

Quantum Mechanics 3 - Class Exercise 8

28.12.2022

Question 1

Consider the Hamiltonian of N interacting electrons,

$$\hat{H} = \hat{H}_0 + \hat{H}_I, \quad (1)$$

where

$$\hat{H}_0 = \sum_{\vec{k}, s} \frac{\hbar^2 |\vec{k}|^2}{2m} \hat{a}_{\vec{k}, s}^\dagger \hat{a}_{\vec{k}, s} \quad s = \uparrow \text{ or } \downarrow, \quad (2)$$

and \hat{H}_I is the Coulomb potential,

$$\hat{H}_I = \frac{e^2}{2V} \sum'_{\vec{k}, \vec{p}, \vec{q}} \sum_{s_1, s_2} \frac{4\pi}{q^2} \hat{a}_{\vec{k}+\vec{q}, s_1}^\dagger \hat{a}_{\vec{p}-\vec{q}, s_2}^\dagger \hat{a}_{\vec{p}, s_2} \hat{a}_{\vec{k}, s_1}. \quad (3)$$

The prime at the first sum is to exclude $\vec{q}=0$. Find $\langle \Phi_0 | \hat{H} | \Phi_0 \rangle$, where $|\Phi_0\rangle$ is the ground state of \hat{H}_0 .

Solution to 1

From Eq. (2) we see that the ground state of \hat{H}_0 corresponds to the state where all the electrons have minimum k . However, due to the Pauli exclusion principle the electrons must be at different quantum states. The ground state therefore corresponds to all the electrons inside the *Fermi sphere*. This sphere is of radius k_F which can be found by requiring that the total number of states inside the Fermi sphere is equal to the number of electrons N .

$$N \stackrel{!}{=} \sum_{|\vec{k}| < k_F} \sum_{s=\uparrow, \downarrow} 1 = \sum_{|\vec{k}| < k_F} 2 = 2 \frac{V \times \frac{4\pi}{3} k_F^3}{(2\pi)^3} = \frac{V k_F^3}{3\pi^2} \implies k_F = (3\pi^2 n)^{1/3}, \quad (4)$$

where $n \equiv N/V$ is the electron number density.

Note: in order to find the number of states inside the Fermi sphere we have to divide the total phase-space volume (which is $V \times \frac{4\pi}{3} k_F^3$) by the volume of each state in phase-space (this volume is $(2\pi)^3$ due to the uncertainty principle). Alternatively, this counting can be viewed as taking the continuum limit, $\sum_{|\vec{k}| < k_F} \rightarrow \int_{|\vec{k}| < k_F} \frac{d^3k}{(2\pi)^3/V} = \frac{V \times \frac{4\pi}{3} k_F^3}{(2\pi)^3}$.

For non-interacting electrons the ground state energy is therefore

$$\begin{aligned}
E_0^{(0)} &= \langle \Phi_0 | \hat{H}_0 | \Phi_0 \rangle = \sum_{|\vec{k}| < k_F} \sum_{s=\uparrow, \downarrow} \frac{\hbar^2 |\vec{k}|^2}{2m} = \frac{\hbar^2}{m} \sum_{|\vec{k}| < k_F} |\vec{k}|^2 = \frac{\hbar^2}{m} \frac{V}{(2\pi)^3} \cdot 4\pi \int_{k=0}^{k_F} k^4 dk \\
&= \frac{\hbar^2}{m} \frac{V}{(2\pi)^3} \frac{4\pi k_F^5}{5} = \frac{3N}{5} \cdot \frac{\hbar^2 k_F^2}{2m}.
\end{aligned} \tag{5}$$

The first-order correction to the ground state energy is

$$E_0^{(1)} = \langle \Phi_0 | \hat{H}_I | \Phi_0 \rangle = \frac{e^2}{2V} \sum'_{\vec{k}, \vec{p}, \vec{q}} \sum_{s_1, s_2} \frac{4\pi}{q^2} \langle \Phi_0 | \hat{a}_{\vec{k}+\vec{q}, s_1}^\dagger \hat{a}_{\vec{p}-\vec{q}, s_2}^\dagger \hat{a}_{\vec{p}, s_2} \hat{a}_{\vec{k}, s_1} | \Phi_0 \rangle. \tag{6}$$

Let us examine the sandwich in Eq. (6). It is the inner product between two states:

1. $|\Phi_0\rangle$ but with two electrons missing: $|\vec{k}, s_1\rangle$ and $|\vec{p}, s_2\rangle$.
2. $|\Phi_0\rangle$ but with two electrons missing: $|\vec{k} + \vec{q}, s_1\rangle$ and $|\vec{p} - \vec{q}, s_2\rangle$.

The sandwich doesn't vanish only if these states are the same, but these states are the same only if the missing electrons (or holes) are the same. There are two options:

1. Consider first $s_1 \neq s_2$. In that case the sandwich doesn't vanish only if $|\vec{k}, s_1\rangle = |\vec{k} + \vec{q}, s_1\rangle$ and $|\vec{p}, s_2\rangle = |\vec{p} - \vec{q}, s_2\rangle$, which implies $\vec{q} = 0$. But $\vec{q} = 0$ is excluded in the summation of Eq. (6) so there aren't any such terms that contribute to $E_0^{(1)}$.
2. Now consider $s_1 = s_2$. This is similar to the previous case but now there is another possibility for which the sandwich won't vanish, this is when $|\vec{k}, s_1\rangle = |\vec{p} - \vec{q}, s_2\rangle$ and $|\vec{k} + \vec{q}, s_1\rangle = |\vec{p}, s_2\rangle$. This can only happen for $\vec{p} = \vec{k} + \vec{q}$.

Thus, we conclude that the only terms that contribute to $E_0^{(1)}$ in Eq. (6) are those which satisfy $s_1 = s_2$ and $\vec{p} = \vec{k} + \vec{q}$.

$$\begin{aligned}
E_0^{(1)} &= \frac{e^2}{2V} \sum'_{\vec{k}, \vec{q}} \sum_{s_1} \frac{4\pi}{q^2} \langle \Phi_0 | \hat{a}_{\vec{k}+\vec{q}, s_1}^\dagger \hat{a}_{\vec{k}, s_1}^\dagger \hat{a}_{\vec{k}+\vec{q}, s_1} \hat{a}_{\vec{k}, s_1} | \Phi_0 \rangle \\
&= -\frac{e^2}{2V} \sum'_{\vec{k}, \vec{q}} \sum_{s_1} \frac{4\pi}{q^2} \langle \Phi_0 | \hat{a}_{\vec{k}+\vec{q}, s_1}^\dagger \hat{a}_{\vec{k}+\vec{q}, s_1} \hat{a}_{\vec{k}, s_1}^\dagger \hat{a}_{\vec{k}, s_1} | \Phi_0 \rangle \\
&= -\frac{e^2}{2V} \sum'_{\vec{k}, \vec{q}} \sum_{s_1} \frac{4\pi}{q^2} \langle \Phi_0 | \hat{n}_{\vec{k}+\vec{q}, s_1} \hat{n}_{\vec{k}, s_1} | \Phi_0 \rangle.
\end{aligned} \tag{7}$$

The state $\hat{n}_{\vec{k}, s_1} | \Phi_0 \rangle$ doesn't vanish only if $|\Phi_0\rangle$ consists the state $|\vec{k}, s_1\rangle$. But $|\Phi_0\rangle$ consists all the states where $|\vec{k}| < k_F$ so only these \vec{k} values contribute to the sum in Eq. (7). In a similar manner, we can deduce that only $|\vec{k} + \vec{q}| < k_F$ contribute. Thus

$$E_0^{(1)} = -\frac{e^2}{2V} \times 2 \sum'_{\vec{k}, \vec{q}} \frac{4\pi}{q^2} \Theta(k_F - |\vec{k}|) \Theta(k_F - |\vec{k} + \vec{q}|), \tag{8}$$

where $\Theta(\cdot)$ is the Heaviside function. This is very similar to what we saw earlier. Each summation can be replaced by $V \int d^3k/(2\pi)^3$. Thus

$$E_0^{(1)} = -\frac{4\pi V^2 e^2}{(2\pi)^6 V} \int d^3q \frac{1}{q^2} \int d^3k \Theta(k_F - |\vec{k}|) \Theta(k_F - |\vec{k} + \vec{q}|). \quad (9)$$

Let's look first on the k integral. This is actually the intersection volume between two spheres of radius k_F located at a distance q apart. This volume is given by

$$\int d^3k \Theta(k_F - |\vec{k}|) \Theta(k_F - |\vec{k} + \vec{q}|) = \left(\frac{4\pi}{3} k_F^3 - \pi k_F^2 q + \frac{\pi q^3}{12} \right) \Theta(2k_F - q). \quad (10)$$

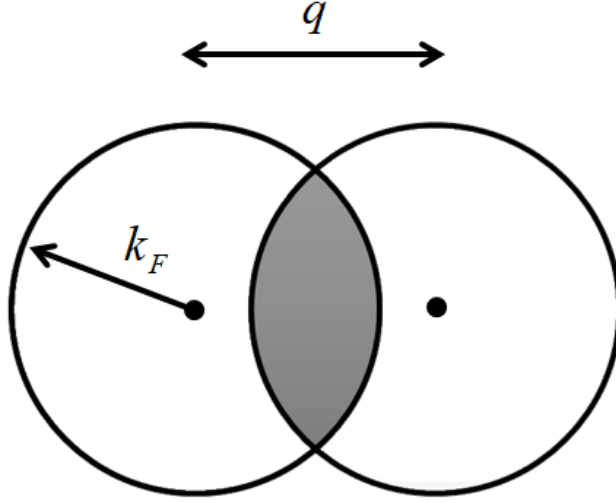


Figure 1: Two spheres of radius k_F at a distance q apart. The volume of interest is shaded in gray.

Plugging this expression back in Eq. (9) yields:

$$\begin{aligned} E_0^{(1)} &= -\frac{V e^2}{16\pi^5} \int_0^{2k_F} q^2 dq \int_{-1}^1 d\cos\theta \int_0^{2\pi} d\phi \frac{1}{q^2} \left(\frac{4\pi}{3} k_F^3 - \pi k_F^2 q + \frac{\pi q^3}{12} \right) \\ &= -\frac{V e^2}{4\pi^4} \int_0^{2k_F} dq \left(\frac{4\pi}{3} k_F^3 - \pi k_F^2 q + \frac{\pi q^3}{12} \right) = -\frac{V e^2 k_F^4}{4\pi^3} = -\frac{3N e^2}{4\pi} (3\pi^2 n)^{1/3}. \end{aligned} \quad (11)$$

The ground state energy of the interacting system is therefore

$$E = E_0^{(0)} + E_0^{(1)} = \frac{3N}{5} \cdot \frac{\hbar^2 k_F^2}{2m} - \frac{3Ne^2}{4\pi} (3\pi^2 n)^{1/3} = N \left[\frac{3\hbar^2 (3\pi^2 n)^{2/3}}{10m} - \frac{3e^2}{4\pi} (3\pi^2 n)^{1/3} \right]. \quad (12)$$

Let us assume that the electrons are packed in atomic spheres of radius r_0 so $n = \left(\frac{4\pi}{3} r_0^3\right)^{-1}$. We will use also the Bohr radius, $a_0 = \hbar^2/me^2$.

$$\frac{E}{N} = \left(\frac{9\pi}{4}\right)^{1/3} \frac{3e^2}{2a_0} \left[\frac{(9\pi/4)^{1/3} a_0^2}{5 r_0^2} - \frac{1}{2\pi} \frac{a_0}{r_0} \right]. \quad (13)$$

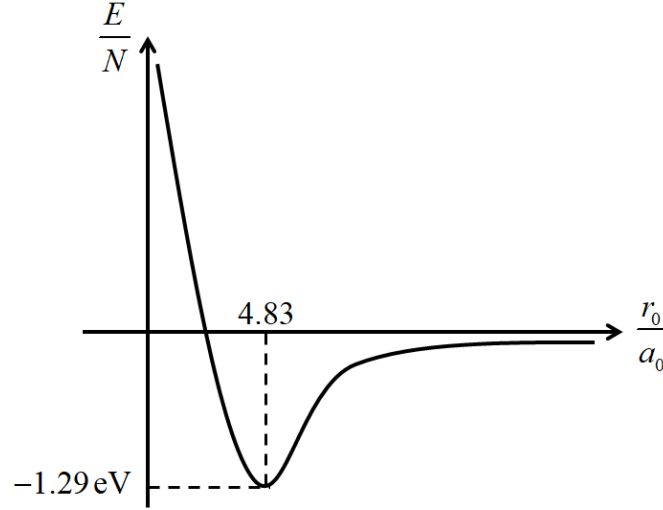


Figure 2: The energy of the system per electron as a function of the electrons spacing.

It is straightforward to find that the minimum energy corresponds to $r_0 = \frac{4\pi(9\pi/4)^{1/3}}{5} a_0 \approx 4.83a_0$. Once we plug this value in Eq. (13) we get

$$\left(\frac{E}{N}\right)_{\min} \approx -0.095 \times \frac{e^2}{2a_0} = -0.095 \times 13.6\text{eV} \approx -1.29\text{eV}. \quad (14)$$

Note: for Sodium metal $E/N = -1.13\text{eV}$ and $r_0 = 3.96a_0$. The model predicts the ground state energy and spacing very well for Sodium, with error of 15-20%.

Question 2

Consider the Hamiltonian

$$\hat{H} = \epsilon \left(\hat{a}_1^\dagger a_1 + \hat{a}_2^\dagger a_2 \right) + \Delta \left(\hat{a}_1^\dagger \hat{a}_2^\dagger + \hat{a}_2 \hat{a}_1 \right), \quad (15)$$

where $\epsilon > \Delta$ are positive and real numbers. Use Bogoliubov transformation to find the eigen-energies of the system. Do it when $\hat{a}_1^\dagger, \hat{a}_2^\dagger$ are

1. bosonic creation operators.
2. fermionic creation operators.

Solution to 1

We use the following Bogoliubov transformation,

$$\hat{c}_1 \equiv u \hat{a}_1 + v \hat{a}_2^\dagger \quad (16)$$

$$\hat{c}_2^\dagger \equiv u \hat{a}_2^\dagger + v \hat{a}_1. \quad (17)$$

where u, v are real numbers. We require the commutation relations

$$[\hat{c}_i, \hat{c}_j^\dagger] = \delta_{i,j} \quad (18)$$

$$[\hat{c}_i, \hat{c}_j] = [\hat{c}_i^\dagger, \hat{c}_j^\dagger] = 0. \quad (19)$$

The requirement of Eq. (18) leads to $u^2 - v^2 = 1$. Let's show this explicitly for $i = j = 1$:

$$1 \stackrel{!}{=} [\hat{c}_1, \hat{c}_1^\dagger] = [u \hat{a}_1 + v \hat{a}_2^\dagger, u \hat{a}_1^\dagger + v \hat{a}_2] = u^2 \underbrace{[\hat{a}_1, \hat{a}_1^\dagger]}_{=1} + uv \underbrace{[\hat{a}_1, \hat{a}_2]}_{=0} + uv \underbrace{[\hat{a}_2^\dagger, \hat{a}_1^\dagger]}_{=0} + v^2 \underbrace{[\hat{a}_2^\dagger, \hat{a}_2]}_{=-1} = u^2 - v^2. \quad (20)$$

Very similarly, you can prove to yourself that Eq. (18) holds for $i = j = 2$ only if $u^2 - v^2 = 1$ (Eq. (18) is true for $i \neq j$ since \hat{c}_1 and \hat{c}_2^\dagger share the same operators which commute between themselves). Eq. (19) is automatically satisfied due to our construction of \hat{c}_1 and \hat{c}_2^\dagger in Eqs. (16) and (17). For example:

$$[\hat{c}_1, \hat{c}_2] = [u \hat{a}_1 + v \hat{a}_2^\dagger, u \hat{a}_2 + v \hat{a}_1^\dagger] = u^2 \underbrace{[\hat{a}_1, \hat{a}_2]}_{=0} + uv \underbrace{[\hat{a}_1, \hat{a}_1^\dagger]}_{=1} + uv \underbrace{[\hat{a}_2^\dagger, \hat{a}_2]}_{=-1} + v^2 \underbrace{[\hat{a}_2^\dagger, \hat{a}_1^\dagger]}_{=0} = uv - uv = 0. \quad (21)$$

It would be convenient to find the inverse transformation:

$$\hat{a}_1 = u \hat{c}_1 - v \hat{c}_2^\dagger \quad (22)$$

$$\hat{a}_2^\dagger = u \hat{c}_2^\dagger - v \hat{c}_1. \quad (23)$$

Let us calculate first:

$$\begin{aligned} \hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2 &= (u \hat{c}_1^\dagger - v \hat{c}_2) (u \hat{c}_1 - v \hat{c}_2^\dagger) + (u \hat{c}_2^\dagger - v \hat{c}_1) (u \hat{c}_2 - v \hat{c}_1^\dagger) \\ &= u^2 (\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2) + v^2 (\hat{c}_1 \hat{c}_1^\dagger + \hat{c}_2 \hat{c}_2^\dagger) - uv (\hat{c}_2 \hat{c}_1 + \hat{c}_1 \hat{c}_2 + \hat{c}_2^\dagger \hat{c}_1^\dagger + \hat{c}_1^\dagger \hat{c}_2^\dagger) \\ &= (u^2 + v^2) (\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2) - 2uv (\hat{c}_1 \hat{c}_2 + \hat{c}_1^\dagger \hat{c}_2^\dagger) + 2v^2 \end{aligned} \quad (24)$$

where the last step comes from the commutation relations of Eqs. (18) and (19). Next, we calculate:

$$\begin{aligned}
\hat{a}_1^\dagger \hat{a}_2^\dagger + \hat{a}_2 \hat{a}_1 &= (u\hat{c}_1^\dagger - v\hat{c}_2) (u\hat{c}_2^\dagger - v\hat{c}_1) + (u\hat{c}_2 - v\hat{c}_1^\dagger) (u\hat{c}_1 - v\hat{c}_2^\dagger) \\
&= -2uv (\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2 \hat{c}_2^\dagger) + (u^2 + v^2) (\hat{c}_2 \hat{c}_1 + \hat{c}_1^\dagger \hat{c}_2^\dagger) \\
&= -2uv (\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2) + (u^2 + v^2) (\hat{c}_1 \hat{c}_2 + \hat{c}_1^\dagger \hat{c}_2^\dagger) - 2uv
\end{aligned} \tag{25}$$

where the last step comes from the commutation relations. We now plug Eqs. (24) and (25) in the Hamiltonian:

$$\hat{H} = [(u^2 + v^2)\epsilon - 2uv\Delta] (\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2) + [(u^2 + v^2)\Delta - 2uv\epsilon] (\hat{c}_1 \hat{c}_2 + \hat{c}_1^\dagger \hat{c}_2^\dagger) + 2v^2\epsilon - 2uv\Delta, \tag{26}$$

The two last terms in the Hamiltonian are scalars in Hilbert space — these have no physical importance and we can therefore omit them in the rest of the calculation. In order to make the Hamiltonian diagonalized we need to require that the off-diagonal term vanishes:

$$(u^2 + v^2)\Delta - 2uv\epsilon \stackrel{!}{=} 0, \tag{27}$$

or (by multiplying Eq. (27) by Δ/u^2):

$$\Delta^2 \frac{v^2}{u^2} - 2\epsilon\Delta \frac{v}{u} + \Delta^2 = 0. \tag{28}$$

Define $x \equiv \Delta v/u$ and the equation becomes

$$x^2 - 2\epsilon x + \Delta^2 = 0. \tag{29}$$

The solution for x is¹

$$\Delta \frac{v}{u} = x = \epsilon - \sqrt{\epsilon^2 - \Delta^2} = \epsilon - E, \quad E \equiv \sqrt{\epsilon^2 - \Delta^2}. \tag{30}$$

We now have two equations with two unknowns:

$$u^2 - v^2 = 1 \tag{31}$$

$$\Delta \frac{v}{u} = \epsilon - E. \tag{32}$$

The solutions for these equations are

$$u^2 = \frac{\Delta^2}{\Delta^2 - (\epsilon - E)^2} = \frac{\epsilon^2 - E^2}{(\epsilon^2 - E^2) - (\epsilon - E)^2} = \frac{\epsilon + E}{(\epsilon + E) - (\epsilon - E)} = \frac{\epsilon}{2E} + \frac{1}{2} \tag{33}$$

$$v^2 = \frac{(\epsilon - E)^2}{\Delta^2 - (\epsilon - E)^2} = \frac{(\epsilon - E)^2}{(\epsilon^2 - E^2) - (\epsilon - E)^2} = \frac{\epsilon - E}{(\epsilon + E) - (\epsilon - E)} = \frac{\epsilon}{2E} - \frac{1}{2} \tag{34}$$

¹We rule out the "+" solution. This is because for that solution, $\Delta = 0$ would then imply $\epsilon = 0$, which is not necessarily true.

We need to compute now several more quantities:

$$(u^2 + v^2) \epsilon = \frac{\epsilon^2}{E} \quad (35)$$

$$2uv\Delta = 2u^2\Delta \frac{v}{u} \stackrel{(1)}{=} 2u^2(\epsilon - E) = \left(\frac{\epsilon}{E} + 1\right)(\epsilon - E) = \frac{\epsilon^2 - E^2}{E}, \quad (36)$$

where equality (1) follows from Eq. (30). Finally, we plug Eqs. (35) and (36) back in the Hamiltonian of Eq. (26) to find

$$\boxed{\hat{H} = E \left(\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2 \right), \quad E \equiv \sqrt{\epsilon^2 - \Delta^2}}. \quad (37)$$

Solution to 2

Let's assume first that the Bogoliubov transformation of Eqs. (16) and (17) still works for fermions. We now need to require the following anti-commutation relations

$$\{ \hat{c}_i, \hat{c}_j^\dagger \} = \delta_{i,j} \quad (38)$$

$$\{ \hat{c}_i, \hat{c}_j \} = \{ \hat{c}_i^\dagger, \hat{c}_j^\dagger \} = 0. \quad (39)$$

We check our assumption by evaluating

$$\{ \hat{c}_1, \hat{c}_2 \} = \left\{ u\hat{a}_1 + v\hat{a}_2^\dagger, u\hat{a}_2 + v\hat{a}_1^\dagger \right\} = u^2 \underbrace{\{ \hat{a}_1, \hat{a}_2 \}}_{=0} + uv \underbrace{\{ \hat{a}_1, \hat{a}_1^\dagger \}}_{=1} + uv \underbrace{\{ \hat{a}_2^\dagger, \hat{a}_2 \}}_{=1} + v^2 \underbrace{\{ \hat{a}_2^\dagger, \hat{a}_1^\dagger \}}_{=0} = uv + uv \neq 0. \quad (40)$$

We see that this anti-commutator does not vanish as it should, so we must think of a different transformation. Thus, we instead use (notice the minus sign at Eq. (42)!):

$$\hat{c}_1 = u\hat{a}_1 + v\hat{a}_2^\dagger \quad (41)$$

$$\hat{c}_2^\dagger = u\hat{a}_2^\dagger - v\hat{a}_1. \quad (42)$$

For this transformation we indeed get that $\{ \hat{c}_1, \hat{c}_2 \} = 0$. However, now we get a different relation between u and v since

$$1 \stackrel{!}{=} \{ \hat{c}_1, \hat{c}_1^\dagger \} = \left\{ u\hat{a}_1 + v\hat{a}_2^\dagger, u\hat{a}_1^\dagger + v\hat{a}_2 \right\} = u^2 \underbrace{\{ \hat{a}_1, \hat{a}_1^\dagger \}}_{=1} + uv \underbrace{\{ \hat{a}_1, \hat{a}_2 \}}_{=0} + uv \underbrace{\{ \hat{a}_2^\dagger, \hat{a}_1^\dagger \}}_{=0} + v^2 \underbrace{\{ \hat{a}_2^\dagger, \hat{a}_2 \}}_{=1} = u^2 + v^2, \quad (43)$$

and we get the same relation for $\{ \hat{c}_2, \hat{c}_2^\dagger \} = 1$. The inverse transformation also slightly changes,

$$\hat{a}_1 = u\hat{c}_1 - v\hat{c}_2^\dagger \quad (44)$$

$$\hat{a}_2^\dagger = u\hat{c}_2^\dagger + v\hat{c}_1, \quad (45)$$

and now the Hamiltonian becomes (you may fill in the details of the algebra):

$$\hat{H} = \left[(u^2 - v^2) \epsilon + 2uv\Delta \right] \left(\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2 \right) + \left[(u^2 - v^2) \Delta - 2uv\epsilon \right] \left(\hat{c}_2 \hat{c}_1 + \hat{c}_1^\dagger \hat{c}_2^\dagger \right) + 2v^2\epsilon - 2uv\Delta. \quad (46)$$

Now, in order to diagonalize the Hamiltonian, we require

$$(u^2 - v^2) \Delta - 2uv\epsilon \stackrel{!}{=} 0, \quad (47)$$

and following the same steps we did in the bosons case, we now find

$$\Delta \frac{v}{u} = -\epsilon + E, \quad E \equiv \sqrt{\epsilon^2 + \Delta^2} \quad (48)$$

So again, we have two equations with two unknowns, whose solutions are

$$u^2 = \frac{1}{2} + \frac{\epsilon}{2E} \quad (49)$$

$$v^2 = \frac{1}{2} - \frac{\epsilon}{2E}, \quad (50)$$

and we end up with the following Hamiltonian:

$$\boxed{\hat{H} = E (\hat{c}_1^\dagger \hat{c}_1 + \hat{c}_2^\dagger \hat{c}_2), \quad E \equiv \sqrt{\epsilon^2 + \Delta^2}.} \quad (51)$$

Notice the different eigen-energies for bosons and fermions.