Solution of electric-field-driven tight-binding lattice coupled to fermion reservoirs

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We study electrons in tight-binding lattice driven by DC electric field with their energy dissipated through on-site fermionic thermostats. Due to the translational invariance in the transport direction, the problem can be block-diagonalized. We solve this time-dependent quadratic problem and demonstrate that the problem has well-defined steady-state. The steady-state occupation number shows that the Fermi surface shifts at small field by the drift velocity, in agreement with the Boltzmann transport theory, but it then deviates significantly at high fields due to strong nonlinear effect. Despite the lack of momentum scattering, the conductivity takes the same form as the semi-classical Ohmic expression from the relaxation-time approximation.

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I. INTRODUCTION

Nonequilibrium phenomena in lattice are the oldest and most fundamental problems in solid state physics. In conventional solids, acceleration due to external field is relatively small compared to electronic energy, and various scattering mechanisms make the transport diffusive enough so that the small field approximation has often been applicable. The quantum Boltzmann method has been applied effectively \cite{1} and linear response limit has been widely used in the solid-state literature. However, recent progress in nano-devices and optical lattice systems has made rigorous high-field formalism necessary to understand their non-perturbative effects such as the Bloch oscillation. In such regime, understanding the interplay of non-perturbative field-effect and the many-body physics has emerged as one of the most pressing problems in nano-science.

Combining the nonequilibrium and quantum many-body effects is an extremely challenging task. Much effort has been exerted towards understanding strong correlation physics in quantum dot physics, especially the prototypical nonequilibrium Kondo problem. Analytical theories \cite{2,3} and many numerical methods have been proposed along the time-dependent \cite{4}, and steady-state simulation \cite{5}. In such systems with localized interacting region, the important question of energy dissipation could have been side-stepped, and the existence of steady-state has not been a major issue.

In the past few years, non-perturbative inclusion of electric-field and many-body effects in lattice systems has been one of the central issues in the field. Theories for lattice nonequilibrium have been formulated \cite{6,7} mostly based on the dynamical mean-field theory (DMFT) for an s-orbital tight-binding (TB) lattice with on-site interaction \cite{8,9}. Various attempts have been made to include dissipation mechanism to the driven lattice by fermion bath \cite{10} and bosonic bath \cite{11}. This work corresponds to the analytic solution of the non-interacting limit of the models considered in Refs. \cite{10,11}. Although a long-held belief in solid-state transport has been that, under a finite electric-field, the Fermi sea is perturbatively shifted by drift velocity, many calculations performed under the DMFT framework have suggested that the system approaches a steady-state with infinitely hot electron gas even for small field. With inclusion of proper dissipation mechanism, one expects the Boltzmann picture of displaced Fermi surface at small fields and a recovery of the Bloch oscillation in the high-field limit.

However, it has been unclear so far what approximations, such as single-band approximation without Landau-Zener tunneling or the nature of on-site interaction, are responsible for the rather peculiar long-time states obtained from numerical theories. One of the goals of this paper is that we provide exact solutions to one of the simplest dissipation models with on-site fermion thermostats and give analytic understanding of the problem, and guide possible future modeling.

Due to the nature of the one-body reservoirs, the problem can be solved exactly (see Fig. 1). With identical reservoirs on each site, the Hamiltonian can be block-diagonalized according to the wave-vector of electrons in the transport direction. The block-diagonal Hamiltonian can then be exactly solved by a time-dependent perturbation theory \cite{12} using the nonequilibrium Green function theory. The calculation of the wave-vector dependent occupation number supports the semi-classical Boltzmann equation result \cite{13}. Based on these findings, we conclude that the fermion thermostat model, despite its crude modeling to realistic dissipation mechanism, can serve as a minimal setup for the studies of strong correlation effects in driven lattice models. Although the model considered here is one-dimensional, the result can be readily extended to any spatial dimensions since the model is one-body and conserves momentum.

II. MODEL

We study a quadratic model of a one-dimensional s-orbital tight-binding model connected to fermionic reser-
voirs (see Fig. 1) under a uniform electric field $E$. The effect of the electric field is absorbed in the temporal gauge as the Peierls phase $\varphi(t) = (eEa)t$ to the hopping integral $\gamma$. The time-dependent Hamiltonian then reads

$$\hat{H}(t) = -\gamma \sum_i (c_i^\dagger d_{i+1} + H.c.) + \sum_{i\alpha} \epsilon_{i\alpha} c_{i\alpha}^\dagger c_{i\alpha} - g \sum_{i\alpha} (c_{i\alpha}^\dagger d_i + H.c.),$$

with $d_i^\dagger$ as the (spinless) electron operator on the tight-binding chain on site $i$, $c_{i\alpha}^\dagger$ with the reservoir fermion states connected to the site $i$ with the continuum index $\alpha$ along each reservoir chain. Here we do not specify the explicit connectivity of the reservoir chains, but each chains are assumed to have an identical dispersion relation $\epsilon_{i\alpha}$. Notice that the electric field is applied only along the reservoir chain direction.

The Peierls phase $\varphi(t)$ is given as

$$\varphi(t) = \begin{cases} 0, & \text{for } t < 0 \\ \Omega t, & \text{for } t > 0 \end{cases}$$

$\Omega = eEa$ is the Bloch-oscillation frequency due to the electric field.

We note that the whole system has discrete translational symmetry in the transport direction and the Hamiltonian is readily block-diagonalized with respect to the wave-vector $k$ as $d_{k}^\dagger = \sqrt{N_d^{-1}} \sum_j e^{ikR_j} d_j^\dagger$ and $c_{k\alpha}^\dagger = \sqrt{N_d^{-1}} \sum_j e^{ikR_j} c_{j\alpha}^\dagger$ (with lattice sites $R_j = aj$ and the number of sites along the TB chain $N_d$),

$$\hat{H}(t) = \sum_k \left[ -2\gamma \cos(k + \varphi(t))d_{k}^\dagger d_k + \sum_{\alpha} \epsilon_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha} - g \sum_{\alpha} (c_{k\alpha}^\dagger d_k + H.c.) \right].$$

Here $\epsilon_d(k) = -2\gamma \cos(k)$ is the tight-binding dispersion at zero $E$-field. Then each $k$-sector can be treated and solved separately. So from now on, we suppress the $k$-subscript until necessary with the following Hamiltonian,

$$\hat{H}_k(t) = -2\gamma \cos(k + \varphi(t))d_k^\dagger d_k + \sum_{\alpha} \epsilon_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha} - g \sum_{\alpha} (c_{k\alpha}^\dagger d_k + H.c.).$$

It is important to note that the $k$-dependence enters the problem as $k + \varphi(t)$ for $t > 0$. This problem is simply a resonant level model where the level is modulated sinusoidally for $t > 0$.

### III. SOLUTION FOR OCCUPATION NUMBER AND CURRENT

The time-dependent Hamiltonian \cite{footnote} can be exactly solved by the nonequilibrium Keldysh Green function method. We write the Hamiltonian as $\hat{H}_k(t) = \hat{H}_0 + \hat{V}(t)$ with the time-independent unperturbed part $\hat{H}_0 = \hat{H}_k(0)$ and the time-dependent perturbation as $\hat{V}(t) = \hat{H}_k(t) - \hat{H}_k(0)$.

$$\hat{V}(t) = -2\gamma [\cos(k + \varphi(t)) - \cos(k)]d_k^\dagger d_k \equiv v(t)d_k^\dagger d_k.$$ (5)

When the perturbation is one-body on discrete states the lesser and greater part of the self-energy is zero, and the lesser $d$-Green function $G^<$ is expressed only in terms of the transient term, symbolically written in the matrix form as\cite{footnote}

$$G^< = [I + G^r V]G^0_0 [I + V G^a]$$ (6)

and the retarded Green function $G^r$ is given by the usual Dyson’s equation

$$G^r = G^0_0 + G^0_0 V G^a,$$ (7)

where the matrix product denotes convolution-integrals in time.

First with the retarded functions, the non-interacting limit has the time-translational symmetry and

$$G^r_0(t-t') = -i\theta(t-t') \int_{-\infty}^{\infty} dt' \frac{\Gamma}{e^2 + \Gamma^2} e^{-i\epsilon(t-t')}$$

$$= -i\theta(t-t')e^{-i\epsilon_d(k)(t-t')-\Gamma|t-t'|},$$ (8)

where we use a flat-band DOS for the reservoir in the infinite-band limit with the hybridization broadening $\Gamma = \gamma/2$. 

\begin{figure}[h]
\centering
\includegraphics[width=\columnwidth]{fig1}
\caption{(Color online) One-dimensional tight-binding lattice of orbital $d_i$ under an electric field $E$. Each lattice site is connected to an identical fermionic bath of $\{c_{i\alpha}\}$ with the continuum index $\alpha$ along the reservoir chain direction.}
\end{figure}
We set the initial lesser Green function with the half-filled $G_{0}^{<}(t, t)$, and finally we have for the full retarded Green function which can be solved as

$$g^r(t, t') = 1 - i \int_{t'}^{t} ds v(s)g^r(s, t'),$$

(9)

and finally we have for the full retarded Green function

$$G^r(t, t') = -i \theta(t-t')e^{-i\epsilon_d(k)(t-t')-\Gamma|t-t'|} \exp\left[ -i \int_{t'}^{t} v(s)ds \right],$$

(10)

For the same-time argument for $G^<$ we have the Dyson’s equation

$$G^<(t, t) = G_0^<(t, t)$$

$$+ \int_{0}^{t} \left[ G^r(t, s)v(s)G_0^<(s, t) + G_0^<(t, s)v(s)G^a(s, t) \right] ds$$

$$+ \int_{0}^{t} \int_{0}^{t} G^r(t, s)v(s)G_0^<(s', t)v(s')G^a(s', t)dsds'.$$

(12)

We set the initial lesser Green function with the half-filled reservoir at zero temperature as

$$G_0^<(t, t') = i \int_{-\infty}^{0} d\omega \frac{\Gamma/\pi}{(\omega - \epsilon_d(k))^2 + \Gamma^2} e^{-i\omega(t-t')}.$$  

(13)

After some straightforward steps, the occupation number for the wave-vector $k$, $n_k(t) = -iG^<(t, t)$, becomes

$$n_k(t) = \int_{-\infty}^{0} d\omega \frac{\Gamma/\pi}{(\omega - \epsilon_d(k))^2 + \Gamma^2} \times \left[ 1 - i \int_{0}^{t} ds v(s)e^{i(\omega - \epsilon_d(k) + \Gamma)(t-t') - i\int_{0}^{t} v(s')ds'} \right].$$

(14)

Fig. 2 shows the above $n_k(t)$ numerically evaluated for $\gamma = 1$, $\Omega = 0.5$, $\Gamma = 0.1$ and at $k = \pi/2 + 0.1$. Due to the exponential factor $e^{-\Gamma(t-t')}$, the integral converges to a steady-state oscillation state after time $t \approx \Gamma^{-1}$ and the transient behavior dies out. Therefore, for long-time behavior, the time-integral range $[0, t]$ can be changed to $[-\infty, t]$ for easier analytic treatment. After an integral-by-parts and some straightforward steps, we have

$$n_k(t) = \frac{\Gamma}{\pi} \int_{-\infty}^{0} d\omega \times \left[ \int_{-\infty}^{0} ds e^{-i(\omega + \Gamma)s - i(2\gamma/\Omega)\sin(k + \Omega(t+s))} \right].$$

(15)

An identity for Bessel functions $J_n(x)$

$$e^{ix\cos \theta} = \sum_{n=-\infty}^{\infty} i^n J_n(x)e^{in\theta}$$

(16)

can be used to perform the integrals as

$$n_k(t) = \frac{\Gamma}{\pi} \sum_{nm} \frac{J_n(\pi/\Omega)J_m(\pi/\Omega)e^{(m-n)(k+\Omega t)}}{1 - (m-n)\Omega + 2i\Gamma} \times$$

$$\left[ \frac{1}{2} \log \frac{m^2\Omega^2 + \Gamma^2}{n^2\Omega^2 + \Gamma^2} + i\chi_{mn} \right]$$

(17)

with

$$\chi_{mn} = \pi + \tan^{-1} \frac{m\Omega}{\Gamma} + \tan^{-1} \frac{n\Omega}{\Gamma}.$$  

(18)

To interpret the $k$-occupation number, we should study the quantities with respect to the physically meaningful gauge-invariant (mechanical) wave-vector $k_m = k + \Omega t$. The occupation number can be easily evaluated by replacing $k + \Omega t$ by $k_m$ in Eq. (17), as shown in FIG. 3 for the damping at $\Gamma = 0.1$. As the field $\Omega$ increases, the $k$-occupation number to the Fermi-Dirac distribution shifted towards the field direction. Despite the lack of momentum scattering in the system, the picture of displaced Fermi sea remains valid for small field. The fermion thermostats acting as particle reservoirs seem to dephase the Peierls factor when an electron is absorbed in the reservoir, hence leading to the similar effect as the momentum scattering. In appendix, it has been shown analytically that the shift of the wave-vector at small field is

$$\delta k = \frac{\Omega}{\Gamma} \propto E \tau,$$

(19)
as expected in the Boltzmann transport picture. The momentum shift $\delta k$, in the low-field limit, corresponds to the drift velocity which is proportional to the electric field $E$ and the lifetime $\tau(\sim \Gamma^{-1})$ of the transport electron given by the reservoir. As the field increases the shift of Fermi surface deviates from the linear relation. As the field is further increased ($\Omega \gg \Gamma$), the distribution significantly deviates from the sharp low temperature distribution and all $k_m$ gradually become equally occupied.

Another gauge-invariant quantities are the local variables. For instance, by taking the $k$-summation of Eq. (17), one obtains the local electron density. Due to the sine-function, the DC current has contributions only from $m - n = \pm 1$ in Eq. (17). After some manipulations, we have

$$\bar{n}_{\text{local}}(t) = \frac{1}{2} \sum_{m=-\infty}^{\infty} \left[ J_m \left( \frac{2\gamma}{\Omega} \right) \right]^2 = \frac{1}{2}. $$

Now we turn to the calculation of electric current,

$$J_k(t) = \frac{\partial \epsilon_k(k + \Omega t)}{\partial k} n_k(t) = 2\gamma \sin(k + \Omega t) n_k(t). \quad (20)$$

Due to the sine-function, the DC current has contributions only from $m - n = \pm 1$ in Eq. (17). After some manipulations, we have

$$J_k = \frac{2\gamma \Gamma}{\pi(\Omega^2 + 4\Gamma^2)} \sum_m J_m \left( \frac{2\gamma}{\Omega} \right) J_{m-1} \left( \frac{2\gamma}{\Omega} \right) \times \left[ \Gamma \log \frac{m^2\Omega^2 + \Gamma^2}{(m-1)^2\Omega^2 + \Gamma^2} + \Omega \chi_{m,m-1} \right]. \quad (21)$$

As in the case for $n_k(t)$, the DC limit of $J_k(t)$ becomes independent of $k$. The total current is shown in Figs. 4 and 3. Similar plot has been obtained in the interacting model from numerical calculation of Hubbard model connected to fermion bath\textsuperscript{21}.

It is instructive to simplify the above expression in the limit of $\Omega, \Gamma \ll \gamma$ where the DC current is reduced to the expression

$$\bar{J} = \frac{4\gamma \Gamma \Omega}{\pi(\Omega^2 + 4\Gamma^2)}. \quad (22)$$

Detailed derivation is provided in Appendix. This approximate expression is shown as dashed lines in Fig. 4. Despite that the formula was derived for $\Omega, \Gamma \ll \gamma$, it shows remarkable accuracy to the DC current for a wide range of $\Gamma$ and $E$.

It is also interesting to note that a similar formula has been derived for a super-lattice system with Ohmic scattering within the semi-classical Boltzmann transport equation\textsuperscript{21}. Although the current has the same dependence on the damping and the electric field, it should be emphasized that the two models have quite different scattering mechanism where in the Boltzmann approach\textsuperscript{21} the momentum relaxation is explicitly built-in while in our case the lattice wave-vector scattering does not happen and a very different Fermi surface structure results. In the low-field limit, the current (22) recovers the form of the Drude conductivity per electron,

$$\bar{J} \approx \frac{\gamma \Omega}{\pi \Gamma} \times \frac{E \tau}{m^*}, \quad (23)$$

with $\gamma \sim 1/m^*$ and $\Gamma \sim 1/\tau$. 

FIG. 3: (color online) Occupation number $n(k_m)$ with respect to the gauge-invariant mechanical wave-vector $k_m = k + \Omega t$ from Eq. (17) at $\Gamma = 0.1$. At zero field ($\Omega = 0$, dashed line), $n(k_m)$ is given by the Fermi-dirac distribution with the smooth steps from the damping $\Gamma$. As the field increases, the distribution shifts to higher wave-vector as predicted by the Boltzmann theory. With higher field ($\Omega > \Gamma$), the distribution develops strong nonlinear effect with increasing effective temperature.

FIG. 4: (color online) DC current as a function of the damping $\Gamma$ and electric field $\Omega = eEA$. For small field, the current has a linear dependence on the $E$-field showing an Ohm’s law-like behavior. As $E$ increases, the Bloch oscillation behavior takes over and the DC current decreases. The dashed lines are the simplified expression, Eq. (22).
FIG. 5: (Color online) Contour plot of DC current as a function of damping and electric field.

IV. CONCLUSIONS

Calculations on electron transport with fermion thermostats confirm salient features of numerical results, and map the model to the Boltzmann transport picture, such as Fermi surface shift in the Brillouin zone by the drift velocity and the Ohmic-like limit of electric current. In particular, the electric current, Eq. (22), recovered the semi-classical transport result even without any momentum scattering. Explicit and exact calculations clarify the steady-state nature of the model which might have different scattering processes from the realistic solid-state transport systems. Nevertheless, its phenomenological similarity to the conventional semi-classical pictures has been established. The findings lead us to conclude that the fermion bath model, despite its drastic simplifications in the one-particle coupling and the lack of momentum scattering, can be considered as a rudimentary and minimal dissipation mechanism which will be invaluable in further modeling strong correlation physics through dynamical mean-field theory.

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Appendix A: Momentum occupation number at small field

In Eq. (15), we rewrite the expression by the gauge-invariant wave-vector \( k_m = k + \Omega t \) and the \( \omega \)-integral first to obtain

\[
\frac{i\Gamma}{\pi} \int_{-\infty}^{\infty} ds \int_{-\infty}^{0} ds' e^{i\Gamma(s+s')-i(2\gamma/\Omega)[\sin(k_m+\Omega t)-\sin(k_m+\Omega t')]}.
\]

For small field \( \Omega \ll \gamma \), the principal part evaluation \( \mathcal{P} \), the \( \delta \)-function part yield a simple contribution of \( \frac{1}{2} \). Redefining the times by the average time \( T = \frac{1}{2} (s + s') \) and the relative time \( t_r = s - s' \), we can express Eq. (15) as

\[
\frac{1}{2} \frac{i\Gamma}{\pi} \int_{-\infty}^{0} dt \int_{-|T|}^{2|T|} dt_r \mathcal{P} e^{i2\Gamma t_r-(4\gamma/\Omega)\cos(k_m+\Omega t)\sin(\Omega t_r/2)}.
\]

We look at the mechanical wave-vector slightly away from \( \pm \pi/2 \) and set \( k_m = \pi/2 + \delta k \). We change variables as \( y = -\Omega T, x = \Omega t_r \). Then we have the integral as

\[
\frac{i\Gamma}{\pi\Omega} \int_{0}^{\infty} dy \int_{-2y}^{2y} dx \mathcal{P} e^{i\Omega y(2\gamma/\Omega)\sin(\delta k - y)\sin(x/2)}.
\]

For small field \( \Omega \ll \Gamma \), the integral has main contribution from \( |x|, y \leq \Omega/\Gamma \ll 1 \). Then the integral can be approximately evaluated for \( |\delta k| \leq \Omega/\Gamma \) as

\[
n(k_m) \approx \frac{1}{2} + \frac{2\gamma \Omega}{\Gamma^2} \left( 1 - \frac{\Gamma}{\Omega} \delta k \right).
\]

Appendix B: Derivation of current at small field

For both \( \Gamma, \Omega \ll \gamma \), we expand Eq. (21) to the leading order of \( m \) as

\[
\tilde{J}_k \approx \frac{2\gamma \Gamma}{\pi(\Omega^2 + 4\Gamma^2)} \sum_m J_m \left( \frac{2\gamma}{\Omega} \right) J_{m-1} \left( \frac{2\gamma}{\Omega} \right) \times
\]

\[
\left[ \frac{2m\Gamma\Omega^2}{m^2\Omega^2 + \Gamma^2} + 2\Omega \tan^{-1} \frac{m\Omega}{\Gamma} \right].
\]

Rearranging the summation and using the identity

\[x[J_{m-1}(x) + J_{m+1}(x)] = 2mJ_m(x),\]

we write

\[
\tilde{J}_k \approx \frac{2\gamma \Gamma}{\pi(\Omega^2 + 4\Gamma^2)} \sum_m J_m [J_{m-1} + J_{m+1}] \times
\]

\[
\left[ \frac{m\Omega^2}{m^2\Omega^2 + \Gamma^2} + \Omega \tan^{-1} \frac{m\Omega}{\Gamma} \right]
\]

\[
= \frac{2\Omega}{(2\Omega^2 + 4\Gamma^2)} \sum_m m\Omega J_m^2 \left( \frac{m\Omega}{m^2\Omega^2 + \Gamma^2} + \tan^{-1} \frac{m\Omega}{\Gamma} \right).
\]

For \( \Omega \ll \gamma \), we define \( x = m\Omega \) in the regime \( m = x/\Omega \gg 1 \), the summation becomes

\[
\int_{-\infty}^{\infty} xJ_n \left( \frac{2\gamma}{\Omega} \right)^2 \left( \frac{x\Gamma}{x^2 + \Gamma^2} + \tan^{-1} \frac{x}{\Gamma} \right) dx/\Omega.
\]

Using the asymptotic expression\(^{[22]}\) for \( x/\Omega, \gamma/\Omega \to \infty \),

\[
[J_n \left( \frac{2\gamma}{\Omega} \right)^2] \sim \begin{cases} \frac{\Omega/\gamma}{\pi \sqrt{1-(x/2\gamma)^2}} & (|x| < 2\gamma) \\ 0 & (|x| > 2\gamma) \end{cases}
\]
the integral simplifies to
\[
\int_{-2\gamma}^{2\gamma} \frac{1}{\pi \sqrt{4\gamma^2 - x^2}} \left( \frac{x^2 \Gamma}{x^2 + \Gamma^2} + x \tan^{-1} \frac{x}{\Gamma} \right) dx.
\]
In the limit \( \Gamma \ll \gamma \), the second term in the parenthesis dominates and we have
\[
J \approx \frac{2\Gamma \Omega}{\pi (\Omega^2 + 4\Gamma^2)} \int_{0}^{2\gamma} \frac{dx}{\sqrt{4\gamma^2 - x^2}} = \frac{4\gamma \Gamma \Omega}{\pi (\Omega^2 + 4\Gamma^2)}.
\]