Journey from the Hubbard Dimer to the Hubbard Model

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Overview of the Process

- Rewrite Hubbard Hamiltonian as sum of two-site Hubbard models
- Express Hamiltonian equation as relation between inverse Greens function matrix elements of full Hubbard model and those of the Hubbard dimer
- Use translational invariance and tight-binding nature to construct full inverse Greens function matrix
- Fourier transform inverse Greens function to diagonalize it
- Invert the diagonal matrix to obtain full Greens function matrix in terms of inverse Greens function matrix elements of the dimer

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Lattice of N sites and Z nearest neighburs 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 $\tau = \hat{n} - \frac{1}{2}$.

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

Writing the Hubbard Model Hamiltonian

- Express entire thing in terms of nearest-neighbour pairs

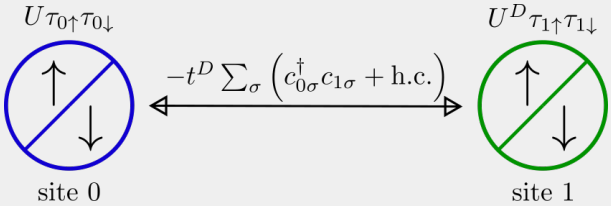
$$
\begin{aligned}
&= -t^H \sum_{\langle ij \rangle} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) + \frac{1}{Z} \sum_{\langle ij \rangle} U^H \left[\tau_{i\uparrow}\tau_{i\downarrow} + \tau_{j\uparrow}\tau_{j\downarrow} \right] \\
&= \frac{1}{Z} \sum_{\langle ij \rangle} \left[-Zt^H \left(c_{i\sigma}^\dagger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

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

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

The final Hamiltonian is a sum of Hubbard dimers

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



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

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.

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

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- 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.

$$\left(G^{-1}\right)_{ij} = \frac{2}{NZ} \times \left(G_D^{-1}\right)_{ij} = \frac{2}{NZ} \left(G_D^{-1}\right)_{\text{o1}}$$

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

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

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

Diagonalizing the inverse Greens function matrix

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

Compute Greens functions and other stuff

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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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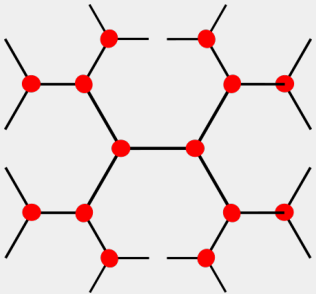
Greens functions give spectral functions as well!

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

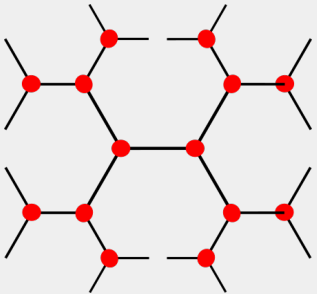
On the Bethe Lattice ($Z \to \infty$)

Also emerges from this formulation:

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

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

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



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