Journey from the Hubbard Dimer to the Hubbard Model

Abhirup Mukherjee, Dr. Siddhartha Lal

Department of Physical Sciences
IISER Kolkata

August 13, 2021

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.

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.

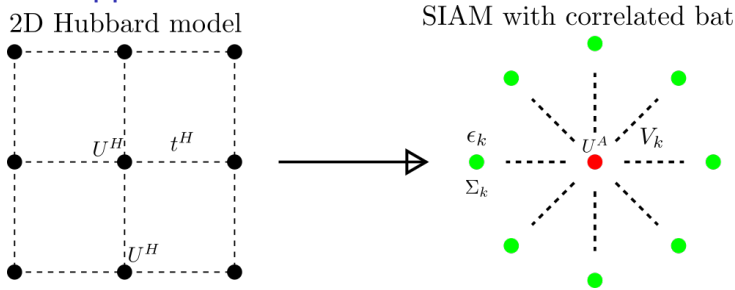
Overview of the Process

- 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.

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.

Auxiliary System Approach



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

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

$$(\tilde{\epsilon}_k = \epsilon_k + \Sigma(k,\omega))$$

RG Analysis of Auxiliary System

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

$$\Big\downarrow \; U_A H^A U_A^\dagger \quad (URG)$$

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

$$(U_b^* = U^{A*})$$

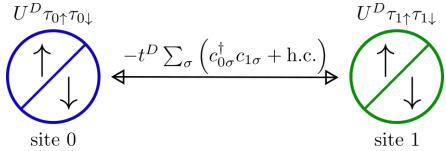
$$\Big\downarrow \; \text{zero mode}$$

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

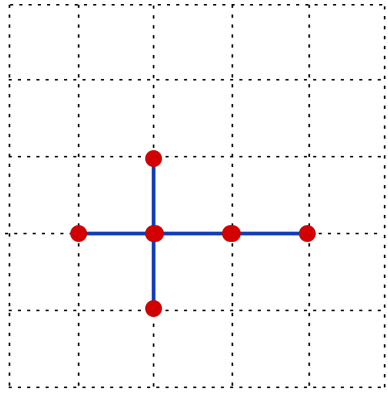
Restoring Translational Invariance

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

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



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



(Tiling 2D square lattice with dimers)
(N sites, w coordination number)

Relating the original and reconstructed Hubbard models

- We chose an auxiliary model appropriate to the original Hubbard model (H^H).
- We then performed the URG on it, and took the zero mode of the stable fixed point theory to obtain a Hubbard dimer.
- Finally, we tiled the 2D square lattice with the dimer to obtain a reconstructed Hubbard model ($\tilde{H}$) with new parameters.

In principle, H^H and $\tilde{H}$ are related via a unitary (or atleast similarity) transformation.

$$\tilde{H} = \mathcal{U} H^H \mathcal{U}^{-1} \quad , \quad \mathcal{U} = TZU_A$$

$$Z: \text{ zero mode projection } , \quad T: \text{ lattice tiling operation}$$

$$\therefore \ \tilde{G}(\tilde{r}, \tilde{r}') = G^H(r, r')$$

$$(\text{where } |\tilde{r}\rangle \equiv \mathcal{U}\,|r\rangle)$$

Inverse Greens function from Hamiltonian

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

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

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

Inverse Greens function from Hamiltonian

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

- Take diagonal matrix element $\langle \tilde{i}| \, G^{-1} \, |\tilde{i}\rangle$, against excitations above the *exact ground state*:

$$|\tilde{i}\rangle \equiv \mathcal{U} \, |i\rangle = \mathcal{U} c_i^\dagger \, |0\rangle$$

On the RHS, there are w terms that have the index i.

$$\left(\tilde{G}^{-1}\right)_{\tilde{i},\tilde{i}} = \left(G^{-1}\right)_{i,i} = \frac{2}{Nw} \times \left(G_D^{-1}\right)_{ii} \times w = \frac{2}{N} \left(G_D^{-1}\right)_{00} \equiv g_0$$

(due to translation invariance)

Inverse Greens function from Hamiltonian

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

- 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.

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

(due to translation invariance)

Inverse Greens function from Hamiltonian

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

- **All other matrix elements are zero**, because no term in the Hamiltonian scatters between non-nearest-neighbour sites
  $\longrightarrow$ **inverse Greens function matrix has contributions only from nearest neighbour sites, and respects the lattice geometry**

Diagonalizing the inverse Greens function matrix

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

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

$k_i \equiv$ projection of $\vec{k}$ on the i^{th} primitive vector, $a_i \equiv$ lattice spacing along i^{th} dimension

$\xi_{\vec{k}}$ arises from lattice geometry and **introduces non-locality in** G^{-1}.

Diagonalizing the inverse Greens function matrix

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

Single-particle Greens functions and related quantities

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

Single-particle Greens functions and related quantities

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

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

Single-particle Greens functions and related quantities

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

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

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

Single-particle Greens functions and related quantities

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

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

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

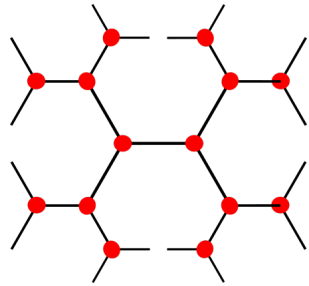
Spectral function: $$A_H(\vec{k},\omega) = -\frac{1}{\pi}\mathrm{Im}(G_H(\vec{k},\omega)) = -\frac{1}{\pi}\mathrm{Im}\left[(g_0 + g_1\xi_{\vec{k}})^{-1}\right]$$

On the Bethe Lattice ($w \to \infty$)

Hamiltonian scaling arguments suggest [1]

$$t^H \to t^H/\sqrt{w}$$

- In an auxiliary model treatment of the Hubbard model on this lattice, **there is only one (direct) path linking the impurity to a given neighbouring bath site.**
- This ensures that the impurity self-energy is related **simply to the local part of the bath Greens function.**



Bethe lattice with $w = 3$

No non-trivial loops on this lattice. Any pair of sites (i, j) are only connected via a direct path (if it exists).

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

On the Bethe Lattice ($w \to \infty$)

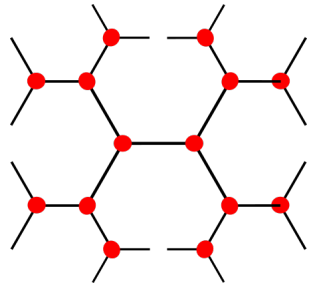
A locality also emerges from our formulation:

$$G_{ii}^{-1} = \frac{2}{N}\left[G_D^{-1}\right]_{00} \to \text{finite}$$

$$\mathbf{G_{ij}^{-1} = \frac{2}{Nw}\left[G_D^{-1}\right]_{00} \to 0} \quad \text{when } w \to \infty$$

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

$$\Sigma_H(\vec{k}, \omega) \to \omega - g_0 + t^H \xi_{\vec{k}}$$



Bethe lattice with $w = 3$

No non-trivial loops on this lattice. Any pair of sites (i, j) are only connected via a direct path (if it exists).

[0] Vollhardt, Krzysztof and Marcus, Dynamical Mean-Field Theory, 2012, Springer Berlin Heidelberg

Choosing ground state wavefunctions

Note that our formulation is in principle exact if we use the exact ground state eigenfunction of the Hubbard model. Putting this into practice is however difficult.

Choosing ground state wavefunctions

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

$$|\tilde{0}\rangle = \sum_{\langle ij \rangle} |0_{ij}^{D}\rangle \otimes |\Phi\rangle$$

  - Analytic expressions for g_0 and g_1
  - However, reduction of many-particle entanglement to only short-ranged

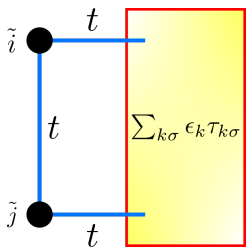
Choosing ground state wavefunctions

- 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 (or any other numerical method)
  - 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:

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

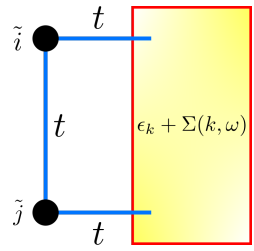


- Allows systematic improvement by increasing number of momentum states in bath
- Introduces more entanglement, because the electrons of the dimer can now traverse through the bath
- Introduces a three peak spectral function , and hence of observing a metal-insulator transition

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:

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



  - 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 for the Hubbard model on (say) the 2D square lattice 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.