Fermionic Hubbard Model for Two-Site System

Shehtab Zaman

May 2017

1 Hubbard Model Hamiltonian for Fermion

$$\mathcal{H} = -t\sum_{\sigma}\left(f^{\dagger}_{1\sigma}f_{2\sigma} + f^{\dagger}_{2\sigma}f_{1\sigma}\right) + U\left(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\right) \tag{1}$$

Where for site i and spin σ, the creation, annihalation and number operators are $f^{\dagger}_{i\sigma}$,$f_{i\sigma}$, $\hat{n}_{i\sigma}$ respectively. The number operator is defined as

$$\hat{n}_{i\sigma} = f^{\dagger}_{i\sigma}f_{i\sigma}$$

2 Fock Space

2.1 Notes on Fock Space

2.1.1 Second Quantizaion

The many body wavefunctions for bosons and fermions are difficult to work with. So we use the occupation-number representation of "second quantizatin: formalism". Essentially for fermions we consider the occupation number for each state. In this example a half-filled two site system is considered and so each state can either be 0 or 1, or each site can only one fermion with the same state and spin.

2.1.2 Creation and Annihilation operators

2.1.3 Anti-Commutation Relations

Unlike bosons, fermions obey the anti-commutation relations. The **anti-commutator** $\{A, B\}$ between two operators A and B are defined as

$$\{A, B\} \equiv AB + BA \tag{2}$$

The fermion creation and annhilation operators satisfies the relations

$$\{c_k, c_{k\prime}\} = 0 \tag{3}$$

$$\{c^{\dagger}_k, c^{\dagger}_{k\prime}\} = 0 \tag{4}$$

$$\{c^{\dagger}_k, c_{k\prime}\} = \delta_{k,k\prime} \tag{5}$$

2.2 Fock Space Basis

The Hubbard model does not change the total number of electron in the system. Thus we can consider a half-filled ($N = 2$) two site system. According to the Pauli Exclusion Principle, for a half-filled two-site system we have 6 basis states.

Fock States		
$\lvert\phi_i\rangle$	State	Spin Diagram
$\lvert\phi_1\rangle$	$c^\dagger_{2\uparrow}c^\dagger_{1\uparrow}\lvert\rangle$	$\uparrow,\uparrow$
$\lvert\phi_2\rangle$	$c^\dagger_{1\downarrow}c^\dagger_{1\uparrow}\lvert\rangle$	$\uparrow\downarrow,\bigcirc$
$\lvert\phi_3\rangle$	$c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}\lvert\rangle$	$\downarrow,\uparrow$
$\lvert\phi_4\rangle$	$c^\dagger_{2\downarrow}c^\dagger_{1\uparrow}\lvert\rangle$	$\uparrow,\downarrow$
$\lvert\phi_5\rangle$	$c^\dagger_{2\downarrow}c^\dagger_{2\uparrow}\lvert\rangle$	$\bigcirc,\uparrow\downarrow$
$\lvert\phi_6\rangle$	$c^\dagger_{1\downarrow}c^\dagger_{2\downarrow}\lvert\rangle$	$\downarrow,\downarrow$

3 Two-Site Hubbard Model Matrix

$$\mathcal{H} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & U & -t & -t & 0 & 0 \\ 0 & -t & 0 & 0 & -t & 0 \\ 0 & -t & 0 & 0 & -t & 0 \\ 0 & 0 & -t & -t & U & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{6}$$

4 Exact Solution