

JOURNEY FROM THE HUBBARD DIMER TO THE HUBBARD MODEL

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OVERVIEW OF THE PROCESS

- Choose correlated Anderson model as the auxiliary model and perform URG analysis and extract zero mode to obtain Hubbard dimer as the effective low energy Hamiltonian.
- Translate this Hubbard dimer Hamiltonian to recreate a new/renormalized Hubbard model. This Hubbard model is assumed to be linked to the parent Hubbard model via a similarity transformation.
- Express equation between renormalized Hubbard and Hubbard dimers as relation between inverse Greens function matrix elements of full Hubbard model and those of the Hubbard dimer.
- Obtain Greens functions of the parent Hubbard model in terms of those of the Hubbard dimer.

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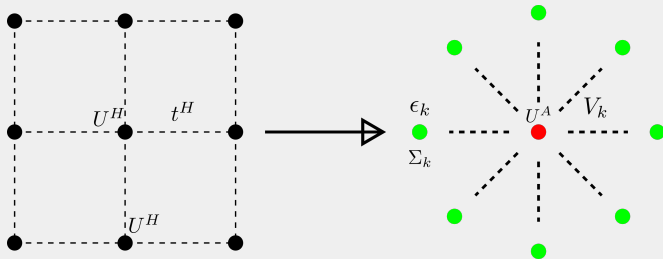
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CLUSTER-BATH APPROACH



$$H^H = -t^H \sum_{\sigma, \langle i,j \rangle} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) + U^H \sum_i \tau_{i\uparrow} \tau_{i\downarrow}$$

$$H^A = \sum_{k\sigma} \tilde{\epsilon}_k \tau_{k\sigma} + U^A \tau_{d\uparrow} \tau_{d\downarrow} + U_b \sum_{kk'} \hat{n}_k \hat{n}_{k'}$$

$$-t^A \sum_{k\sigma} \left(c_{d\sigma}^\dagger c_{k\sigma} + \text{h.c.} \right)$$

RG ANALYSIS OF AUXILIARY SYSTEM

$$\sum_{k\sigma} \tilde{\epsilon}_k \tau_{k\sigma} + U \tau_{d\uparrow} \tau_{d\downarrow} + U_b \sum_{kk'} \hat{n}_k \hat{n}_{k'} - t \sum_{k\sigma} \left(c_{d\sigma}^\dagger c_{k\sigma} + \text{h.c.} \right)$$

$$\downarrow U H U^\dagger$$

$$\sum_{k\sigma}^* \left[\tilde{\epsilon}_k \tau_{k\sigma} - t^* \left(c_{d\sigma}^\dagger c_{k\sigma} + \text{h.c.} \right) \right] + U^* \tau_{d\uparrow} \tau_{d\downarrow} + U^* \sum_{kk'}^* \hat{n}_k \hat{n}_{k'}$$

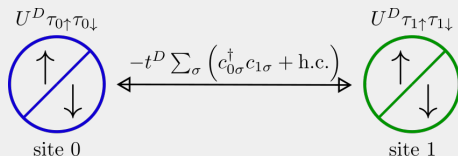
$$\downarrow \text{zero mode}$$

$$-t^* \sum_{\sigma} \left(c_{d\sigma}^\dagger c_{z\sigma} + \text{h.c.} \right) + U^* \tau_{d\uparrow} \tau_{d\downarrow} + U^* \tau_{z\uparrow} \tau_{z\downarrow}$$

RESTORING TRANSLATIONAL INVARIANCE

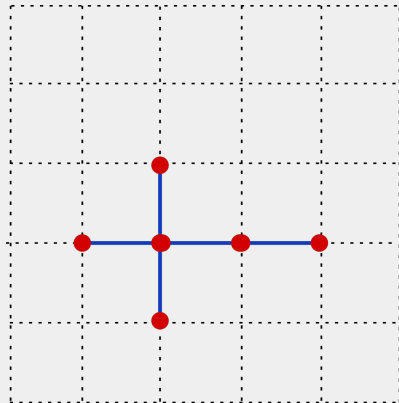
$$\tilde{H}(\tilde{t}, \tilde{U}) = \frac{2}{N_W} \sum_{\langle ij \rangle} H^D(i, j)$$

$$H^D = -t^D \sum_{\sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) + U^D (\tau_{i\uparrow} \tau_{i\downarrow} + \tau_{j\uparrow} \tau_{j\downarrow})$$



$$\tilde{t} \equiv \frac{2}{N_W} t^D, \quad \tilde{U} \equiv \frac{2}{N_W} U^D$$

$$\tilde{H} = \mathcal{U} H^D \mathcal{U}^{-1} \quad \left[\tilde{G}(\tilde{r}, \tilde{r}') = G^H(r, r') \right]$$



INVERSE GREENS FUNCTION FROM HAMILTONIAN

Write equation in terms of inverse Greens function $G^{-1}(\omega) = \omega - H$

$$\begin{aligned}\omega - \tilde{G}^{-1} &= \frac{2}{Nw} \sum_{\langle ij \rangle} [\omega - G_D^{-1}(\omega, i, j)] \\ \longrightarrow \tilde{G}^{-1} &= \frac{2}{Nw} \sum_{\langle ij \rangle} G_D^{-1}(\omega, i, j)\end{aligned}$$

- Take diagonal matrix element $\langle \tilde{i} | G^{-1} | \tilde{i} \rangle$, against excitations above the *exact ground state*. On the RHS, there are w terms that have the index i .

$$(\tilde{G}^{-1})_{\tilde{i}, \tilde{i}} = (G^{-1})_{i, i} = \frac{2}{Nw} \times (G_D^{-1})_{ii} \times w = \frac{2}{N} (G_D^{-1})_{oo} \equiv g_o$$

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- Take nearest-neighbour matrix element $\langle \tilde{i} | \tilde{G}^{-1} | \tilde{j} \rangle$. On the RHS, there's just one term that has both indices i and j .

$$(\tilde{G}^{-1})_{\tilde{i}\tilde{j}} = (G^{-1})_{i,j} = \frac{2}{N_W} \times (G_D^{-1})_{ij} = \frac{2}{N_W} (G_D^{-1})_{01} \equiv g_1$$

INVERSE GREENS FUNCTION FROM HAMILTONIAN

Write equation in terms of inverse Greens function $G^{-1}(\omega) = \omega - H$

$$\omega - \tilde{G}^{-1} = \frac{2}{N_W} \sum_{\langle ij \rangle} [\omega - G_D^{-1}(\omega, i, j)]$$

$$\longrightarrow \tilde{G}^{-1} = \frac{2}{N_W} \sum_{\langle ij \rangle} G_D^{-1}(\omega, i, j)$$

- **All other matrix elements are zero**, because no term in the Hamiltonian scatters between non-nearest-neighbour sites
 \longrightarrow **tri-diagonal inverse Greens function matrix**

DIAGONALIZING THE INVERSE GREENS FUNCTION MATRIX

$$G^{-1} = \begin{pmatrix} g_0 & g_1 & 0 & \dots & g_1 \\ g_1 & g_0 & g_1 & 0 & \dots \\ 0 & g_1 & g_0 & g_1 & \dots \\ 0 & 0 & \dots & \dots & \dots \end{pmatrix} \xrightarrow{\text{Fourier transform to } k\text{-space}} g_0 + g_1 \begin{pmatrix} \xi_{\vec{k}_1} & 0 & 0 & \dots \\ 0 & \xi_{\vec{k}_2} & 0 & \dots \\ 0 & 0 & \xi_{\vec{k}_3} & \dots \\ 0 & 0 & \dots & \dots \end{pmatrix}$$

$$\xi_{\vec{k}} = \sum_{i=1}^w \cos(a_i q_i)$$

DIAGONALIZING THE INVERSE GREENS FUNCTION MATRIX

$$G^{-1} = g_0 + g_1 \begin{pmatrix} \xi_{\vec{k}_1} & & \\ & \xi_{\vec{k}_2} & \\ & & \xi_{\vec{k}_3} \end{pmatrix} \xrightarrow{\text{invert the diagonal matrix}} G = \begin{pmatrix} G_{\vec{k}_1} & & \\ & G_{\vec{k}_2} & \\ & & G_{\vec{k}_3} \end{pmatrix}$$

\vec{k} -space Greens function:
$$G_H(\vec{k}, \omega) = \frac{N}{2} \left\{ [G_D^{-1}(\omega)]_{00} + \frac{1}{W} [G_D^{-1}(\omega)]_{01} \xi_{\vec{k}} \right\}^{-1}$$

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\vec{r} -space Greens function: $G_H(\vec{r}, \omega) = \frac{1}{2} \sum_{\vec{k}} e^{i\vec{k} \cdot \vec{r}} \left\{ [G_D^{-1}(\omega)]_{00} + \frac{1}{W} [G_D^{-1}(\omega)]_{01} \xi_{\vec{k}} \right\}^{-1}$

COMPUTE SINGLE-PARTICLE GREENS FUNCTIONS AND OTHER STUFF

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self-energy: $\Sigma_H(\vec{k}, \omega) = \omega - g_0 + (t^H - g_1) \xi_{\vec{k}}$

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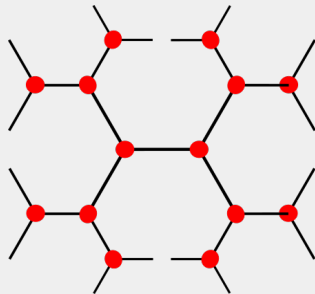
Spectral function: $A_H(\vec{k}, \omega) = -\frac{1}{\pi} \text{Im}(G_H(\vec{k}, \omega)) = -\frac{1}{\pi} \text{Im} [(g_0 + g_1 \xi_{\vec{k}})^{-1}]$

ON THE BETHE LATTICE ($w \rightarrow \infty$)

Hamiltonian scaling arguments suggest ¹

$$G_{ij} = G_{ii}\delta_{ij}$$

(**Greens function becomes local**)



Bethe lattice with $w = 3$

¹Vollhardt, Krzysztof and Marcus, Dynamical Mean-Field Theory, 2012, Springer Berlin Heidelberg

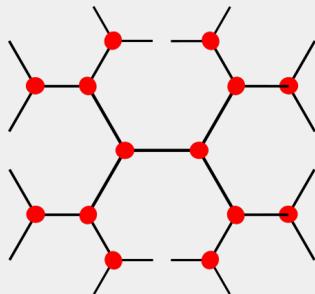
ON THE BETHE LATTICE ($w \rightarrow \infty$)

Also emerges from this formulation:

$$G_{ii}^{-1} = \frac{2}{N} [G_D^{-1}]_{oo} \rightarrow \text{finite}$$

$$\mathbf{G}_{ij}^{-1} = \frac{2}{Nw} [\mathbf{G}_D^{-1}]_{oo} \rightarrow \mathbf{0} \quad \text{when } w \rightarrow \infty$$

G_{ii}^{-1} becomes diagonal $\longrightarrow G_{ij}$ becomes diagonal



Bethe lattice with $w = 3$

CHOOSING GROUND STATE WAVEFUNCTIONS

These are some strategies for choosing the ground state with which to measure the Greens functions:

- Localized limit:

$$|\tilde{o}\rangle = \sum_{\langle ij \rangle} |o_{ij}^D\rangle \otimes |\Phi\rangle$$

- ▶ Simple expressions for g_0 and g_1
- ▶ However, huge loss in entanglement

CHOOSING GROUND STATE WAVEFUNCTIONS

These are some strategies for choosing the ground state with which to measure the Greens functions:

- Compute exact wavefunctions numerically for given values of U^H and t^H :
 - ▶ In principle exact, however size of lattice has to be small to allow exact diagonalization
 - ▶ High accuracy but no analytical insight

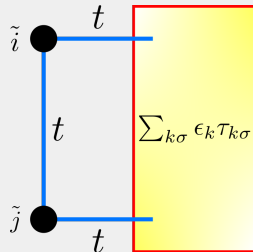
CHOOSING GROUND STATE WAVEFUNCTIONS

These are some strategies for choosing the ground state with which to measure the Greens functions:

- Improve the wavefunction by connecting the Hubbard dimer to a bath:

$$\underbrace{H^D}_{\text{Hubbard dimer}} + \underbrace{\sum_{k\sigma} \epsilon_{k\sigma} \tau_{k\sigma}}_{\text{bath}} - \underbrace{t \sum_{k\sigma} \left(c_{i\sigma}^\dagger c_{k\sigma} + c_{j\sigma}^\dagger c_{k\sigma} + \text{h.c.} \right)}_{\text{bath-dimer hybridisation}}$$

- ▶ Allows systematic improvement by increasing number of momentum states in bath
- ▶ Introduces more entanglement, because the electrons of the dimer can now traverse through the bath
- ▶ Introduces a three peak spectral function , and hence of observing a metal-insulator transition



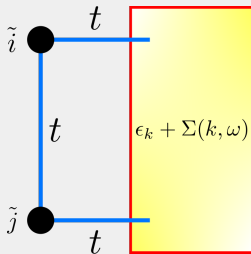
CHOOSING GROUND STATE WAVEFUNCTIONS

These are some strategies for choosing the ground state with which to measure the Greens functions:

- Further improve the wavefunction by introducing self-energy into the bath:

$$\epsilon_k \rightarrow \epsilon_k + \Sigma(k, \omega)$$

- ▶ Singular Σ would introduce gap in bath spectrum and potentially lead to insulating phase
- ▶ Regular Σ (for eg., $\sim \omega^2$) allows low energy excitations and might result in metallic phase
- ▶ Overall, greater control over the physics



FUTURE GOALS

- Obtain expressions for two-particle Greens functions, in order to study holon/doublon excitations
- Recreate the metal-insulator transition, either just from the dispersive bath, or by inserting suitable self-energy $\Sigma(k, \omega)$ in the bath dispersion.
- Once some numerical accuracy is achieved, we can extend the method to other strongly-correlated models like the Heiseberg model for spins, or the periodic Anderson and Kondo models

Thank you for your attention.