PHY 742 Quantum Mechanics II
12-12:50 PM MWF Olin 103

Notes for Lecture 35

Review

- Schedule
- Correction to Hubbard model notes
- Time for filling out course evaluations

27	Fri: 04/08/2022		Multi electron atoms	#21	04/11/2022
28	Mon: 04/11/2022		Multi electron atoms	#22	04/18/2022
29	Wed: 04/13/2022		Multi electron atoms		
	Fri: 04/15/2022	*No class*	Holiday		
30	Mon: 04/18/2022		Hubbard model with multiple electrons	#23	04/22/2022
31	Wed: 04/20/2022		Hubbard model with multiple electrons		
32	Fri: 04/22/2022		BCS model of superconductivity		
33	Mon: 04/25/2022		BCS model of superconductivity		
34	Wed: 04/27/2022		Review		
35	Fri: 04/29/2022		Review		

More comments on the 2-site Hubbard model

Two-site Hubbard model

$$H = -t\left(c^{\dagger}_{1\uparrow}c_{2\uparrow} + c^{\dagger}_{2\uparrow}c_{1\uparrow} + c^{\dagger}_{1\downarrow}c_{2\downarrow} + c^{\dagger}_{2\downarrow}c_{1\downarrow}\right) + U\left(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}\right)$$

Matrix elements of Hamiltonian for all 2 particle states with spin 0:

$$H = \begin{array}{c} \\ A \\ B \\ C \end{array} \begin{array}{c} \begin{array}{ccc} A & B & C \end{array} \\ \begin{pmatrix} U & 0 & -\sqrt{2}t \\ 0 & U & -\sqrt{2}t \\ -\sqrt{2}t & -\sqrt{2}t & 0 \end{pmatrix} \end{array}$$

$$|A\rangle \equiv c^{\dagger}_{1\uparrow}c^{\dagger}_{1\downarrow}|0\rangle$$

$$|B\rangle \equiv c^{\dagger}_{2\uparrow}c^{\dagger}_{2\downarrow}|0\rangle$$

$$|C\rangle \equiv \frac{1}{\sqrt{2}}\left(c^{\dagger}_{1\uparrow}c^{\dagger}_{2\downarrow} + c^{\dagger}_{2\uparrow}c^{\dagger}_{1\downarrow}\right)|0\rangle$$

Note that this is corrected from the original slides

We claim that these states correspond to a total spin S=0; how can we analyze this?

Total spin S=0:

$$|A\rangle \equiv c^{\dagger}{}_{1\uparrow} c^{\dagger}{}_{1\downarrow} |0\rangle$$

$$|B\rangle \equiv c^{\dagger}{}_{2\uparrow} c^{\dagger}{}_{2\downarrow} |0\rangle$$

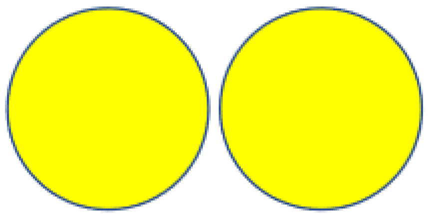
$$|C\rangle \equiv \frac{1}{\sqrt{2}}\left(c^{\dagger}{}_{1\uparrow} c^{\dagger}{}_{2\downarrow} + c^{\dagger}{}_{2\uparrow} c^{\dagger}{}_{1\downarrow}\right)|0\rangle$$

Possible total spin S=1 states:

$$|D\rangle = c^{\dagger}_{1\uparrow} c^{\dagger}_{2\uparrow} |0\rangle$$

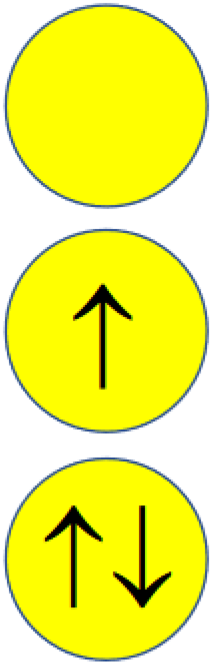
$$|E\rangle = \frac{1}{\sqrt{2}}\left(c^{\dagger}_{1\uparrow} c^{\dagger}_{2\downarrow} - c^{\dagger}_{2\uparrow} c^{\dagger}_{1\downarrow}\right)|0\rangle$$

$$|F\rangle = c^{\dagger}_{1\downarrow} c^{\dagger}_{2\downarrow} |0\rangle$$



l = 1 2

Possible configurations of a single site



$$|0\rangle$$

$$c^{\dagger}_{\uparrow}|0\rangle$$

$$c^{\dagger}_{\uparrow} c^{\dagger}_{\downarrow}|0\rangle$$

How can we calculate the total spin for our states?

Basic properties of indistinguishable Fermi particles

$$\Psi(1,2) = -\Psi(2,1)$$

Typically, we can write $\Psi(1,2) = \psi_{space}(\mathbf{r}_1, \mathbf{r}_2)\psi_{spin}(\sigma_1, \sigma_2)$

$$\Rightarrow \text{If } \psi_{space}(\mathbf{r}_1, \mathbf{r}_2) = \psi_{space}(\mathbf{r}_2, \mathbf{r}_1) \text{ then } \psi_{spin}(\sigma_1, \sigma_2) = -\psi_{spin}(\sigma_2, \sigma_1) \quad (S = 0)$$

$$\Rightarrow \text{If } \psi_{space}(\mathbf{r}_1, \mathbf{r}_2) = -\psi_{space}(\mathbf{r}_2, \mathbf{r}_1) \text{ then } \psi_{spin}(\sigma_1, \sigma_2) = \psi_{spin}(\sigma_2, \sigma_1) \quad (S = 1)$$

How can we analyze this in second quantization?

Total spin S=0

$$\left|A\right\rangle \equiv c^{\dagger}{}_{1\uparrow}c^{\dagger}{}_{1\downarrow}\left|0\right\rangle$$

$$\left|B\right\rangle \equiv c^{\dagger}{}_{2\uparrow}c^{\dagger}{}_{2\downarrow}\left|0\right\rangle$$

$$\left|C\right\rangle \equiv \frac{1}{\sqrt{2}}\left(c^{\dagger}{}_{1\uparrow}c^{\dagger}{}_{2\downarrow} + c^{\dagger}{}_{2\uparrow}c^{\dagger}{}_{1\downarrow}\right)\left|0\right\rangle$$

Total spin S=1

$$\left|D\right\rangle = c^{\dagger}_{1\uparrow}c^{\dagger}_{2\uparrow}\left|0\right\rangle$$

$$\left|E\right\rangle = \frac{1}{\sqrt{2}}\left(c^{\dagger}_{1\uparrow}c^{\dagger}_{2\downarrow} - c^{\dagger}_{2\uparrow}c^{\dagger}_{1\downarrow}\right)\left|0\right\rangle$$

$$\left|F\right\rangle = c^{\dagger}_{1\downarrow}c^{\dagger}_{2\downarrow}\left|0\right\rangle$$

How do you calculate total spin for these second-quantized basis states?

Answer thanks to Professor William C. Kerr and his student Professor Will Hodge (Ph. D. 2008, currently a physics professor at Stevenson University in Maryland)

For system with states $\{i\}$, need to evaluate operator

$$\left(\sum_i \mathbf{S}_i\right)^2 = \sum_i \mathbf{S}_i^2 + \sum_{i \neq i} \mathbf{S}_i \cdot \mathbf{S}_j$$

The single particle operators $\mathbf{S}_i^2$ are all the same with expectation value $\frac{3}{4}\hbar^2$

The two-particle operators are more complicated and require that we sum over all quantum numbers except spin.

Famous Kerr-Hodge formula --

$$\mathbf{S}^2 = \hbar^2 \left[\frac{3}{4}\hat{N} + \frac{1}{4}\sum_{\sigma} \left(\sum_{n_1 \neq n_2} \hat{n}_{n_1,\sigma}\hat{n}_{n_2,\sigma} - \sum_{n_1,n_2} \hat{n}_{n_1,\sigma}\hat{n}_{n_2,-\sigma} \right) + \sum_{n_1,n_2} c^\dagger_{n_1,\uparrow} c^\dagger_{n_2,\downarrow} c_{n_2,\uparrow} c_{n_1,\downarrow} \right]. \qquad (2.27)$$

$$\mathbf{S}^2 = \hbar^2\Bigg[\frac{3}{4}\hat{N} + \frac{1}{4}\sum_{\sigma}\Bigg(\sum_{n_1\neq n_2}\hat{n}_{n_1,\sigma}\hat{n}_{n_2,\sigma} - \sum_{n_1,n_2}\hat{n}_{n_1,\sigma}\hat{n}_{n_2,-\sigma}\Bigg) + \sum_{n_1,n_2} c^{\dagger}_{n_1,\uparrow}c^{\dagger}_{n_2,\downarrow}c_{n_2,\uparrow}c_{n_1,\downarrow}\Bigg]. \tag{2.27}$$

$$\mathbf{S}^2|A\rangle = \hbar^2\left(\frac{3}{4}\hat{N} - \frac{2}{4}\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + c^{\dagger}_{1\uparrow}c^{\dagger}_{1\downarrow}c_{1\uparrow}c_{1\downarrow}\right)c^{\dagger}_{1\uparrow}c^{\dagger}_{1\downarrow}|0\rangle = \hbar^2\left(\frac{6}{4} - \frac{2}{4} - 1\right)c^{\dagger}_{1\uparrow}c^{\dagger}_{1\downarrow}|0\rangle = 0$$

$$\mathbf{S}^2|C\rangle = \hbar^2\left(\frac{3}{4}\hat{N} - \frac{1}{4}\hat{n}_{1\uparrow}\hat{n}_{2\downarrow} - \frac{1}{4}\hat{n}_{2\uparrow}\hat{n}_{1\downarrow} + c^{\dagger}_{1\uparrow}c^{\dagger}_{2\downarrow}c_{2\uparrow}c_{1\downarrow} + c^{\dagger}_{2\uparrow}c^{\dagger}_{1\downarrow}c_{1\uparrow}c_{2\downarrow}\right)\frac{1}{\sqrt{2}}\left(c^{\dagger}_{1\uparrow}c^{\dagger}_{2\downarrow} + c^{\dagger}_{2\uparrow}c^{\dagger}_{1\downarrow}\right)|0\rangle$$

$$=\hbar^2\left(\frac{6}{4} - \frac{2}{4} - 1\right)\frac{1}{\sqrt{2}}\left(c^{\dagger}_{1\uparrow}c^{\dagger}_{2\downarrow} + c^{\dagger}_{2\uparrow}c^{\dagger}_{1\downarrow}\right)|0\rangle = 0$$

$$\mathbf{S}^2|E\rangle = \hbar^2\left(\frac{3}{4}\hat{N} - \frac{1}{4}\hat{n}_{1\uparrow}\hat{n}_{2\downarrow} - \frac{1}{4}\hat{n}_{2\uparrow}\hat{n}_{1\downarrow} + c^{\dagger}_{1\uparrow}c^{\dagger}_{2\downarrow}c_{2\uparrow}c_{1\downarrow} + c^{\dagger}_{2\uparrow}c^{\dagger}_{1\downarrow}c_{1\uparrow}c_{2\downarrow}\right)\frac{1}{\sqrt{2}}\left(c^{\dagger}_{1\uparrow}c^{\dagger}_{2\downarrow} - c^{\dagger}_{2\uparrow}c^{\dagger}_{1\downarrow}\right)|0\rangle$$

$$=\hbar^2\left(\frac{6}{4} - \frac{2}{4} + 1\right)\frac{1}{\sqrt{2}}\left(c^{\dagger}_{1\uparrow}c^{\dagger}_{2\downarrow} - c^{\dagger}_{2\uparrow}c^{\dagger}_{1\downarrow}\right)|0\rangle = 2\hbar^2\frac{1}{\sqrt{2}}\left(c^{\dagger}_{1\uparrow}c^{\dagger}_{2\downarrow} - c^{\dagger}_{2\uparrow}c^{\dagger}_{1\downarrow}\right)|0\rangle$$