Electric-field-driven resistive switching in dissipative Hubbard model

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We study how strongly correlated electrons on a dissipative lattice evolve from equilibrium when driven by a constant electric field, focusing on the extent of the linear regime and hysteretic non-linear effects at higher fields. We access the non-equilibrium steady states, non-perturbatively in both the field and the electronic interactions, by means of a non-equilibrium dynamical mean-field theory in the Coulomb gauge. The linear response regime is limited by Joule heating effects and breaks down at fields orders of magnitude smaller than the quasi-particle energy scale. For large electronic interactions, strong but experimentally accessible electric fields can induce a resistive switching by driving the strongly correlated metal into a Mott insulator. Hysteretic I-V curves suggest that the non-equilibrium current is carried through a spatially inhomogeneous metal-insulator mixed state.

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Understanding of solids driven out of equilibrium by external fields [1, 2] has been one of the central goals in condensed matter physics for the past century and is very relevant to nanotechnology applications such as resistive transitions. Multiple studies of this phenomenon have been performed in semiconductors and oxides [3–10]. In oxides, the application of an electric field can lead to a dramatic drop of resistivity up to 5 orders of magnitude. The relatively accessible threshold fields $E_{th} \sim 10^3-6$ V/m and the hysteretic I-V curves make them good candidates for the fabrication of novel electronic memories. A Landau-Zener type of mechanism [11] seems unlikely as it predicts a threshold field on the order of $10^8-9$ V/m. In narrow gap chalcogenide Mott insulators, an avalanche breakdown was suggested with $E_{th} \sim E_{gap}^{2.5}$ [3]. Yet, the resistive switchings in other classes of correlated materials do not seem to involve solely electronic mechanisms. In organic charge-transfer complexes, it is believed to occur via the electro-chemical migration of ions [4, 5]. Finally, there are strong indications that a Joule heating mechanism occurs in some binary oxides such as NiO [7] and VO$_2$ [8–10]: the electric-field-driven current locally heats up the sample which experiences a temperature-driven resistive switching.

These experiments raise basic questions such as how a strongly correlated state continuously evolves out of equilibrium when driven by an external field, how to describe the non-equilibrium steady states that consequently emerge, and the development of a basic microscopic theory of the driven metal-insulator transition is much needed.

Building on earlier theoretical efforts [11–19, 21–25] we identify in a canonical model of strongly interacting electrons a region where electric-field-driven resistive switching takes place. We demonstrate how Joule heating effects modify the linear response regime and how, away from the linear regime, the same Joule physics is again the key to describe the hysteretic resistive transitions of the strongly correlated system. The derived energy scales for resistive transitions are orders of magnitude smaller than bare model parameters, within the feasible experimental range. This scenario suggests a highly inhomogeneous distribution of resistivity and temperature in real materials.

We study the Hubbard model in a constant and homogeneous electric field $E$ which induces a current of electrons $J$. After a transient regime, a non-equilibrium steady state establishes if the power injected in the system, $J \cdot E$, is balanced by coupling the system to a thermostat which can absorb the excess of energy via heat transfer [14, 15, 21–24]. For simplicity, we start with an infinite one-dimensional tight-binding (TB) chain. The thermostat is modeled by identical fermion reservoirs attached to each TB sites. In the Coulomb gauge, the electric field amounts in an electrostatic potential $-\ell E$ imposed on the $\ell$-th TB site ($\ell = -\infty, \cdots, \infty$) and on its associated fermion bath [15]. The model is fully consistent with gauge-covariant models [23]. The non-interacting Hamiltonian reads,

$\hat{H}_0 = -\gamma \sum_{\ell \sigma} (d_{\ell+1,\sigma}^† d_{\ell,\sigma} + \text{H.c.}) - \frac{g}{\sqrt{\ell}} \sum_{\ell \sigma} (d_{\ell,\sigma}^† c_{\ell,\sigma} + \text{H.c}) + \sum_{\ell \alpha \sigma} c_{\ell,\sigma}^† c_{\ell,\sigma} - \sum_{\ell \sigma} \ell E (d_{\ell,\sigma}^† d_{\ell,\sigma} + c_{\ell,\sigma}^† c_{\ell,\sigma}), \quad (1)$

where $d_{\ell,\sigma}^†$ are the tight-binding electron creation operators at the $\ell$-th site with spin $\sigma = \uparrow$ or $\downarrow$, and $c_{\ell,\sigma}^†$ are the corresponding reservoir electron operators attached. $\alpha$ is a continuum index corresponding to the reservoir dispersion relation $\epsilon_{\alpha}$ defined with respect to the electrostatic potential $-\ell E$. $g$ is the overlap between the TB chain and the reservoirs of length $L$ which will be sent to infinity, assuming furthermore that the reservoirs remain in equilibrium at bath temperature $T_B$. The ele-
tric field does not act within each reservoir whose role is to extract energy but not electric charge from the system. We use a flat density of states (infinite bandwidth) for the reservoir spectra $\epsilon_\alpha$, and define the damping parameter as $\Gamma = L^{-1} \pi g^2 \sum_\alpha \delta(\epsilon_\alpha)$. We work with $\hbar = e = k_B = a = 1$ in which $e$ is the electronic charge and $a$ is the lattice constant. In the rest of this Letter, we measure energies in units of the TB hopping parameter $\gamma$ and set $\gamma = 1$. The exact solution of the non-interacting model in Eq. (1) has been shown [14, 15] to reproduce the conventional Boltzmann transport theory despite the lack of momentum transfer scattering. In a homogeneous lattice under a uniform electric-field, there is no net particle flux into each reservoir [15]. The Hubbard model $H = H_0 + H_1$ is defined with the on-site Coulomb interaction parameter $U$ as

$$H_1 = U \sum (d_{\uparrow}^\dagger d_{\uparrow} - \frac{1}{2}) (d_{\downarrow}^\dagger d_{\downarrow} - \frac{1}{2}).$$

(2)

Our calculations are in the particle-hole symmetric limit.

We use the dynamical mean-field theory (DMFT [16, 26]) to treat the many-body interaction via a self-consistent local approximation of the self-energies. Note that the self-energy has contributions from both the many-body interaction $\hat{H}_1$ and the coupling to the reservoirs: $\Sigma_{\ell \ell'}^{r}(\omega) = -2i \Pi^{r}(\omega)$ and $\Sigma_{\ell \ell'}^{<}(\omega) = 2i \Pi^{<}(\omega) + \Pi_{\ell \ell'}^{r}(\omega) + \Pi_{\ell \ell'}^{<}(\omega)$ with the Fermi-Dirac (FD) distribution $f_{\Pi}(\omega) \equiv [1 + \exp(\omega/T_{b})]^{-1}$. Once the local retarded and lesser self-energies are computed, one can access the full retarded and lesser Green’s functions (GFs). Note that in a homogeneous non-equilibrium steady state, all the TB sites are equivalent. In the Coulomb gauge, this translates formally into the relation $G_{\ell \ell'}^{r}(\omega) = G_{\ell \ell'}^{<}(\omega + kE)$ and similarly for the self-energies [15].

Below, we present the real-space implementation of our DMFT scheme in the Coulomb gauge, and directly in the non-equilibrium steady states. It consists in solving out one TB site — say $\ell = 0$— (often referred as impurity) and replacing its direct environment (i.e. two semi-infinite dissipative Hubbard chains and its own reservoir) with a self-consistently determined non-interacting environment (often referred as Weiss “fields”). The local electronic interaction of the single site problem is then treated by means of an impurity solver which provides for the local self-energy.

Assuming for a moment that the local self-energies $\Sigma_{\ell \ell'}^{r}(\omega) \equiv \Sigma_{\ell \ell'}^{<}(\omega + \ell E)$ are known, the on-site Green’s functions obey the following Dyson equations

$$G_{\ell \ell'}^{r}(\omega)^{-1} = \omega - \Sigma_{\ell \ell'}^{r}(\omega) - \gamma^2 F_{\ell \ell'}^{r}(\omega),$$

$$G_{\ell \ell'}^{<}(\omega) = |G_{\ell \ell'}^{r}(\omega)|^2 \Sigma_{\ell \ell'}^{<}(\omega) + \gamma^2 F_{\ell \ell'}^{<}(\omega),$$

(3)

(4)

in which $\gamma^2 F_{\ell \ell'}^{<}$ are the total hybridization functions to the left and right semi-infinite chains, $F_{\ell \ell'}^{<}(\omega) = F_{\ell \ell'}^{+<}(\omega + E) + F_{\ell \ell'}^{-<}(\omega - E)$. $F_{\ell \ell'}(\omega)$ is the on-site retarded GF at the end of the RHS-chain ($\ell = 1$) which obeys the self-similar Dyson equation

$$F_{\ell \ell'}^{r}(\omega)^{-1} = \omega - \Sigma_{\ell \ell'}^{r}(\omega) - \gamma^2 F_{\ell \ell'}^{r}(\omega + E),$$

(5)

which can be solved recursively after more than 500 iterations. $F_{\ell \ell'}(\omega)$ corresponds to the GF of the LHS-chain and can be obtained similarly. The non-interacting parts of the impurity GFs, $G$, are constructed using

$$G_{\ell \ell'}^{r}(\omega)^{-1} = \omega + i \Gamma - \gamma^2 F_{\ell \ell'}^{<}(\omega),$$

$$G_{\ell \ell'}^{<}(\omega) = |G_{\ell \ell'}^{r}(\omega)|^2 [2i \Pi_{\ell \ell'}^{r}(\omega) + \gamma^2 F_{\ell \ell'}^{<}(\omega)].$$

(6)

(7)

The local self-energies are obtained by means of the iterative-perturbation theory (IPT) with a second order perturbation theory in the Coulomb parameter $U$: $\Sigma_{\ell \ell'}^{r}(t) = U[\Sigma_{\ell \ell'}^{<}(t)]^2 [\Sigma_{\ell \ell'}^{r}(t)]^2$. The GFs are updated with this self-energy using the above Dyson’s equations and the procedure is repeated until convergence is achieved.

We generalize the above method to higher dimensions. Assuming that the electric-field is oriented along the principal axis direction, $E = E\hat{x}$, the lattice is translation invariant in the perpendicular direction and the above construction of the Dyson’s equation can be carried out independently per each perpendicular momentum vector. See Supplementary Material for a detailed discussion. Below, we present results of the model in one, two and three dimensions.

We first discuss the linear response regime. Within the DMFT, the DC conductivity in the limit of zero temperature and zero electric field can be obtained via the Kubo formula as $\sigma_{DC} \propto \lim_{\nu \to 0} \sum_{k} d\nu \rho_{k}(\nu) \rho_{-k}(\nu - E)$ with the spectral function at a given wave-vector $k$, $\rho_{k}(\nu) = -\pi^{-1} \text{Im} \nu - \epsilon_{k} + i\gamma \Sigma_{\ell \ell'}^{r}(\nu - E)^{-1}$. Therefore, as long as $\Sigma_{\ell \ell'}^{r}(\nu) \approx 0$ as $\nu \approx 0$, $T \rightarrow 0$, the DC conductivity is independent of the interaction. This argument is similar to the one used by Prange and Kadanoff [27] for the electron-phonon interaction. Recent calculations were restricted to the single polaron case [22] or did not have access to the linear response regime [21, 23, 24].

FIG. 1 confirms the validity of the linear response analysis. The initial slope of the current $J$ vs. the electric-field $E$ is independent of the interaction strength $U$ both in (a) one and (b) three-dimension. The linear behavior deviates at the field $E_{lin} \approx 0.02 - 0.03$, orders of magnitude smaller than the renormalized (half)-bandwidth $W^{\ast} = z \times (2\Gamma) \approx 1.0$ with the renormalization factor $z$.

As the field $E$ increases further, the current is enhanced over its value at $U = 0$. The contribution at $E = U/2$ is a two-step resonant process which can be viewed in the Coulomb gauge as the consequence of the overlap between the lower/upper Hubbard bands of the left/right neighboring sites with the in-gap states present at the Fermi level [25]. The current peak at $E = U$ is due to the direct overlap of the Hubbard bands on neighboring sites [18, 25].
The immediate departure from the linear conductivity at very small fields can be well understood with a Joule heating scenario in which the Coulombic interaction is the dominant scattering process and is rapidly modified by an increasing effective temperature as the field is increased. We first demonstrate this effective temperature effect by showing in Fig. 2(a) that the scattering rates from the Coulomb interaction, \( \tau_U^{-1} = -\text{Im} \Sigma_U(\omega = 0) \), for different sets of the damping \( \Gamma \) collapse onto a scaling curve as a function of \( (E/\Gamma)^2 \) for small \( E \). This scaling is clearly evocative of the well known \( T^2 \) behavior of equilibrium retarded self-energies.

In the non-interacting 1-d chain with fermion baths at zero temperature, the hot-electron effective temperature has been obtained in the small field limit as \[ T_{\text{eff}} = \frac{\sqrt{6}}{\pi} \frac{E}{\Gamma}. \] (8)

Inserting this \( T_{\text{eff}} \) into the equilibrium perturbative self-energy [28], we obtain

\[ \tau_U^{-1} = -\text{Im} \Sigma_{\text{eq}}^r(\omega = 0, T_{\text{eff}}) \approx \frac{\pi^3}{2} A_0(0)^3 U^2 T_{\text{eff}}^2, \] (9)

which is represented by the dashed lines in Fig. 2(a).

Here \( A_0(0) = (\pi \sqrt{T^2 + 4\gamma^2})^{-1} \) is the non-interacting DOS at \( \omega = 0 \). The robust agreement between this estimate and the actual non-equilibrium self-energy leaves no doubt that the electron scattering is dominated by the Joule heating in the small field limit.

The scattering rate can be directly related to the electric current via the Drude conductivity \( J(E) = \sigma_{\text{DC}}(E)E \) with the non-linear DC conductivity \( \sigma_{\text{DC}}(E) \). In the non-interacting limit, the linear conductivity can be written as \( \sigma_{\text{DC}} = 2\gamma^2/(\pi \Gamma \sqrt{T^2 + 4\gamma^2}) \) [15]. In Fig. 2(b), we plot also the Drude formula with the scattering rate \( \Gamma \) of the fermion baths replaced by the total scattering \( \Gamma_{\text{tot}} = \Gamma + \tau_U^{-1} \). The qualitative agreement with the numerical results extends over a wide range of the \( E \)-field, well beyond the linear regime. Naturally, the agreement is perfect in the low field limit where the linear response theory is exact.

Using Eq. (9), the current at small field can be approximated as \( J = \sigma_{\text{DC}} E/(1 + E^2 / E_{\text{lin}}^2) \) with the departure from the linear behavior occurring around (from the condition \( \Gamma \approx \tau_U^{-1} \) at \( E = E_{\text{lin}} \))

\[ E_{\text{lin}} \approx \sqrt{\frac{8\pi^2 \gamma^2 \Gamma^3/2}{3}} \frac{U}{T}. \] (10)

This estimate is valid away from \( U = 0 \) and the metal-insulator limit, and agrees well with FIG. 2(b) [29]. We emphasize that, while negative-differential-resistance (NDR) behaviors occur typically in periodic structures due to the Bloch oscillations [30] as the dashed lines \( (U = 0) \) in Fig. 1, the NDR here with a strong interaction comes from strong non-linear scattering due to the Joule heating.

In the presence of weak dissipation and strong electronic interactions, the non-equilibrium evolution becomes more dramatic. With the effective temperature, Eq. (8), having a singular limit as \( \Gamma \rightarrow 0 \), the electron temperature tends to rise very sharply as the field is applied. This effect, together with a small value of the renormalized coherent energy scales, causes the system to immediately deviate from the linear response regime, preventing itself from overheating. This mechanism, in a vicinity of a quantum phase transition, can strongly modify the state of a system. Indeed, we will show that there is a region of the parameters \( U \) and \( E \) for which the non-equilibrium Dyson’s equations have two distinct solutions, one corresponding to an incoherent metal and the other to an insulator.

With a small damping \( \Gamma = 0.01 \), the MIT can be sharply defined at the bath temperature \( T_b = 0.01 \). In
Fig. 3(a), we start from a metallic state at $U = 11.6$, and increase the electric-field from zero. We use the self-consistent solution at a certain $E$-field for the initial self-energy of the next $E$ run. As seen above, the system has an extremely narrow linear response window with $E_{\text{lin}} < 0.001$, followed by an NDR behavior. As the electric-field is further increased, an electric-field-driven metal-to-insulator occurs at $E_{\text{MIT}} \approx 0.03$. Similar strong non-linear $I$-$V$ behavior followed by a resistive transition has been observed in NiO [7]. The spectral functions in Fig. 3(b) show that the change leading up to the MIT is abrupt. The quasi-particle spectral weight rapidly disappears near the MIT driven by the electric-field, opening an insulating gap. The non-equilibrium energy distribution function indicates that the system undergoes a highly non-monotonic cold-hot-cold temperature evolution near the MIT.

![FIG. 3: (color online) (a) Electric-field driven metal-to-insulator transition (MIT) in the vicinity of a Mott-insulator at $U = 11.6$, $\Gamma = 0.01$ and $T_b = 0.02$ in a two-dimensional square lattice with electric field in $x$-direction. The metallic state at zero field becomes insulating at electric field of magnitude orders of magnitude smaller than bare energy scales. Depending on whether the electric-field is increased or decreased, metal-insulator hysteresis occurs with a window for phase-coexistence. (b) Spectral function and distribution function $f_{\text{loc}}(\omega)$ with increasing electric-field. The quasi-particle spectral weight rapidly disappears near the MIT driven by the electric-field, opening an insulating gap. The non-equilibrium energy distribution function indicates that the system undergoes a highly non-monotonic cold-hot-cold temperature evolution near the MIT.

![FIG. 4: (color online) (a) Phase diagram of metal-insulator transition in a square lattice driven by the electric field (upper panel) and temperature (lower panel). The metal-insulator coexistence driven by electric field has similar structure as that driven by temperature, while we observe non-trivial re-entrant behavior at high fields as a function of the Coulomb parameter $U$. $\Gamma = 0.01$. (b) Critical electric field $E_{\text{MIT}}$, at $U = 12$, vs. damping $\Gamma$ with the approximate dependence $E_{\text{MIT}} \propto \sqrt{\Gamma}$ (red dashed line).]

Even though the calculations performed here are on homogeneous lattices, the phase coexistence suggests that, under a uniform field, the system can be spatially segregated into a mixed state of metal and insulator regions which in turn have inhomogeneous temperature distribution with complex thermodynamic states. The hot metallic regions will be oriented in the direction of the field, forming experimentally observed current-carrying filaments.

The Joule heating scenario has been previously invoked in the literature for resistive switching in disordered films [33]. Our discovery of the coexistence of two distinct non-equilibrium steady-state solutions in the framework of a relatively simple quantum mechanical model could be applicable to NiO [7] and V$_2$O$_3$ systems where metal-to-insulator transitions are known to occur with increasing temperature. Further extensions to cluster DMFT would allow a realistic treatment of the electronic structure and could successfully address the case of VO$_2$.

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Supplementary Material: Metal-to-insulator phase transition in field-driven electron lattice coupled to dissipation

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Fig. S1: One-dimensional tight-binding chain place in a uniform electric-field within the Coulomb gauge. On each orbital along the transport chain is attached a semi-infinite fermion chain which dissipates the excess energy accumulated by the Joule heating.

Formulation of one-dimensional chain under electric-field: We model a one-dimensional Hubbard model in the Coulomb gauge, as shown in Fig. S1, with the Hamiltonian

\[
H = -\gamma \sum_{\ell,\sigma} (d_{\ell+1,\sigma}^d d_{\ell,\sigma} + \text{h.c.}) + U \sum_{\ell} \left( n_{\ell\uparrow} - \frac{1}{2} \right) \left( n_{\ell\downarrow} - \frac{1}{2} \right) + \sum_{\ell,\alpha,\sigma} \epsilon_\alpha c_{\ell\alpha\sigma}^d c_{\ell\alpha\sigma}^c - \frac{g}{\sqrt{L}} \sum_{\ell,\alpha,\sigma} (d_{\ell\alpha\sigma}^d c_{\ell\alpha\sigma}^c + \text{h.c.}) - \sum_{\ell} {\ell} E \left( d_{\ell\alpha\sigma}^d d_{\ell\alpha\sigma}^c + \sum_{\alpha} c_{\ell\alpha\sigma}^d c_{\ell\alpha\sigma}^c \right),
\]

where all orbitals on the \( \ell \)-th TB site are shifted by \( \ell E \) and also the chemical potential by \( \mu_\ell = -\ell E \). Here we use the unit \( e = a = 1 \). The fermion reservoir chains (with yellow circles) act as energy drain from energetically excited electrons on the main tight-binding (TB) lattice. This Hamiltonian in the Coulomb gauge [2] is equivalent to the temporal gauge [3] and the gauge-covariant form [4]. In a long-time limit, we assume we have already-reached a well-defined nonequilibrium steady-state in the presence of reservoirs. With respect to \( d_\ell \), we have two sources for the electronic self-energy, one from the fermion reservoirs and the other from the Coulomb interaction, which we denote as \( \Sigma_\Gamma \) and \( \Sigma_U \), respectively. Here we make a dynamical mean-field theory (DMFT) assumption that the self-energies are local and identical, except that the energies are shifted by the voltage drop along the TB lattice [1],

\[
G^{r,\ell\ell}(\omega) = G^{r,\ell\ell}(\omega + \ell E) \quad \text{and} \quad \Sigma^{r,\ell\ell}_{\ell\ell}(\omega) = \Sigma^{r,\ell\ell}_{\ell\ell}(\omega + \ell E),
\]

\( \ell = -\infty, \infty \) denotes the lattice site [2]. Here the subscript ‘loc’ refers to the local quantity at the central site \( \ell = 0 \). The Dyson’s equation in the steady-state for the full retarded Green’s function can be expressed in the familiar form as

\[
G^r(\omega)^{-1} = \begin{bmatrix}
\ldots & \ldots & \ldots & \ldots \\
\omega - \Sigma^{r}_{U,\text{loc}}(\omega) & \gamma & 0 & \gamma \\
\gamma & \omega - \Sigma^{r}_{U,\text{loc}}(\omega + \ell E) & \gamma & 0 \\
0 & \gamma & \omega + \ell E - \Sigma^{r}_{U,\text{loc}}(\omega + \ell E) & \gamma \\
\ldots & \ldots & \ldots & \ldots \\
\end{bmatrix}
= [\omega + \ell E + i\Gamma - \Sigma^{r}_{U,\text{loc}}(\omega)]\delta_{\ell\ell'} + \gamma \delta_{\ell,-1,1}. \quad (3)
\]
The Weiss-field Green function $\mathcal{G}$ can be expressed similarly except that the interacting self-energy is omitted at the central site,

$$[G^r(\omega)^{-1}]_{\ell\ell'} = [G^r(\omega)^{-1}]_{\ell\ell'} + \Sigma_{U,loc}(\omega)\delta_{\ell 0}\delta_{\ell' 0} \equiv [G^r(\omega)^{-1} + \Sigma_{U,loc}^r]_{\ell\ell'},$$

with $\Sigma_{U,loc}^r = \text{diag}[\cdots, 0, 0, \Sigma_{U,loc}^r(\omega), 0, 0, \cdots]$.

Inversion of the above infinite matrix can be achieved efficiently by a recursive method. We divide the lattice into three parts with the central site $\ell = 0$, the left ($\ell = -1, -2, \cdots, -\infty$) and right ($\ell = 1, 2, \cdots, \infty$) semi-infinite chains. We denote the retarded GF matrix $F^r_\ell$ on the RHS semi-infinite chain as

$$[F^r_\ell(\omega)^{-1}]_{\ell\ell'} = [\omega + \ell E + i\Gamma - \Sigma_{U,loc}^r(\omega + \ell E)]\delta_{\ell\ell'} + \gamma\delta_{|\ell-\ell'|,1},$$

with $\ell, \ell' = 1, 2, \cdots, \infty$. The local GF at the end of the chain ($\ell = 1$) $[F^r_\ell(\omega + E) \equiv F^r_\ell(\omega)_{11}]$ can be expressed as a continued fraction

$$F^r_\ell(\omega + E) = \frac{1}{\omega + E + i\Gamma - \Sigma_{U,loc}^r(\omega + E) - \gamma^2 F^r_\ell(\omega + 2E) - \cdots}$$

$$= [\omega + E + i\Gamma - \Sigma_{U,loc}^r(\omega + E) - \gamma^2 F^r_\ell(\omega + 2E)]^{-1},$$

or

$$F^r_\ell(\omega + E)^{-1} = \omega + E + i\Gamma - \Sigma_{U,loc}^r(\omega + E) - \gamma^2 F^r_\ell(\omega + 2E),$$

from the self-similarity of the semi-infinite chain. The recursive relation Eq. (7) is solved numerically with iteration number $M$ over 500. Practically, we start from an initial GF $F^r_\ell(\omega + ME) = [\omega + ME + i\Gamma - \Sigma_{U,loc}^r(\omega + ME)]^{-1}$ and by Eq. (7) we generate $F^r_\ell(\omega + (M - 1)E)$. We repeat the process Eq. (7) until we reach $F^r_\ell(\omega + E)$. The LHS GF, $F^r_\ell(\omega - E)$, can be similarly obtained through

$$F^r_\ell(\omega - E)^{-1} = \omega - E + i\Gamma - \Sigma_{U,loc}^r(\omega - E) - \gamma^2 F^r_\ell(\omega - 2E).$$

Once we obtain fully convergent GFs $F^r_{\pm}(\omega \pm E)$, the full local GF for the infinite chain can be constructed as

$$G^r_{loc}(\omega)^{-1} = \omega + i\Gamma - \Sigma_{U,loc}^r(\omega) - \gamma^2 [F^r_+(\omega + E) + F^r_-(\omega - E)].$$

The Weiss-field GF $G^r(\omega)$, omits the interacting self-energy only on the central site ($\ell = 0$) and we have

$$G^r(\omega)^{-1} = \omega + i\Gamma - \gamma^2 [F^r_+(\omega + E) + F^r_-(\omega - E)] = G^r_{loc}(\omega)^{-1} + \Sigma_{U,loc}^r(\omega).$$

Now, we turn to the Dyson’s equation for lesser GFs. When the lattice of $d_\ell$ is connected to the reservoirs and the interaction, its steady-state dynamics is governed by the transport equation

$$G_{\ell\ell'}^<(\omega) = \sum_p G_{\ell p}^r(\omega)\Sigma_{p,\text{tot}}^<(\omega)G_{p\ell'}^a(\omega),$$

with $p = -\infty, \cdots, \infty$ running over all TB sites and $\Sigma_{\text{tot}}^<$ being the sum of contributions from the fermion baths and the Hubbard interaction. For the central site $\ell = \ell' = 0$, we use a similar trick as above to group $p$ into the central site and left and right chains,

$$G_{loc}^<(\omega) = G_{loc}^r(\omega)\Sigma_{\text{tot,loc}}^<(\omega)G_{loc}^a(\omega) + \sum_{p<0} G_{0p}^r(\omega)\Sigma_{\text{tot,p}}^<(\omega)G_{p0}^a(\omega) + \sum_{p>0} G_{0p}^r(\omega)\Sigma_{\text{tot,p}}^<(\omega)G_{p0}^a(\omega).$$
For the RHS summation \((p > 0)\), one can write the Dyson’s equation \(G^r_{0p}(\omega) = G^r_{\text{loc}}(\omega)(-\gamma)F^\pm_{+,1p}(\omega)\) and similarly for the advanced FGs, and therefore we have the third term as
\[
\gamma^2|G^r_{\text{loc}}(\omega)|^2 \sum_{p>0} F^r_{+,1p}(\omega) \Sigma^\pm_{\text{tot},p}(\omega) F^a_{+,p1}(\omega).
\] (13)

The summed expression is nothing but the local lesser GF \(F^\pm_\pm(\omega + E) = F^\pm_{+,11}(\omega)\) within the LHS semi-infinite chain, and we obtain
\[
F^\pm_\pm(\omega \pm E) = |G^r_{\text{loc}}(\omega)|^2 \left\{ \Sigma^\pm_{\text{tot},\text{loc}}(\omega) + \gamma^2[F^\pm_\pm(\omega + E) + F^\pm_\pm(\omega - E)] \right\},
\] (14)

\(F^\pm_\pm(\omega \pm E)\) can be obtained from \(\Sigma^\pm_{\text{loc}}(\omega)\) following similar steps.

To summarize, given the local self-energies \(\Sigma^\pm_{\text{loc}}(\omega)\), GFs for the semi-infinite chains \(F^\pm_{+,p}\) are calculated via Eqs. (7,8,15). The retarded GFs are obtained via Eqs. (9,10), and finally the lesser GFs follow via Eqs. (14,17). This procedure, formulated on real-space, corresponds to the \(k\)-summation of the impurity GF in equilibrium DMFT formalism.

**Multi-dimensional lattice under electric-field:** For higher dimensional cubic lattice with the field along an axial direction \((\mathbf{E} = E\hat{x})\), the lattice has translational invariance perpendicular to the field, and the problem is block-diagonalized with the transverse wave-vector \(k_\perp\).

We solve the Dyson’s equation as above with the \(k_\perp\)-space (the self-energy \(\Sigma^r_{\text{loc}}(\omega)\) does not have \(k_\perp\) dependence), and then sum over \(k_\perp\) to get the local GF. For hypercubic TB lattice the dispersion is \(\epsilon_k = -2\gamma \cos(k_x) + \epsilon(k_\perp)\). Then adding \(\epsilon(k_\perp)\) to the on-site energy of the 1-d tight-binding chain and carrying out the 1-d Dyson’s equation in the previous section, we obtain the GF \(G^r_{k_\perp,\text{loc}}(\omega)\). By summing over \(k_\perp\) in the \(d - 1\) dimensional Brillouin zone, we get the full local GFs
\[
G^r_{\text{loc}}(\omega) = \int_{\text{BZ}} \frac{d^{d-1}k_\perp}{(2\pi)^{d-1}} G^r_{k_\perp}(\omega) = \int d\epsilon_\perp D_{d-1}(\epsilon_\perp) G^r_{\epsilon,\text{loc}}(\epsilon_\perp,\omega),
\] (18)
with the $d−1$ dimensional DoS $D_{d−1}(\epsilon_\perp)$. The Weiss-field GFs are obtained via Eqs. (10,17).

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