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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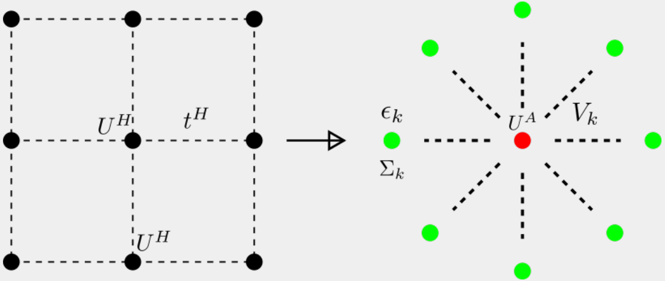


$$-t^H \sum_{\sigma,\langle i,j\rangle} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} \right) + U^H \sum_i \tau_{i\uparrow}\tau_{i\downarrow}$$

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

RG Analysis of Auxiliary System

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

$$\Big\downarrow UHU^\dagger$$

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

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

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

Lattice of N sites and Z nearest neighbours at each site

$$H = -t^H \sum_{\langle ij \rangle} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} \right) + \sum_i U^H \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu^H \hat{N}$$

- For particle-hole symmetry, choose $U^H = \frac{1}{2}\mu^H$
- Define $\tau = \hat{n} - \frac{1}{2}$.

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

RG Analysis of Auxiliary System

- Express entire thing in terms of nearest-neighbour pairs

$$= -t^H \sum_{\langle ij \rangle} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} \right) + \frac{1}{Z} \sum_{\langle ij \rangle} U^H \left[\tau_{i\uparrow}\tau_{i\downarrow} + \tau_{j\uparrow}\tau_{j\downarrow} \right]$$

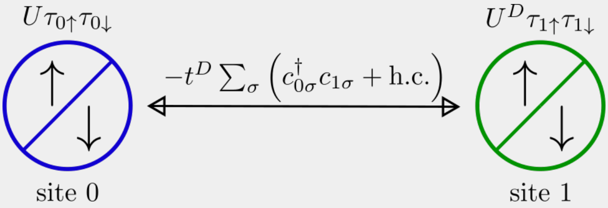
$$= \frac{1}{Z} \sum_{\langle ij \rangle} \left[-Zt^H \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} \right) + U^H \left(\tau_{i\uparrow}\tau_{i\downarrow} + \tau_{j\uparrow}\tau_{j\downarrow} \right) \right]$$

- Since total number of nearest neighbours pairs is $\frac{NZ}{2}$, pull out the same factor

$$H = \frac{2}{NZ} \sum_{\langle ij \rangle} \left[-\frac{NZt^H}{2} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.} \right) + \frac{NU^H}{2} \left(\tau_{i\uparrow}\tau_{i\downarrow} + \tau_{j\uparrow}\tau_{j\downarrow} \right) \right] \tag{1}$$

The final Hamiltonian is a sum of Hubbard dimers

$$H = \frac{2}{NZ}\sum_{\langle ij\rangle} H^D\left(i, j, t^D = \frac{NZt^H}{2}, U^D = \frac{NU^H}{2}\right)$$



$$H^D = -t^D\left(c^\dagger_{0\sigma}c_{1\sigma} + \text{h.c.}\right) + U^D\left(\tau_{0\uparrow}\tau_{0\downarrow} + \tau_{1\uparrow}\tau_{1\downarrow}\right)$$

Inverse Greens function from Hamiltonian

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

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

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

- Take diagonal matrix element $\langle i | G^{-1} | i \rangle$. On the RHS, there are Z terms that have the index i. Because of translational invariance, all such terms will be same.

$$\left(G^{-1}\right)_{ii} = \frac{2}{NZ} \times \left(G_D^{-1}\right)_{ii} \times Z = \frac{2}{N} \left(G_D^{-1}\right)_{oo}$$

Inverse Greens function from Hamiltonian

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

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

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

$$\left(G^{-1}\right)_{ij} = \frac{2}{NZ} \times \left(G_D^{-1}\right)_{ij} = \frac{2}{NZ} \left(G_D^{-1}\right)_{01}$$

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

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

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

- **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

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

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

Diagonalizing the inverse Greens function matrix

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Compute Greens functions and other stuff

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

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

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

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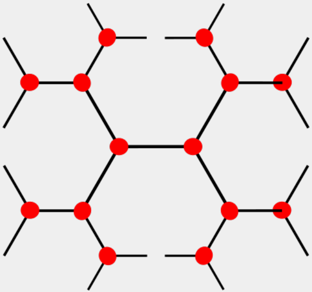
Greens functions give spectral functions as well!

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

Hamiltonian scaling arguments suggest [1]

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

(**Greens function becomes local**)



Bethe lattice with $Z = 3$

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

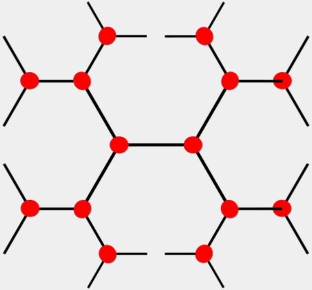
On the Bethe Lattice ($Z \to \infty$)

Also emerges from this formulation:

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

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

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



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