Second quantization and Exact diagonalization

For more info, see Negele, etc Chapter 1 of Quantum Many-Particle Systems

June 3, 2015

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- One could represent the operators in matrix form with a orthonormal basis

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- Normalized state (state to form a orthonoramal basis)
  $|\alpha_1...\alpha_N\rangle = \frac{1}{\sqrt{\prod_\alpha n_\alpha!}} |\alpha_1...\alpha_N\}$

Express many-body operators

- A elegant way to derive the expression is through a basis transformation
- $U = \sum_\alpha U_\alpha n_\alpha = \sum_\alpha U_\alpha c_\alpha^\dagger c_\alpha$ and $\{|\alpha\rangle\} \to \{|\mu\rangle\}$ results $U = \sum_{\lambda\mu} \langle\lambda|U|\mu\rangle c_\lambda^\dagger c_\mu$. For example:

$$T = -\frac{\hbar^2}{2m}\int d^3x \psi^\dagger(x)\nabla^2\psi(x) = \int \frac{d^3k}{(2\pi)^3}\frac{\hbar^2 k^2}{2m} c_k^\dagger c_k$$

$$U = \int d^3x U(x)\psi^\dagger(x)\psi(x) = \int \frac{d^3k}{(2\pi)^3} U_k c_k^\dagger c_k$$

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- $V|\alpha\beta) = V_{\alpha\beta}|\alpha\beta)$ Notice there is no self-interaction. So $V = \frac{1}{2}\sum_{\alpha\beta} n_\alpha(n_\beta - \delta_{\alpha\beta}) = \frac{1}{2}\sum_{\alpha\beta}(\alpha\beta|V|\alpha\beta)a_\alpha^\dagger a_\beta^\dagger a_\beta a_\alpha$
- And a basis change will lead $V = \frac{1}{2}\int d^3xd^3y\psi^\dagger(x)\psi^\dagger(y)V(x-y)\psi(y)\psi(x)$

Construct and Represent Basis

- For either spin $\frac{1}{2}$ or fermionic lattice model, one could use 0 and 1 to describe the local states
- For example, one site Hubbard model, $|n_{\uparrow} n_{\downarrow}\rangle$, we have four states $|0\rangle = 00$;$|\downarrow\rangle = 01$; $|\uparrow\rangle = 10$; $|\uparrow\downarrow\rangle = 11$.
- It is convient to seperate orbitals into two parts according to spin, i.e $|n_{1\uparrow} n_{2\uparrow} ... n_{N\uparrow} n_{1\downarrow} ... n_{N\downarrow}\rangle$
- Use symmetry to block diagonalize the Hamiltonian

Examples (one site Hubbard model)

- $H = Un_\uparrow n_\downarrow - \mu(n_\uparrow + n_\downarrow)$
- Particle conservation: $F = F_0 \oplus F_1 \oplus F_2$
- $F_0 = \{|0\rangle\}$ $H_0 = [0]$
- $F_1 = \{|\uparrow\rangle, |\downarrow\rangle\}$ $H_1 = \begin{bmatrix} -\mu & 0 \\ 0 & -\mu \end{bmatrix}$. (one could further use spin rotation symmetry, or S_z is conserved)
- $F_2 = \{|\uparrow\downarrow\rangle\}$, $H_2 = [U]$

Examples (two sites Hubbard model)

- $H = U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}) - t\sum_\sigma(c^\dagger_{1\sigma}c_{2\sigma} + c^\dagger_{2\sigma}c_{1\sigma}) - \mu N$
- Particle conservation: $F = F_0 \oplus F_1 \oplus F_2 \oplus F_3 \oplus F_4$
- It is trival to consider the zero particle state and one particle state. Also, particle hole symmetry. so does three and four particle state
- There are 4 states with S_z zero $|n_{1\uparrow}n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle$: 1010, 1001, 0110, 0101
- Notice, pay attention to sign for hopping term

Examples (two sites Hubbard model)

- There are 4 states with S_z zero $|n_{1\uparrow}n_{2\uparrow}n_{1\downarrow}n_{2\downarrow}\rangle$: 1010, 1001, 0110, 0101

$$H = \begin{pmatrix} -2\mu + U & -t & -t & 0 \\ -t & -2\mu & 0 & -t \\ -t & 0 & -2\mu & -t \\ 0 & -t & -t & -2\mu + U \end{pmatrix}$$

Examples (two sites Hubbard model)

- One could use translational symmetry to block diagonalize the Hamiltonian, i.e, eigenstates of momentum:

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|1010\rangle - |0101\rangle)$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|1001\rangle - |0110\rangle)$$

$$H = \begin{bmatrix} -2\mu + U & 0 \\ 0 & -2\mu \end{bmatrix}$$

$$E = \{U - 2\mu, -2\mu\}$$

Examples (two sites Hubbard model)

- One could use translational symmetry to block diagonalize the Hamiltonian, i.e, eigenstates of momentum:

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|1010\rangle + |0101\rangle)$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|1001\rangle + |0110\rangle)$$

$$H = \begin{bmatrix} -2\mu + U & -2t \\ -2t & -2\mu \end{bmatrix}$$

$$E = \{\frac{1}{2}\left(-4\mu - \sqrt{16t^2 + U^2} + U\right), \frac{1}{2}\left(-4\mu + \sqrt{16t^2 + U^2} + U\right)\}$$

Examples (two sites Hubbard model)

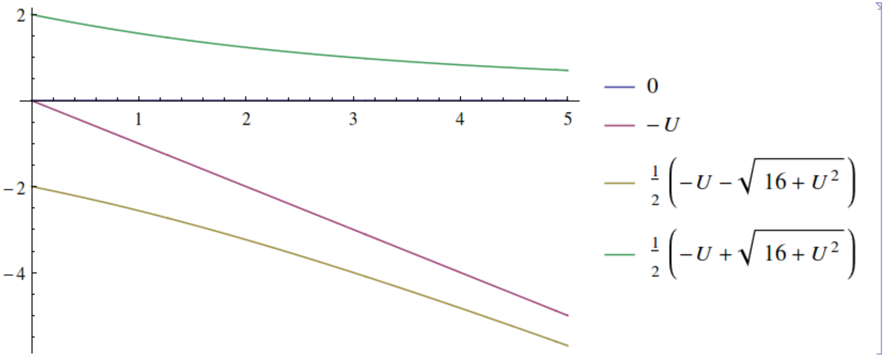

Figure : Two sites Hubbard model (eigenvalues for different U)

Examples (two sites Hubbard model)

- $H = H_0 + \alpha \sum_i S_{iz}$
- For two-particle states, we add more states with $S_z \neq 0$ $|n_{1\uparrow} n_{2\uparrow} n_{1\downarrow} n_{2\downarrow}\rangle$: 1100, 0011 ($S_z = 0$ includes 1010, 1001, 0110, 0101)
- For 1100, 0011, $H = \begin{bmatrix} 2\alpha - 2\mu & 0 \\ 0 & -2\alpha - 2\mu \end{bmatrix}$

Examples (two sites Hubbard model)

- Plot 6 eigenstates

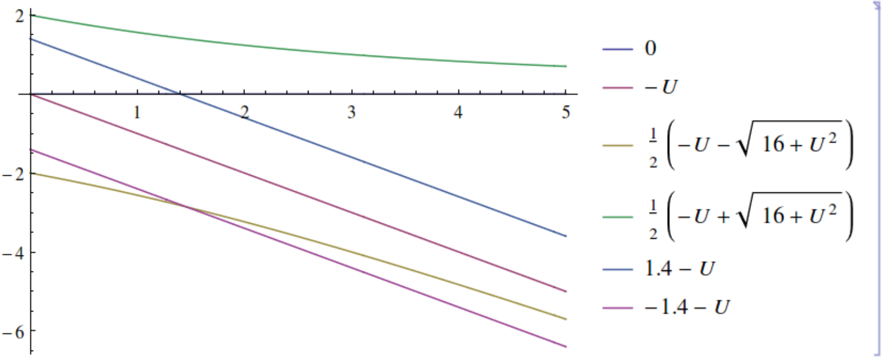

Figure : Two sites Hubbard model (eigenvalues for different U) with magnetic field $\alpha = 0.7$

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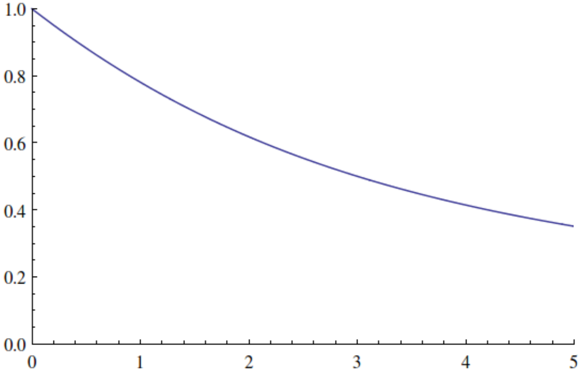

Figure : The critical magnetic field B_c with U. $t = 1$.