Phys 726 - Assignment 2 Solutions

1(a) Substitute $\hat{\psi}_\alpha(\vec{r}) = \sum_{j=1,2} \phi_j(\vec{r})\, \chi_\alpha\, c_{j\alpha}$ into

$$\hat{H} = \sum_\alpha \int d^3r\, \hat{\psi}^\dagger_\alpha(\vec{r})\, T(\vec{r})\, \hat{\psi}_\alpha(\vec{r})$$

$$= \sum_\alpha \int d^3r \sum_j \phi_j^* \chi_\alpha^\dagger c_{j\alpha}^\dagger\, T \sum_{j'} \phi_{j'} \chi_\alpha c_{j'\alpha}$$

$$= \sum_\alpha \sum_{jj'} \cancelto{1}{\chi_\alpha^\dagger \chi_\alpha} \int d^3r\, \phi_j^*(\vec{r})\, T(\vec{r})\, \phi_{j'}(\vec{r})\, c_{j\alpha}^\dagger c_{j'\alpha}$$

$$= \sum_\alpha \begin{pmatrix} c_{1\alpha}^\dagger & c_{2\alpha}^\dagger \end{pmatrix} \begin{pmatrix} \varepsilon_1 & -t \\ -t^* & \varepsilon_2 \end{pmatrix} \begin{pmatrix} c_{1\alpha} \\ c_{2\alpha} \end{pmatrix}$$

where
$$\varepsilon_1 = \int d^3r\, \phi_1^* T \phi_1$$
$$\varepsilon_2 = \int d^3r\, \phi_2^* T \phi_2$$
$$-t = \int d^3r\, \phi_1^* T \phi_2$$
$$-t^* = \int d^3r\, \phi_2^* T \phi_1$$

1(b) For $\varepsilon_1 = \varepsilon_2 = \varepsilon$, the matrix in the Hamiltonian has the form

$$\begin{pmatrix} \varepsilon & -t \\ -t^* & \varepsilon \end{pmatrix} = \begin{pmatrix} \varepsilon & -|t|e^{i\phi} \\ -|t|e^{-i\phi} & \varepsilon \end{pmatrix}$$

We identify the eigenstates

$$① \quad \begin{pmatrix} \varepsilon & -|t|e^{i\phi} \\ -|t|e^{-i\phi} & \varepsilon \end{pmatrix}\begin{pmatrix} 1 \\ e^{-i\phi} \end{pmatrix} = \begin{pmatrix} \varepsilon - |t| \\ -|t|e^{-i\phi} + \varepsilon e^{-i\phi} \end{pmatrix} = (\varepsilon - |t|)\begin{pmatrix} 1 \\ e^{-i\phi} \end{pmatrix}$$

$$② \quad \begin{pmatrix} \varepsilon & -|t|e^{i\phi} \\ -|t|e^{-i\phi} & \varepsilon \end{pmatrix}\begin{pmatrix} 1 \\ -e^{-i\phi} \end{pmatrix} = \begin{pmatrix} \varepsilon + |t| \\ -|t|e^{-i\phi} - \varepsilon e^{-i\phi} \end{pmatrix} = (\varepsilon + |t|)\begin{pmatrix} 1 \\ -e^{-i\phi} \end{pmatrix}$$

Populate a basis transformation matrix with the normalized eigenvectors:

$$U = \begin{pmatrix} U_{1+} & U_{1-} \\ U_{2+} & U_{2-} \end{pmatrix} = \left(① \,\middle|\, ② \right) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ e^{-i\phi} & -e^{-i\phi} \end{pmatrix}$$

Define fermion operators d such that $c = Ud$ and thus $H \sim c^\dagger M c = (Ud)^\dagger M U d = d^\dagger \underbrace{U^\dagger M U}_{\begin{pmatrix} \varepsilon - |t| & 0 \\ 0 & \varepsilon + |t| \end{pmatrix}} d$

$$\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ e^{-i\phi} & -e^{-i\phi} \end{pmatrix} \begin{pmatrix} d_+ \\ d_- \end{pmatrix}$$

$$\Rightarrow \quad c_1 = \frac{1}{\sqrt{2}} (d_+ + d_-)$$

$$c_2 = \frac{e^{-i\phi}}{\sqrt{2}} (d_+ - d_-)$$

$$\Rightarrow \quad \sqrt{2}\, c_1 = d_+ + d_-$$

$$\sqrt{2}\, e^{i\phi} c_2 = d_+ - d_-$$

$$\Rightarrow \quad d_+ = \frac{1}{\sqrt{2}} (c_1 + e^{i\phi} c_2)$$

$$d_- = \frac{1}{\sqrt{2}} (c_1 - e^{i\phi} c_2)$$

Then $\hat{H} = \sum_\alpha \left(d^\dagger_{+\alpha} \; d^\dagger_{-\alpha} \right) \begin{pmatrix} \varepsilon - |t| & 0 \\ 0 & \varepsilon + |t| \end{pmatrix} \begin{pmatrix} d_{+\alpha} \\ d_{-\alpha} \end{pmatrix}$

$$= \sum_\alpha \left\{ (\varepsilon - |t|) d^\dagger_{+\alpha} d_{+\alpha} + (\varepsilon + |t|) d^\dagger_{-\alpha} d_{-\alpha} \right\}$$

$$= \sum_{\alpha = \uparrow, \downarrow} \sum_{n = \pm} (\varepsilon - n|t|) d^\dagger_{n\alpha} d_{n\alpha}$$

The one-particle ground state is

$$d_{+\alpha}^{\dagger}|vac\rangle = \frac{1}{\sqrt{2}}\left(c_{1\alpha}^{\dagger} + e^{-i\phi}c_{2\alpha}^{\dagger}\right)|vac\rangle = \frac{1}{\sqrt{2}}\left(|\alpha,0\rangle + e^{-i\phi}|0,\alpha\rangle\right)$$

for either $\alpha = \uparrow$ or $\alpha = \downarrow$

The two-particle ground state is

$$d_{+\uparrow}^{\dagger}d_{+\downarrow}^{\dagger}|vac\rangle = \frac{1}{\sqrt{2}}\left(c_{1\uparrow}^{\dagger} + e^{-i\phi}c_{2\uparrow}^{\dagger}\right)\frac{1}{\sqrt{2}}\left(c_{1\downarrow}^{\dagger} + e^{-i\phi}c_{2\downarrow}^{\dagger}\right)|vac\rangle$$

$$= \frac{1}{2}\left(c_{1\uparrow}^{\dagger}c_{1\downarrow}^{\dagger} + e^{-i\phi}c_{1\uparrow}^{\dagger}c_{2\downarrow}^{\dagger} + e^{-i\phi}c_{2\uparrow}^{\dagger}c_{1\downarrow}^{\dagger} + e^{-2i\phi}c_{2\uparrow}^{\dagger}c_{2\downarrow}^{\dagger}\right) \times |vac\rangle$$

$$= \frac{1}{2}\left(|\uparrow\downarrow,0\rangle + e^{-i\phi}\left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) + e^{-2i\phi}|0,\uparrow\downarrow\rangle\right)$$

(c) Now consider $\varepsilon_1 = \varepsilon - \Delta$ and $\varepsilon_2 = \varepsilon + \Delta$

$$\begin{pmatrix} \varepsilon_1 & -t \\ -t^* & \varepsilon_2 \end{pmatrix} = \begin{pmatrix} \varepsilon-\Delta & -|t|e^{i\phi} \\ -|t|e^{-i\phi} & \varepsilon+\Delta \end{pmatrix} = \underbrace{(\varepsilon-\Delta)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}_{\text{trivial part}} + \begin{pmatrix} 0 & -|t|e^{i\phi} \\ -|t|e^{-i\phi} & 2\Delta \end{pmatrix}$$

Solve for eigenvectors ...

$$\begin{pmatrix} 0 & -|t|e^{i\phi} \\ -|t|e^{-i\phi} & 2\Delta \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -|t|e^{i\phi}y \\ -|t|e^{-i\phi}x + 2\Delta y \end{pmatrix} = \lambda\begin{pmatrix} x \\ y \end{pmatrix}$$

$$-|t|e^{i\phi}y = \lambda x$$

$$-|t|e^{-i\phi}x + 2\Delta y = -|t|e^{-i\phi}\left(-\frac{1}{\lambda}|t|e^{i\phi}y\right) + 2\Delta y = \lambda y$$

$$\Rightarrow |t|^2 + 2\Delta\lambda = \lambda^2 \quad \text{or} \quad \lambda^2 - 2\Delta\lambda - |t|^2 = 0$$

Eigenvalues $\varepsilon - \Delta + \left(\frac{2\Delta \pm \sqrt{4\Delta^2 + 4|t|^2}}{2}\right)$

$$= \varepsilon - \Delta + \Delta \pm \sqrt{\Delta^2 + |t|^2} = \varepsilon \pm \sqrt{\Delta^2 + |t|^2}$$

Eigenvectors

$$\begin{pmatrix} -|t|e^{i\phi}y \\ -|t|e^{-i\phi}x + 2\Delta y \end{pmatrix} = \left(\Delta \pm \sqrt{\Delta^2 + |t|^2}\right)\begin{pmatrix} x \\ y \end{pmatrix}$$

$$\Rightarrow -|t|e^{i\phi}y = \left(\Delta \pm \sqrt{\Delta^2 + |t|^2}\right)x$$

$$-|t|e^{-i\phi}x + 2\Delta y = \left(\Delta \pm \sqrt{\Delta^2 + |t|^2}\right)y$$

$$\Rightarrow \begin{pmatrix} x \\ y \end{pmatrix} \sim \begin{pmatrix} 1 \\ \dfrac{\Delta \pm \sqrt{\Delta^2 + |t|^2}}{-|t|e^{i\phi}} \end{pmatrix}$$

Normalization $1+\left(\frac{\Delta \pm \sqrt{\Delta^2+|t|^2}}{|t|}\right)^2$

$$= 1 + \frac{\Delta^2 \pm 2\Delta\sqrt{\Delta^2+|t|^2} + \Delta^2 + |t|^2}{|t|^2} = \frac{1}{|t|^2}\left(2|t|^2 + 2\Delta^2 \pm 2\Delta\sqrt{\Delta^2+|t|^2}\right)$$

$$= \frac{2}{|t|^2}\left(|t|^2+\Delta^2 \pm \Delta\sqrt{\Delta^2+|t|^2}\right)$$

Hence, $\begin{pmatrix} x \\ y \end{pmatrix} = \frac{|t|}{\sqrt{2}}\left(|t|^2+\Delta^2 \pm \Delta\sqrt{\Delta^2+|t|^2}\right)^{1/2} \begin{pmatrix} 1 \\ \frac{\Delta \pm \sqrt{\Delta^2+|t|^2}}{-|t|e^{i\phi}} \end{pmatrix}$

$$= \frac{1}{\sqrt{2}}\left(|t|^2+\Delta^2 \pm \Delta\sqrt{\Delta^2+|t|^2}\right)^{-1/2} \begin{pmatrix} 1 \\ \frac{\Delta \pm \sqrt{\Delta^2+|t|^2}}{-|t|e^{i\phi}} \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}}\left(|t|^2+\Delta^2 \pm \Delta\sqrt{\Delta^2+|t|^2}\right)^{-1/2} \begin{pmatrix} |t| \\ -e^{-i\phi}\left(\Delta \pm \sqrt{\Delta^2+|t|^2}\right) \end{pmatrix}$$

Matrix $U = \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{|t|}{\sqrt{|t|^2+\Delta^2-\Delta\sqrt{\Delta^2+|t|^2}}} & \frac{|t|}{\sqrt{|t|^2+\Delta^2+\Delta\sqrt{\Delta^2+|t|^2}}} \\ \frac{-e^{-i\phi}\left(\Delta-\sqrt{\Delta^2+|t|^2}\right)}{\sqrt{|t|^2+\Delta^2-\Delta\sqrt{\Delta^2+|t|^2}}} & \frac{-e^{-i\phi}\left(\Delta+\sqrt{\Delta^2+|t|^2}\right)}{\sqrt{|t|^2+\Delta^2+\Delta\sqrt{\Delta^2+|t|^2}}} \end{pmatrix}$

So the average occupation on site j is

$$\langle \hat{n}_j \rangle = \langle vac | d_{+\uparrow} \left(\sum_{\alpha=\uparrow,\downarrow} c^\dagger_{j\alpha} c_{j\alpha} \right) d^\dagger_{+\uparrow} | vac \rangle$$

$$= \langle vac | d_{+\uparrow} \sum_\alpha \left(\sum_{n=\pm} U_{jn} d_{n\alpha} \right)^\dagger \left(\sum_{m=\pm} U_{jm} d_{m\alpha} \right) d^\dagger_{+\uparrow} | vac \rangle$$

$$= \sum_\alpha \sum_{m,n} U^*_{jn} U_{jm} \langle vac | d_{+\uparrow} d^\dagger_{n\alpha} \underbrace{d_{m\alpha} d^\dagger_{+\uparrow} | vac \rangle}_{= \delta_{m,+} \delta_{\alpha\uparrow} | vac \rangle}$$

$$= \sum_{n=\pm} U^*_{jn} U_{j+} \langle vac | \underbrace{d_{+\uparrow} d^\dagger_{n\uparrow} | vac \rangle}_{\delta_{n,+} | vac \rangle} = |U_{j+}|^2$$

i.e. $$\langle \hat{n}_1 \rangle = \frac{|t|^2}{2\left(|t|^2 + \Delta^2 - \Delta\sqrt{\Delta^2 + |t|^2} \right)} = \frac{1}{2}\left(1 + \frac{\Delta\sqrt{\Delta^2+|t|^2} - \Delta^2}{|t|^2 + \Delta^2 - \Delta\sqrt{\Delta^2+|t|^2}} \right)$$

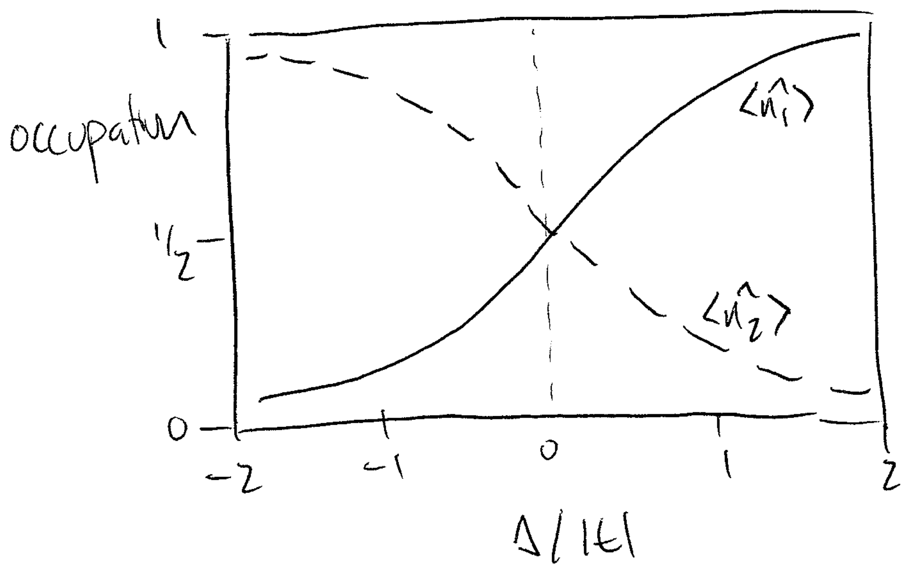
$$\langle \hat{n}_2 \rangle = \frac{\left(\Delta - \sqrt{\Delta^2+|t|^2} \right)^2}{2\left(|t|^2 + \Delta^2 - \Delta\sqrt{\Delta^2+|t|^2} \right)} = \frac{\Delta^2 - 2\Delta\sqrt{\Delta^2+|t|^2} + \Delta^2 + |t|^2}{2\left(|t|^2 + \Delta^2 - \Delta\sqrt{\Delta^2+|t|^2} \right)}$$

$$= \frac{1}{2}\left(1 - \frac{\Delta\sqrt{\Delta^2+|t|^2} - \Delta^2}{|t|^2 + \Delta^2 - \Delta\sqrt{\Delta^2+|t|^2}} \right)$$

Note that $\langle \hat{n}_1 \rangle + \langle \hat{n}_2 \rangle = 1$. There's still exactly one electron in the system, but as Δ increases it spends more of its time on atom 1.

$$\langle \hat{n}_1 \rangle \sim \frac{1}{2} + \frac{\Delta}{2|t|} - \frac{\Delta^3}{4|t|^3} + \dots$$

$$\langle \hat{n}_2 \rangle \sim \frac{1}{2} - \frac{\Delta}{2|t|} + \frac{\Delta^3}{4|t|^3} + \dots$$



2. $\hat{H} = \varepsilon a^\dagger a + \frac{\Delta}{2}\left[a^2 + (a^\dagger)^2\right]$

(a) $\hat{A} = c(a + \lambda a^\dagger)$

We'll take c and λ real.

$$[\hat{A}, \hat{A}^\dagger] = c^2[a^\dagger + \lambda a, a + \lambda a^\dagger]$$

$$= c^2\left([a^\dagger, a] + \lambda^2[a, a^\dagger]\right)$$

$$= c^2(\lambda^2 - 1) := 1$$

Hence $\hat{A} = \dfrac{i}{\sqrt{1-\lambda^2}}(a + \lambda a^\dagger)$ for $|\lambda| < 1$

Confirm that $[\hat{A}, \hat{A}] = \dfrac{1}{\lambda^2 - 1}[a + \lambda a^\dagger, a + \lambda a^\dagger]$

$$= \frac{1}{\lambda^2 - 1}\left(\lambda[a, a^\dagger] + \lambda[a^\dagger, a]\right) = 0$$

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So $\hat{A}$, $\hat{A}^\dagger$ are bosonic annihilation and creation operators

(b) $\hat{H} = \tilde{\varepsilon}\hat{A}^{\dagger}\hat{A}$

$$= \tilde{\varepsilon} \cdot \frac{-i}{\sqrt{1-\lambda^2}}(a^{\dagger}+\lambda a) \cdot \frac{i}{\sqrt{1-\lambda^2}}(a+\lambda a^{\dagger})$$

$$= \frac{\tilde{\varepsilon}}{1-\lambda^2}\left(a^{\dagger}a + \lambda(a^{\dagger})^2 + \lambda a^2 + \lambda^2 a a^{\dagger}\right)$$

$$= \frac{\tilde{\varepsilon}}{1-\lambda^2}\left\{a^{\dagger}a + \lambda^2(1+a^{\dagger}a) + \lambda\left((a^{\dagger})^2+a^2\right)\right\}$$

$$= \tilde{\varepsilon}\left(\frac{1+\lambda^2}{1-\lambda^2}\right)a^{\dagger}a + \frac{\tilde{\varepsilon}\lambda}{1-\lambda^2}\left((a^{\dagger})^2+a^2\right) + \text{const}$$

$$\equiv \varepsilon a^{\dagger}a + \frac{\Delta}{2}\left((a^{\dagger})^2+a^2\right)$$

(c) Ground state is the bosonic vacuum $|0\rangle$.

The first excited state is

$$\underset{\substack{\uparrow \\ \text{A basis}}}{|\hat{1}\rangle} = \hat{A}^{\dagger}|0\rangle = \frac{-i}{\sqrt{1-\lambda^2}}(a^{\dagger}+\lambda a)|0\rangle = \frac{-i}{\sqrt{1-\lambda^2}}\underset{\substack{\uparrow \\ \text{a basis}}}{|1\rangle}$$

The second excited state is

$$|\hat{2}\rangle = \frac{1}{2!}\hat{A}^{+}\hat{A}^{+}|0\rangle = \frac{1}{2}\hat{A}^{+}|\hat{1}\rangle$$

$$= \frac{1}{2}\left(\frac{-i}{\sqrt{1-\lambda^2}}(a^{+}+\lambda a)\right)\left(\frac{-i}{\sqrt{1-\lambda^2}}|1\rangle\right)$$

$$= -\frac{1}{2(1-\lambda^2)}(a^{+}+\lambda a)|1\rangle$$

$$= -\frac{1}{2(1-\lambda^2)}\left(\sqrt{2}\,|2\rangle + \lambda|0\rangle\right)$$

The third excited state is

$$|\hat{3}\rangle = \frac{1}{3!}\hat{A}^{+}\hat{A}^{+}\hat{A}^{+}|0\rangle = \frac{1}{3}\hat{A}^{+}\left(\frac{1}{2!}\hat{A}^{+}\hat{A}^{+}|0\rangle\right)$$

$$= \frac{1}{3}\left(\frac{-i}{\sqrt{1-\lambda^2}}(a^{+}+\lambda a)\right)\left(-\frac{1}{2(1-\lambda^2)}\left(\sqrt{2}\,|2\rangle+\lambda|0\rangle\right)\right)$$

$$= \frac{i}{6(1-\lambda^2)^{3/2}}\left(\sqrt{2\cdot 3}\,|3\rangle + \lambda|1\rangle + \lambda\sqrt{2\cdot 2}\,|1\rangle + 0\right)$$

$$= \frac{i}{6(1-\lambda^2)^{3/2}}\left(\sqrt{6}\,|3\rangle + 3\lambda|1\rangle\right)$$