Real Time Green's Functions from NCA based Impurity Solver

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Introduction

Strongly correlated materials.

- Idea of description of electrons in solids as independent particles
  $\rightarrow$ wave-like picture
- Materials in which electrons tend to *localize*
  $\rightarrow$particle-like picture
- Strong electronic correlations brings out a variety of phenomena, e.g. metal-to-Mott-insulator transitions

Description of the lattice

Hubbard model.

$$H_{\text{Hubbard}} = -\sum_{\langle i,j\rangle,\sigma} v_{ij} d^\dagger_{i\sigma} d_{j\sigma} + \sum_i U(d^\dagger_{i\uparrow} d_{i\uparrow} - \frac{1}{2})(d^\dagger_{i\downarrow} d_{i\downarrow} - \frac{1}{2})$$

- $v_{ij} \simeq$ overlap between orbitals on neighbouring atomic sites $\sim$ eV
- Coulomb repulsion U, screened value $\sim$ eV

$\rightarrow$ competition between energy scales

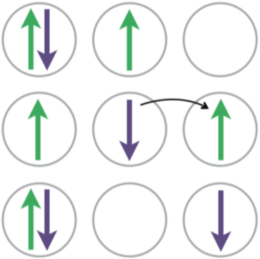

Figure: Lattice model

source: H. Aoki, N. Tsuji, M. Eckstein, M. Kollar, T. Oka, and P. Werner, Rev. Mod. Phys. 86, 779 (2014)

Dynamical Mean Field Theory

Idea of mapping.

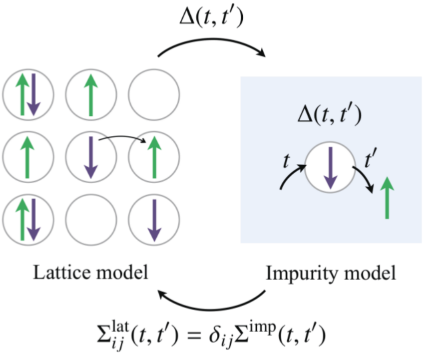

Figure: Mapping of the lattice problem onto an Impurity problem

- Approximate lattice problem with many degrees of freedom by *single-site problem*

Dynamical Mean Field Theory

Set of self-consistent equations.

- compute local Greens function $G^{\sigma}_{ii}(t-t') = -i\langle \mathscr{T} d_{i\sigma}(t) d^{\dagger}_{i\sigma}(t')\rangle$ from an effective impurity model with action

$$S = i\int_c dt U n_{\uparrow}(t) n_{\downarrow}(t) - i\sum_{\sigma}\int_c dt dt' d^{\dagger}_{\sigma}(t) \triangle(t-t') d_{\sigma}(t').$$

- use impurity self energy, defined via $G^{-1}_{ii}(\omega) = \omega + \mu - \triangle(\omega) - \Sigma^{imp}(\omega)$, to obtain the lattice Greens function

$$G^{-1}_{ij}(\omega) = \delta_{ij}[\omega + \mu - \Sigma_{ii}(\omega)] - v_{ij}$$

$$\Sigma_{ii}(\omega) \simeq \Sigma_{imp}(\omega); \Sigma_{i\neq j}(\omega) \simeq 0$$

- average over the Brillouin zone to get the on-site component:

$$G_{ii}(\omega) = \frac{1}{L}\sum_k G_k(\omega) = \frac{1}{L}\sum_k \frac{1}{\omega + \mu + \Sigma(\omega) - \varepsilon_k}$$

Dynamical Mean Field Theory

Set of self-consistent equations.

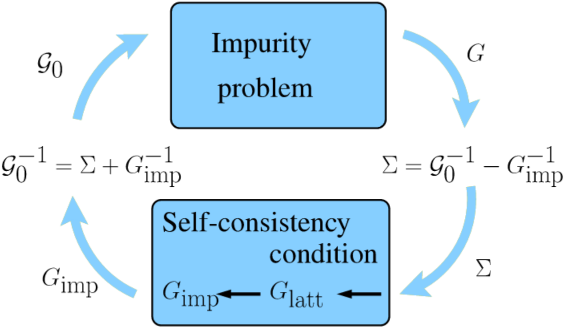

Figure: DMFT iterative loop

source: B. Amadon, Journal of Physics: Condensed Matter, Volume 24, Number 7

Real Time Impurity Solver

Pertubative expansion.

Single-orbital Anderson impurity model

$$H_{imp} = H_{loc} + H_{bath} + H_{hyb}$$

$$H_{loc} = \sum_{\sigma \in \uparrow,\downarrow} \varepsilon_\sigma d_\sigma^\dagger d_\sigma + U(n_\uparrow - \frac{1}{2})(n_\downarrow - \frac{1}{2})$$

$$H_{bath} = \sum_{\sigma,\lambda} \varepsilon_\lambda b_\lambda^\dagger b_\lambda$$

$$H_{hyb} = \sum_{\sigma,\lambda} (v_{\sigma\lambda} b_\lambda^\dagger d_\sigma + v_{\sigma\lambda}^* d_\sigma^\dagger b_\lambda)$$

- Write impurity Hamiltonian as a sum $H_{imp} = H_0 + H_{int}$
- Exact time evolution for H_0, pertubative expansion for H_{int}

Real Time Impurity Solver

Calculation of expectation values.

- Goal is to evaluate objects like $G^{\prec}(t,t') = i\langle d^{\dagger}(t')d(t)\rangle$ and $G^{\succ}(t,t') = -i\langle d(t)d^{\dagger}(t')\rangle$
- Expectation values are given by $\langle O(t)\rangle = \mathrm{Tr}\left(\rho U^{\dagger}(t)\hat{O}U(t)\right)$
- Interaction picture propagator $U(t) = \exp^{iH_0 t}\exp^{-iHt}$ and operator $\hat{O}(t) = \exp^{iH_0 t}\, O \exp^{-iH_0 t}$
- Reduced Hamiltonian $H_0 = H_{\mathrm{Imp}} - H_{\mathrm{Hyb}}$

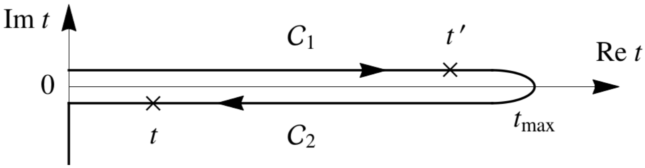

Figure: Keldysh Contour

source: H. Aoki, N. Tsuji, M. Eckstein, M. Kollar, T. Oka, and P. Werner, Rev. Mod. Phys. 86, 779 (2014)

Real Time Impurity Solver

Hybridization expansion.

- Expansion of $\mathrm{U(t)}$ and $\mathrm{U^\dagger(t)}$ in terms of $\widehat{\mathrm{H}}_{\mathrm{hyb}}$:

$$\mathrm{U(t)} = \sum_{\mathrm{n=0}}^{\infty} (-\mathrm{i})^{\mathrm{n}} \int_0^{\mathrm{t}} \mathrm{dt_1} \int_0^{\mathrm{t_1}} \mathrm{dt_2} \cdots \int_0^{\mathrm{t_{n-1}}} \mathrm{dt_n} \widehat{\mathrm{H}}_{\mathrm{hyb}}(\mathrm{t_1}) \widehat{\mathrm{H}}_{\mathrm{hyb}}(\mathrm{t_2}) \cdots \widehat{\mathrm{H}}_{\mathrm{hyb}}(\mathrm{t_n})$$

- Insert expansion for $\mathrm{U(t)}$ into propagator between many body states:

$$\mathrm{G}_{\alpha\beta}(\mathrm{t}) = \langle\langle \alpha \mid \rho_{\mathrm{D}} \exp^{-\mathrm{iHt}} \mid \beta \rangle\rangle_{\mathrm{B}} = \langle\langle \alpha \mid \rho_{\mathrm{D}} \exp^{-\mathrm{iH_0 t}} \mathrm{U(t)} \mid \beta \rangle\rangle_{\mathrm{B}}$$

- many body states are $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$

- $\langle \cdots \rangle_{\mathrm{B}} = \mathrm{Tr}\{\rho_{\mathrm{B}} \cdots\}$

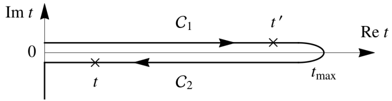

Figure: Keldysh Contour

Real Time Impurity Solver

Hybridization expansion.

$$G_{\alpha\beta}(t) = G^{(0)}_{\alpha\beta}(t) - \sum_{\gamma\delta} \int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_{\alpha\beta}(t-t_1) G^{(0)}_{\gamma\delta}(t_1-t_2) \triangle^{\gamma\delta}_{\alpha\beta}(t_1-t_2) G^{0}_{\alpha\beta}(t_2) - \cdots$$

with bare propagators

$$G^{(0)}_{\alpha\beta}(t) = \langle\langle \alpha \mid \rho_D \exp^{-iH_0 t} \mid \beta \rangle\rangle_B = \delta_{\alpha\beta} \exp^{-i\varepsilon_\alpha t}$$

and Hybridization

$$\begin{aligned} \triangle^{\gamma\delta}_{\alpha\beta}(t_1-t_2) = \langle \alpha \mid d_\sigma \mid \beta \rangle \langle \beta \mid d^\dagger_\sigma \mid \alpha \rangle \triangle^{\prec}(t_1-t_2) + \\ \langle \alpha \mid d^\dagger_\sigma \mid \beta \rangle \langle \beta \mid d_\sigma \mid \alpha \rangle \triangle^{\succ}(t_1-t_2) \end{aligned}$$

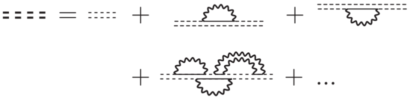

Figure: Example of diagrammatic expansion for bold propagators

Real Time Impurity Solver

Hybridization expansion.

Dyson equation

$$G_{\alpha\alpha}(t) = G^{(0)}_{\alpha\alpha}(t) + \int_0^t dt_1 \int_0^{t_1} dt_2 G^{(0)}_{\alpha\alpha}(t-t_1)\Sigma_{\alpha\alpha}(t_1-t_2)G_{\alpha\alpha}(t_2)$$

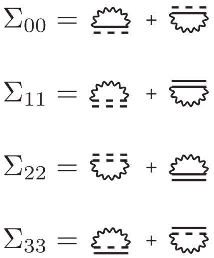

Figure: NCA self-energy

Self-consistent solution

1. Initialize $G_{\alpha\alpha}(t)$ with $G^{(0)}_{\alpha\alpha}(t)$
2. Compute self-energy $\Sigma_{\alpha\alpha}(t)$
3. Update $G_{\alpha\alpha}(t)$
4. go back to step 2

source: G. Cohen, D. R. Reichman, A. J. M. and E. Gull; Phys. Rev. B89, 112139(2014)

Real Time Impurity Solver

Hybridization expansion.

Vertex functions

$$K_{\alpha\beta}(t,t') = K^{(0)}_{\alpha\beta}(t,t') + \sum_{\gamma\delta}\int_0^t dt_1 \int_0^{t'} dt_2 K_{\alpha\gamma}(t_1,t_2) \triangle_{\gamma\delta}(t_1,t_2) K_{\delta\beta}(t-t_1,t'-t_2).$$

$$K^{(0)}_{\alpha\beta}(t,t') = G^{\dagger}_{\alpha\beta}(t) G_{\alpha\beta}(t')$$

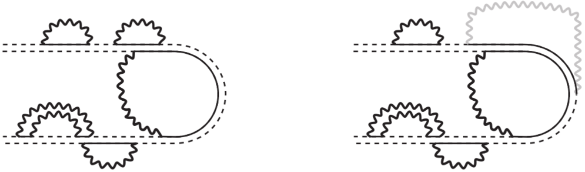

Figure: Diagrammatic expansion for Vertex functions

source: G. Cohen, D. R. Reichman, A. J. M. and E. Gull; Phys. Rev. B89, 112139(2014)

Results

Bethe lattice.

Self-consistency equation for Bethe lattice

$$\triangle(t-t') = v^2 G(t-t')$$

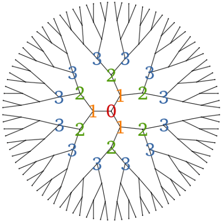

Figure: Bethe lattice

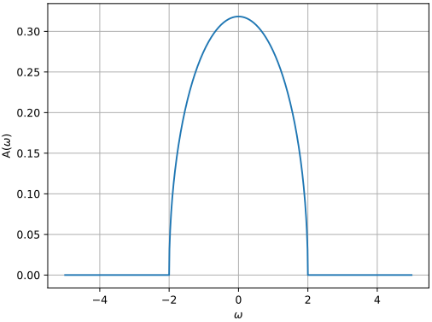

Figure: semicircular Density of States for Bethe lattice

Results

Spectral function for Bethe lattice with increasing interaction strength.

- Single particle spectral function $\mathrm{A}(\omega) = -\frac{1}{\pi}\mathrm{Im}\mathrm{G}^{\mathrm{r}}(\omega)$ represents the density of single-particle excitations at energy ω
- $\mathrm{G}^{\mathrm{r}}(\mathrm{t},\mathrm{t}') = \Theta(\mathrm{t}-\mathrm{t}')(\mathrm{G}^{\succ}(\mathrm{t},\mathrm{t}') - \mathrm{G}^{\prec}(\mathrm{t},\mathrm{t}'))$

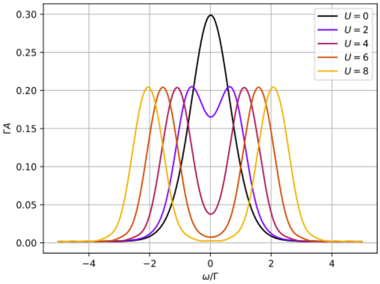

Figure: Spectral function for $\beta = 10$ and $\Gamma\mathrm{t} = 4$

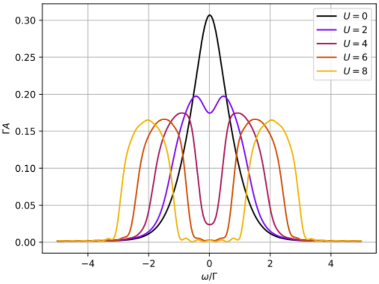

Figure: Spectral function for $\beta = 10$ and $\Gamma\mathrm{t} = 8$

Results

Limiting cases.

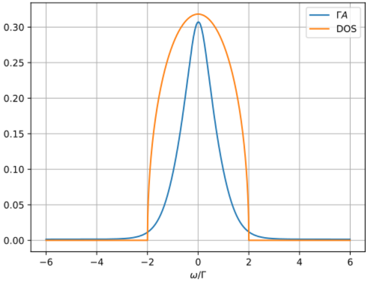

Figure: Spectral function for $\mathrm{U} = 0$, $\beta = 10$ and $\Gamma \mathrm{t} = 10$

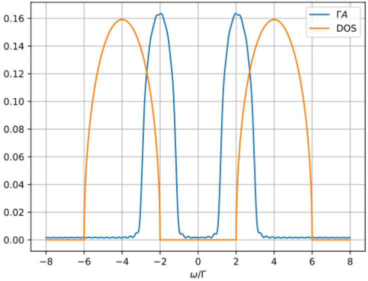

Figure: Spectral function for $\mathrm{U} = 8\Gamma$, $\beta = 10$ and $\Gamma \mathrm{t} = 10$

Results

Dependence on the initial state.

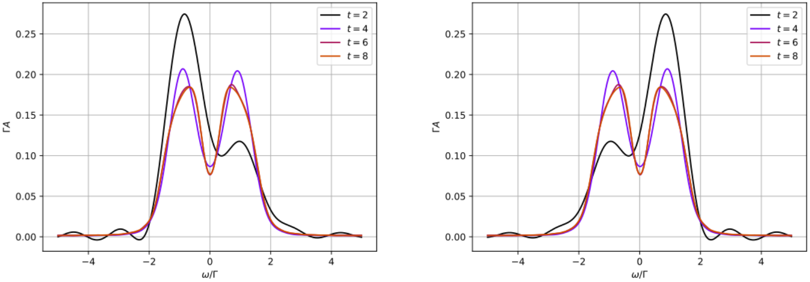

Figure: Spectral function for the inital dot state$|0\rangle$[left] and $|\uparrow\downarrow\rangle$[right]. The parameters areU $= 3\Gamma$, $\Gamma\beta = 1$

Results

Kondo physics.

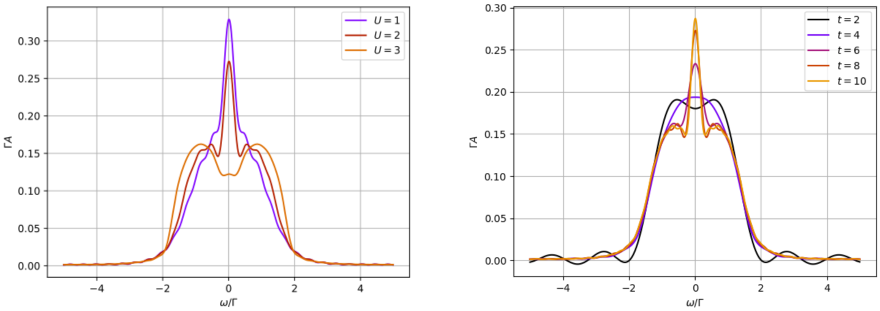

Figure: left: Kondo physics for parameters $\Gamma\beta = 16$, $\Gamma \mathrm{t} = 8$ right: Kondo peak for different timescales with parameters $\mathrm{U} = 2\Gamma$, $\Gamma\beta = 16$

Outlook

1. Apply a spatially homogeneous time-dependent electric field F(t) using a gauge with pure vector potential A(t)

- time-dependent hopping $v_{ij} \rightarrow v_{ij}(t) = v_{ij}^{0} \exp^{ie(R_j - R_i)A(t)}$
  - Self-consistency equation for Bethe lattice $\triangle(t,t') = v(t)G(t,t')v(t')$

1. Extention to an arbitrary lattice
2. Replace single-site by 4x4 cluster