Electric field-driven Mott transition: The role of phonons in strongly correlated systems out of equilibrium

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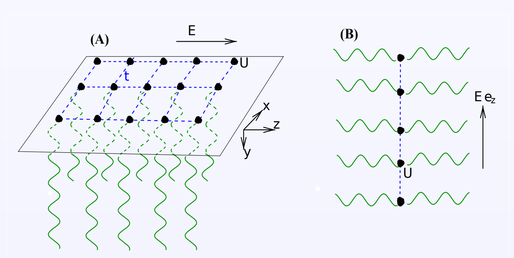
Motivation



Figures (A) and (B). Phonons (green wiggly lines) draining heat perpendicular to the electric field.

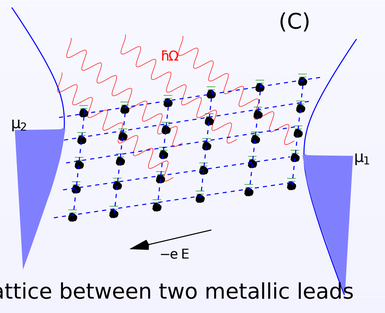
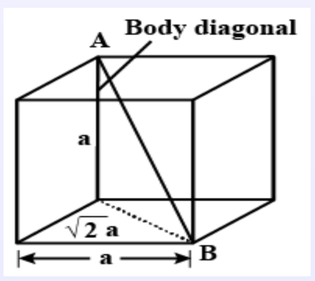


Figure (C). Lattice between two metallic leads

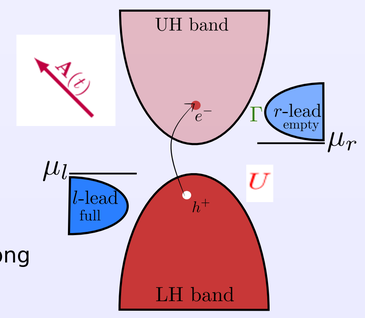
- Electric field-driven Mott transitions: strongly correlated systems turning from insulating- to metallic-behavior due to static electric field [1][2].
- Main questions. Can we use phonons to drain Joule heat? Which approximation do we stick to? Are "bare" phonons (NSCMA) well suited for dissipation or do we need more sophistication (RPA)?

Electronic reservoirs [3]



Simple cubic lattice. Electric field along direction (1,1,1).

Lower- and upper-Hubbard bands



Joule heat gets dissipated by metallic leads

$$\hat{H}_c(t) = -t_c \sum_{<i,j>\sigma} e^{-i\mathbf{A}(t)\cdot(\mathbf{R}_j - \mathbf{R}_i)} \left(\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + h.c.\right) + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

$$H_{coupling} = \sum_{i\in layer,\sigma} v_l(f^\dagger_{l_i,\sigma}c_{i,\sigma}) + v_r(f^\dagger_{r_i,\sigma}c_{i,\sigma}) + h.c$$

$$H_\gamma = -t_\gamma \sum_{<ij>,\sigma} f^\dagger_{i,\sigma}f_{j,\sigma} + \varepsilon_\gamma \sum_i f^\dagger_i f_i, \quad \gamma \in \{l, r\}, \qquad \Gamma \equiv \frac{|v|^2}{t_\gamma}$$

- Generalization to d-dimensional Hubbard lattices coupled to metallic leads with different chemical potentials. A static electric field is turned on according to $\mathbf{A}(t) = A(t)\,(1, 1, \dots 1)$ and $A(t) = -Et$

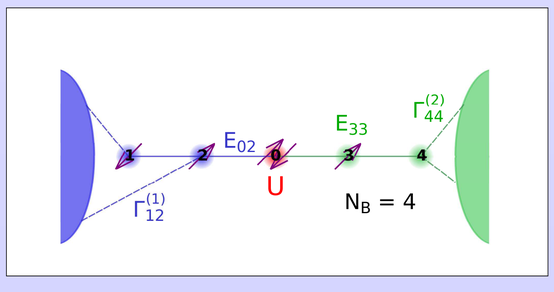
Floquet-DMFT procedure [4][5]

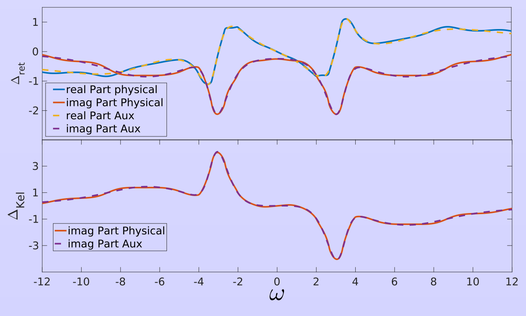
- Floquet representation of Nonequilibrium Green's Functions:
  - $\underline{G}_{mn}(\omega) = \int_{-\infty}^{+\infty} dt_{\rm rel} \frac{1}{\tau} \int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} dt_{\rm av} e^{{\rm i}(\omega + \frac{m+n}{2})t_{\rm rel}} e^{{\rm i}(m-n)\Omega t_{\rm av}} \underline{G}(t,t'),\ -\Omega/2 \le \omega \le \Omega/2, \quad m,n \in \mathbb{Z} \qquad \underline{G} = \begin{pmatrix} G^{\rm R} & G^{\rm K} \\ 0 & G^{\rm A} \end{pmatrix}$
- Interacting Green's Function of the central correlated layer:
  - $\underline{G}^{-1}_{{\rm ph},mn}(\omega_n, \boldsymbol{k}_{||}) = \underline{g}^{-1}_{{\rm ph},mn}(\omega_n, \boldsymbol{k}_{||}) - \underline{\Delta}_{{\rm ph},mn}(\omega, \boldsymbol{k}_{||}) - \underline{\Sigma}_{{\rm ph},mn}(\omega_n, \boldsymbol{k}_{||}), \qquad \omega_n = \omega + n\Omega$

    $\underline{\Sigma}_{{\rm ph},mn}(\omega_n, \boldsymbol{k}_{||}) = \underline{\Sigma}_{{\rm imp},mn}(\omega_n)$ DMFT approximation
- Mapping to the impurity problem:
  - Impurity hybridization function: $\underline{\Delta}^{-1}_{{\rm imp},mn}(\omega_n) = \underline{g}^{-1}_{{\rm imp},mn}(\omega_n) - \underline{G}^{-1}_{{\rm imp},mn}(\omega_n) - \underline{\Sigma}_{{\rm imp},mn}(\omega_n)$
- A time-independent hybridization function is needed to use AMEA [4][5] as impurity solver. Therefore:
  - Floquet Diagonal Self-energy Approximation (FDSA): $\underline{\Sigma}_{{\rm imp},mn}(\omega_n) = \underline{\Sigma}_{\rm imp}(\omega_n)\delta_{mn}$
- Finally, time-average over a period and mapping to the auxiliary problem

Auxiliary Master Equation Approach (AMEA) [6][7]

- It is a nonperturbative nonequilibrium impurity solver that has a controlled and systematically improvable accuracy and is valid, in principle, for both strong and weak interactions and impurity hybridizations
- It maps the impurity system to an auxiliary open quantum system described by Lindblad equation for reduced density matrix operator ρ





Lindblad equation:

Unitary part: $\mathcal{L}_H\rho = -i[H,\rho], \quad H = \sum_{ij,\sigma} E_{ij} d^\dagger_{i,\sigma} d_{j,\sigma} + \frac{U}{2}\sum_\sigma n_\sigma n_{\bar\sigma}$

Dissipator: $\mathcal{L}_D\rho = \sum_{ij,\sigma}\left[\Gamma^{(1)}_{ij}(d^\dagger_{i,\sigma}\rho d_{j,\sigma} - \frac{1}{2}\{d^\dagger_{i,\sigma}d_{j,\sigma},\rho\}) + \Gamma^{(2)}_{ij}(d_{i,\sigma}\rho d^\dagger_{j,\sigma} - \frac{1}{2}\{d_{i,\sigma}d^\dagger_{j,\sigma},\rho\})\right]$

Parameters E_{ij}, $\Gamma^{(1)}_{ij}$ and $\Gamma^{(2)}_{ij}$ determined by a fit of $\underline{\Delta}_{\rm aux}(\omega) \approx \underline{\Delta}_{\rm ph}(\omega)$

Overall accuracy of the method is determined by how well $\underline{\Delta}_{\rm aux}(\omega)$ mimics $\underline{\Delta}_{\rm ph}(\omega)$

Electron-phonon interaction [8]

- Insertion of Holstein (local, i.e. no dispersion) phonons in the lattice Hamiltonian:
  - $H_{\rm ph} = \omega_0 \sum_i a^\dagger_i a_i$
  - $H_{\text{e-ph}} = g\sum_i (a_i + a^\dagger_i)(n_{i,\uparrow} + n_{i,\downarrow} - \alpha)$

Dyson equation in frequency domain - electronic bath

$$\left[\mathbf{G^{-1}}(\omega,\mathbf{k})\right]_{mn} = \left[\mathbf{G_0^{-1}}(\omega,\mathbf{k})\right]_{mn} - \delta_{mn}\left(\left[\mathbf{\Sigma^{(el)}}(\omega)\right]_m + \Gamma\left[\mathbf{g_{bath}}(\omega)\right]_m\right)$$

Both ***electron*** and *phonon* self-energies are ***k-independent*** (**DMFT**) and diagonal in Floquet matrix indices

Dyson equation in frequency domain - heat dissipation by phonons

$$\left[\mathbf{G^{-1}}(\omega,\mathbf{k})\right]_{mn} = \left[\mathbf{G_0^{-1}}(\omega,\mathbf{k})\right]_{mn} - \delta_{mn}\left(\left[\mathbf{\Sigma^{(el)}}(\omega)\right]_m + \left[\mathbf{\Sigma^{(el-ph)}}(\omega)\right]_m\right)$$

Isolated lattice Retarded Green's Function

$$\left[\mathbf{G_0^{-1}}(\omega,\mathbf{k})\right]^R_{mn} = \omega - \varepsilon_0 + i\eta - (\epsilon_{\mathbf{k}})_{m-n}$$

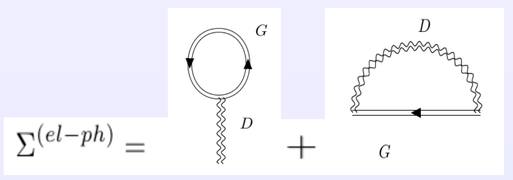
Simple cubic Floquet dispersion relation

$$(\epsilon_{\mathbf{k}})_{m-n} = \frac{1}{2}\left[(\epsilon^{sc}_{\mathbf{k}} + i\,\bar\epsilon^{sc}_{\mathbf{k}})\,\delta_{m-n,1} + (\epsilon^{sc}_{\mathbf{k}} - i\,\bar\epsilon^{sc}_{\mathbf{k}})\,\delta_{m-n,-1}\right]$$

$$\epsilon^{sc}_{\mathbf{k}} = -2t\sum_{\alpha=1}^{d} cos(k_\alpha) \qquad \bar\epsilon^{sc}_{\mathbf{k}} = -2t\sum_{\alpha=1}^{d} sin(k_\alpha)$$

Out of equilibrium a *sine-like* contribution is added to the equilibrium *cosine-like* dispersion.

Migdal Approximation [8] - A first-order expansion in the phonon propagator



Migdal approximation involves only ***Hartree*** (left) and ***Fock*** (right) ***diagrams*** for ***electron-phonon Self-Energy***

Hartree diagram is a ***mean field*** contribution. It is an overall ***energy-shift***.

Non Self-Consistent Migdal Approximation (NSCMA) [8]

Zero-th order truncation for phonon propagator.

- ***Only electrons*** treated ***dynamically*** - "***bare***" ***phonon*** propagator.
- ***No feedback*** from electrons to phonons.

Self-Consistent Migdal Approximation (RPA)

Exact expansion for phonon propagator.

- Both ***electrons*** and ***phonons*** treated ***dynamically***.
- ***Feedback effect*** from electrons to phonons - ***phonon*** propagator is "***dressed***" by electron Green's Function.

Goals

- Investigating the role of phonons as major dissipation mechanism of heat induced by a steady-state current.
- Investigating the effect of electron-phonon interaction: "undressed" phonons vs RPA treatment.

Further developments and applications

- Migdal approximation ("bare" or RPA) applied to overcome the need for *ad hoc* fermionic baths to address the steady-state resistive switch Mott transition [1].

Technical extensions of AMEA

- Development of AMEA-DMFT impurity solver including electron-phonon interaction nonperturbatively.
- Implementation of quantum jump solution of auxiliary Lindblad problem [9] for electron-phonon interaction.
- Full Floquet AMEA-DMFT impurity solver
  - Going beyond diagonal Self-Energies (FDSA)
  - Addressing correlated quantum dots or molecular electronics
- Extension to multi-orbital correlated impurities
  - Multi-orbital DMFT is necessary to address more realistic models or materials

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