average time dependence into this framework if it exists in the system, and we established an exact equivalence between the quantum Boltzmann equation approach and the Kubo approach for the *dc* conductivity.

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