Problem set 4

1) Exchange Hamiltonian

$$\mathcal{H} = \epsilon_a a^\dagger a + \epsilon_b b^\dagger b - J(a^\dagger b + b^\dagger a)$$

$$= (a^\dagger \;\; b^\dagger) \underbrace{\begin{pmatrix} \epsilon_a & -J \\ -J & \epsilon_b \end{pmatrix}}_{H_1} \begin{pmatrix} a \\ b \end{pmatrix}$$

We can diagonalize H_1 as

$$H_1 = U \mathcal{E} U^\dagger$$

where

$$U = \begin{pmatrix} \cos\theta/2 & -\sin\theta/2 \\ \sin\theta/2 & \cos\theta/2 \end{pmatrix}$$

$$\tan\theta = \frac{-2J}{\epsilon_a - \epsilon_b}$$

$$\mathcal{E} = \begin{pmatrix} \mathcal{E}_+ & 0 \\ 0 & \mathcal{E}_- \end{pmatrix}$$

$$\mathcal{E}_\pm = \frac{(\epsilon_a + \epsilon_b)}{2} \pm \frac{1}{2}\sqrt{(\epsilon_a - \epsilon_b)^2 + 4J^2}$$

we then define

$$c_+ = a\cos\theta/2 + b\sin\theta/2$$

$$c_- = -a\sin\theta/2 + b\cos\theta/2$$

or

$$\begin{pmatrix} c_+ \\ c_- \end{pmatrix} = U \begin{pmatrix} a \\ b \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} a \\ b \end{pmatrix} = U^+ \begin{pmatrix} c_+ \\ c_- \end{pmatrix}$$

We then get

$$\mathcal{H} = \varepsilon_+ c_+^+ c_+ + \varepsilon_- c_-^+ c_-$$

which is the sought for diagonal form.

2) Bosonic ladder

$$\mathcal{H} = \sum_i \left(\epsilon_a a_i^\dagger a_i + \epsilon_b b_i^\dagger b_i \right) - g_a \sum_i \left(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i \right)$$
$$- g_b \sum_i \left(b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i \right)$$
$$- J \sum_i \left(a_i^\dagger b_i + b_i^\dagger a_i \right)$$

we can write this as

$$\mathcal{H} = \mathcal{H}_a + \mathcal{H}_b + V_{ab}$$

where

$$\mathcal{H}_a = \sum_i \epsilon_a a_i^\dagger a_i - g_a \sum_i \left(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i \right)$$

$$\mathcal{H}_b = \sum_i \epsilon_b b_i^\dagger b_i - g_b \sum_i \left(b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i \right)$$

$$V_{ab} = -J \sum_i \left(a_i^\dagger b_i + b_i^\dagger a_i \right)$$

The Hamiltonians $\mathcal{H}_a$ and $\mathcal{H}_b$ are just individual tight-binding Hamiltonians.

we now go to Fourier space by introducing

$$a_k^\dagger = \frac{1}{\sqrt{N}} \sum_j e^{ikj} a_j^\dagger$$

$$b_k^\dagger = \frac{1}{\sqrt{N}} \sum_j e^{ikj} b_j^\dagger$$

This will diagonalize $\mathcal{H}_a$ and $\mathcal{H}_b$ individually

$$\mathcal{H}_a = \sum_k (\epsilon_a - 2g_a \cos k)\, a_k^\dagger a_k$$

$$\mathcal{H}_b = \sum_k (\epsilon_b - 2g_b \cos k)\, b_k^\dagger b_k$$

As for V_{ab}:

$$\sum_j a_j^\dagger b_j = \frac{1}{N} \sum_{j,k,q} e^{i(k-q)j}\, a_k^\dagger b_q$$

$$= \sum_{k,q} \Big(\underbrace{\frac{1}{N} \sum_j e^{i(k-q)j}}_{\delta_{k,q}} \Big) a_k^\dagger b_q$$

$$= \sum_k a_k^\dagger b_k$$

thus

$$V_{ab} = -J \sum_k (a_k^\dagger b_k + b_k^\dagger a_k)$$

The total Hamiltonian in Fourier space then becomes

$$\mathcal{H} = \sum_k \left\{ \epsilon_a^k a_k^\dagger a_k + \epsilon_b^k b_k^\dagger b_k - J\,(a_k^\dagger b_k + b_k^\dagger a_k) \right\}$$

where $\epsilon_\alpha^k = \epsilon_\alpha - 2g_\alpha \cos k$.

This Hamiltonian is not yet diagonal. But now a_k only interacts with b_k for the same k. The Hamiltonian is thus split in the form

$$\mathcal{H} = \sum_k \mathcal{H}_k$$

where

$$\mathcal{H}_k = \epsilon_a^k a_k^\dagger a_k + \epsilon_b^k b_k^\dagger b_k - J\,(a_k^\dagger b_k + b_k^\dagger a_k)$$

To finish, we need to diagonalize each $\mathcal{H}_k$ individually. This Hamiltonian is again a non-interacting Hamiltonian, with single particle matrix

$$H_1^k = \begin{pmatrix} \epsilon_a^k & -J \\ -J & \epsilon_b^k \end{pmatrix}$$

This matrix is diagonalized by

$$U_k = \begin{pmatrix} \cos\frac{\theta_k}{2} & -\sin\frac{\theta_k}{2} \\ \sin\frac{\theta_k}{2} & \cos\frac{\theta_k}{2} \end{pmatrix}$$

$$\tan\theta_k = \frac{-2J}{\epsilon_a^k - \epsilon_b^k}$$

The eigenenergies are

$$E_{k,\pm} = \frac{\epsilon_a^k + \epsilon_b^k}{2} \pm \frac{1}{2}\sqrt{(\epsilon_a^k - \epsilon_b^k)^2 + 4J^2}$$

If we now define new operators

$$c_{k+} = a_k \cos\theta_k/2 + b_k \sin\theta_k/2$$

$$c_{k-} = -a_k \sin\theta_k/2 + b_k \cos\theta_k/2$$

then (as you may verify), we get

$$\mathcal{H} = \sum_k \left\{ E_{k+} c_{k+}^{\dagger} c_{k+} + E_{k-} c_{k-}^{\dagger} c_{k-} \right\}$$

This is the diagonal structure and $E_{k\pm}$ are the energy bands.

3) Fermionic triple well

$$\mathcal{H} = U \sum_i \hat{n}_i \hat{n}_{i+1} - g \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i)$$

(a) Since there are exactly 2 fermions, there will be 3 possible states. I choose to label them as

$$|1,2\rangle := c_1^\dagger c_2^\dagger |0\rangle$$

$$|2,3\rangle := c_3^\dagger c_2^\dagger |0\rangle$$

$$|3,1\rangle := c_3^\dagger c_1^\dagger |0\rangle$$

(b) In all 3, the interaction $\hat{n}_i \hat{n}_{i+1}$ is always present

thus

$$U \sum_i \hat{n}_i \hat{n}_{i+1} = \begin{pmatrix} U & 0 & 0 \\ 0 & U & 0 \\ 0 & 0 & U \end{pmatrix}$$

Next:

$$(c_1^\dagger c_2 + c_2^\dagger c_1)|1,2\rangle = 0$$

$$\begin{aligned}(c_2^\dagger c_3 + c_3^\dagger c_2)|1,2\rangle &= c_3^\dagger c_2 |1,2\rangle \\ &= c_3^\dagger c_2 c_1^\dagger c_2^\dagger |0\rangle \\ &= - c_3^\dagger c_1^\dagger c_2 c_2^\dagger |0\rangle \\ &= - c_3^\dagger c_1^\dagger (1 - c_2^\dagger c_2)|0\rangle \end{aligned}$$

will annihilate $|0\rangle$

$$\begin{aligned} &= - c_3^\dagger c_1^\dagger |0\rangle \\ &= -|3,1\rangle \end{aligned}$$

and

$$(c_3^\dagger c_1 + c_1^\dagger c_3)\,|1,2\rangle = c_3^\dagger c_1\,|1,2\rangle$$

$$= c_3^\dagger c_1\, c_1^\dagger c_2^\dagger\,|0\rangle$$

$$= c_3^\dagger\,(1 - c_1^\dagger c_1)\,c_2^\dagger\,|0\rangle$$

$$= c_3^\dagger c_2^\dagger\,|0\rangle$$

$$= -\,c_2^\dagger c_3^\dagger\,|0\rangle$$

$$= -\,|2,3\rangle .$$

thus, if we define

$$V = \sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right)$$

Then

$$\langle 1,2|\,V\,|1,2\rangle = 0$$

$$\langle 2,3\,|\,V\,|\,1,2\rangle = -1$$

$$\langle 3,1\,|\,V\,|\,1,2\rangle = -1$$

this gives the 1st column of V

$$V = \begin{pmatrix} 0 & \cdots & \cdots \\ -1 & \cdots & \cdots \\ -1 & \cdots & \cdots \end{pmatrix}$$

The other columns can be guessed by symmetry:

$$V = \begin{pmatrix} 0 & -1 & -1 \\ -1 & 0 & -1 \\ -1 & -1 & 0 \end{pmatrix}$$

Thus, we finally arrive at

$$\mathcal{H} = \begin{pmatrix} U & g & g \\ g & U & g \\ g & g & U \end{pmatrix}$$

(c) the eigenvalues of $\mathcal{H}$ are

$$E_1 = E_2 = U - g$$

$$E_3 = U + 2g$$

and the eigenvectors are

$$|E_1\rangle = \frac{|1,2\rangle - |3,1\rangle}{\sqrt{2}}$$

$$|E_2\rangle = \frac{|1,2\rangle - |2,3\rangle}{\sqrt{2}}$$

$$|E_3\rangle = \frac{|1,2\rangle + |2,3\rangle + |3,1\rangle}{\sqrt{3}}$$

4) Bogoliubov transformation

$$\mathcal{H} = \epsilon\,(a^\dagger a + b^\dagger b) + g\,(a^\dagger b^\dagger + ba)$$

$$a = uc - v d^\dagger$$

$$b = ud + v c^\dagger$$

(a) $$\underbrace{\{a, a^\dagger\}}_{1} = \{uc - v d^\dagger,\; u^* c^\dagger - v^* d\}$$

$$= |u|^2 \underbrace{\{c, c^\dagger\}}_{1} + |v|^2 \underbrace{\{d, d^\dagger\}}_{1}$$

$$\therefore \quad |u|^2 + |v|^2 = 1$$

the condition $\{b, b^\dagger\}$ imposes the same thing

(b) $$a^\dagger a = (u^* c^\dagger - v^* d)(uc - v d^\dagger)$$

$$= |u|^2 c^\dagger c + |v|^2 d d^\dagger - u^* v\, c^\dagger d^\dagger - u v^* dc$$

$$b^\dagger b = (u^* d^\dagger + v^* c)(ud + v c^\dagger)$$

$$= |u|^2 d^\dagger d + |v|^2 c c^\dagger + u^* v\, d^\dagger c^\dagger + u v^*\, cd$$

writing $dd^\dagger = 1 - d^\dagger d$, etc., we get

$$a^\dagger a + b^\dagger b = 2|v|^2 + (|u|^2 - |v|^2)(c^\dagger c + d^\dagger d)$$

$$- 2u^* v\, c^\dagger d^\dagger - 2u v^* dc$$

Next :

$$a^\dagger b^\dagger = (u^* c^\dagger - v^* d)(u^* d^\dagger + v^* c)$$

$$= u^* v^* (c^\dagger c - d d^\dagger) + (u^*)^2 c^\dagger d^\dagger - (v^*)^2 dc$$

$$b a = (a^\dagger b^\dagger)^\dagger$$

$$= u v (c^\dagger c - d d^\dagger) + u^2 dc - v^2 c^\dagger d^\dagger$$

Thus

$$a^\dagger b^\dagger + ba = (u^* v^* + uv)(c^\dagger c + d^\dagger d - 1)$$

$$+ ((u^*)^2 - v^2) c^\dagger d^\dagger + (u^2 - (v^*)^2) dc$$

Combining everything, we get

$$\mathcal{H} = \epsilon \Big\{ 2|v|^2 + (|u|^2 - |v|^2)(c^\dagger c + d^\dagger d)$$
$$- 2u^* v \, c^\dagger d^\dagger - 2 u v^* dc \Big\}$$
$$+ g \Big\{ (u^* v^* + uv)(c^\dagger c + d^\dagger d - 1)$$
$$+ ((u^*)^2 - v^2) c^\dagger d^\dagger + (u^2 - (v^*)^2) dc \Big\}$$

$\therefore$

$$\mathcal{H} = 2|v|^2 \epsilon - g(u^* v^* + uv)$$
$$+ \left[\epsilon(|u|^2 - |v|^2) + g(u^* v^* + uv) \right] (c^\dagger c + d^\dagger d)$$
$$+ \left[-2\epsilon u^* v + g((u^*)^2 - v^2) \right] c^\dagger d^\dagger$$
$$+ \left[-2\epsilon u v^* + g(u^2 - (v^*)^2) \right] dc$$

—//

We now choose u and v such as to kill the two blue terms. Since $|u|^2 + |v|^2 = 1$, we may parametrize

$$u = \cos\theta/2$$

$$v = \sin\theta/2$$

Although u, v may be complex, choosing them real is enough.

Then, the term multiplying $c^\dagger d^\dagger$ becomes

$$-2\epsilon\cos\frac{\theta}{2}\sin\frac{\theta}{2} + g\left(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}\right) = 0$$

or

$$-\epsilon\sin\theta + g\cos\theta = 0$$

this means we can eliminate this term if we choose

$$\tan\theta = g/\epsilon$$

As for the other terms in H, we then get

$$\left[\epsilon\left(|u|^2 - |v|^2\right) + g\left(u'v^* + uv\right)\right] = \epsilon\cos\theta + g\sin\theta$$
$$= \sqrt{\epsilon^2 + g^2}$$

and

$$2|v|^2\epsilon - g\left(u^*v^* + uv\right) = 2\epsilon\sin^2\frac{\theta}{2} - g\sin\theta$$
$$= 2\epsilon\left(\frac{1-\cos\theta}{2}\right) - g\sin\theta$$
$$= \epsilon - \left(\epsilon\cos\theta + g\sin\theta\right)$$
$$= \epsilon - \sqrt{\epsilon^2 + g^2}$$

The Hamiltonian thus finally becomes

$$\mathcal{H} = E_0 + \sqrt{\epsilon^2 + g^2}\,(c^\dagger c + d^\dagger d)$$

$$E_0 = \epsilon - \sqrt{\epsilon^2 + g^2}$$