Journey from the Hubbard Dimer to the Hubbard Model

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- 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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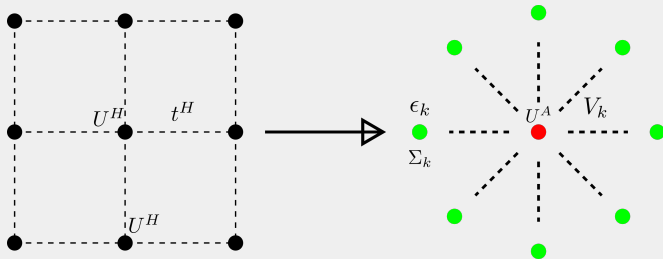
Overview of the Process

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

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

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

$$\downarrow UHU^{\dagger}$$

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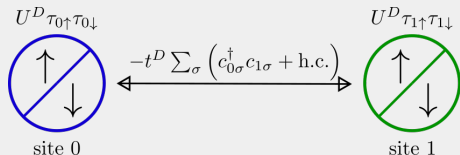
$$\downarrow \text{zero mode}$$

$$-t^* \sum_{\sigma} \left(c_{d\sigma}^{\dagger} c_{z\sigma} + \text{h.c.} \right) + U^* \tau_{d\uparrow}\tau_{d\downarrow} + U^* \tau_{z\uparrow}\tau_{z\downarrow}$$
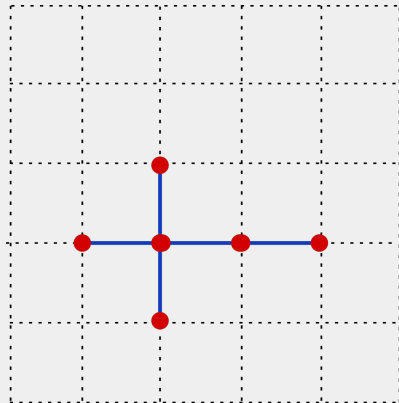
$$\tilde{H}(\tilde{t}, \tilde{U}) = \frac{2}{Nw} \sum_{\langle ij \rangle} H^D(i,j)$$

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

$U^D \tau_{0\uparrow}\tau_{0\downarrow}$

$U^D \tau_{1\uparrow}\tau_{1\downarrow}$

$-t^D \sum_\sigma \left(c_{0\sigma}^\dagger c_{1\sigma} + \text{h.c.} \right)$

site 0

site 1

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

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

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

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

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

- 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.

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

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

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

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

- 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.

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

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

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

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

- **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**

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

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

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

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

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

$\vec{k}$-space Greens function:
$$G_H(\vec{k}, \omega) = \frac{N}{2} \left\{ \left[G_D^{-1}(\omega) \right]_{oo} + \frac{1}{W} \left[G_D^{-1}(\omega) \right]_{o1} \xi_{\vec{k}} \right\}^{-1}$$

$\vec{r}$-space Greens function:
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self-energy:
$$\Sigma_H(\vec{k}, \omega) = \omega - g_o + \left(t^H - g_1 \right) \xi_{\vec{k}}$$

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

Spectral function: $\quad A_H(\vec{k}, \omega) = -\dfrac{1}{\pi} \mathrm{Im}(G_H(\vec{k}, \omega)) = -\dfrac{1}{\pi} \mathrm{Im} \left[(g_o + g_1 \xi_{\vec{k}})^{-1} \right]$

Hamiltonian scaling arguments suggest [1]

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

(**Greens function becomes local**)
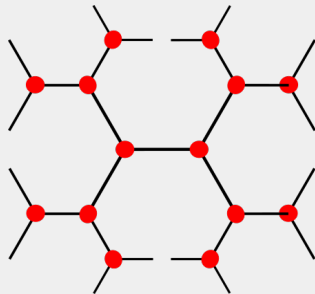
Bethe lattice with $w = 3$

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[1]Vollhardt, Krzysztof and Marcus, Dynamical Mean-Field Theory, 2012, Springer Berlin Heidelberg
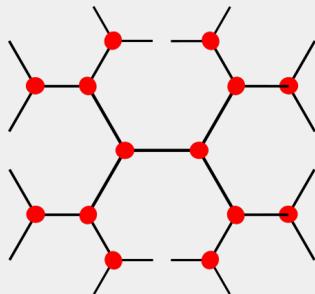
Also emerges from this formulation:

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

$$\mathbf{G_{ij}^{-1} = \frac{2}{Nw} \left[G_D^{-1} \right]_{oo} \to o} \quad \text{when } w \to \infty$$

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

Bethe lattice with $w = 3$

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

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
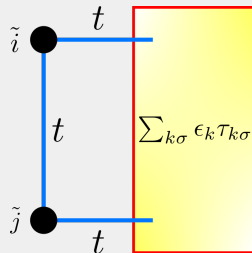 - High accuracy but no analytical insight

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:

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

- ▶ 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 introducint 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
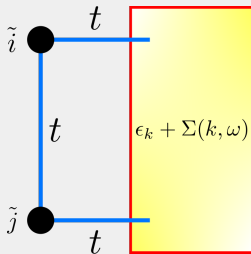
FUTURE GOALS

- 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