I. Kramers Degeneracy

(a) Show that the energy levels of a system that is time-reversal invariant and with half-odd integer angular momentum j (like one consisting of an odd number of electrons) will be at least two-fold degenerate.

Solution:
Suppose that we have an energy eigenket $|n\rangle$ and that H and the time-reversal operator Θ commute with each other. Note that $\Theta|n\rangle$ is the time-reversed state of $|n\rangle$. Then, we have

$$E_n\Theta|n\rangle = H\Theta|n\rangle = \Theta H|n\rangle \tag{1}$$

which shows that $|n\rangle$ and $\Theta|n\rangle$ belong to the same energy eigenvalue E_n. This means that these two states should differ by a phase factor at most:

$$\Theta|n\rangle = e^{i\delta}|n\rangle \tag{2}$$

Then, we get

$$\Theta^2|n\rangle = \Theta\left(e^{i\delta}|n\rangle\right) = e^{-i\delta}\Theta|n\rangle = e^{-i\delta}e^{i\delta}|n\rangle = |n\rangle \tag{3}$$

However, for a system with half-odd integer angular momentum j, $\Theta^2 = -1$ always. Thus, we have here a contradiction which means that $\Theta|n\rangle$ must be a distinct state from $|n\rangle$ with the same energy (*i.e.* a degeneracy in the system). There might be other degeneracies other than this so the said system will at least be two-fold degenerate

(b) Argue that this degeneracy is not lifted by an external electric field, but can be lifted by an external magnetic field.

Solution:
Since Θ is anti-unitary, x must be even while p and S must be odd under time reversal to preserve the commutation relation

$$[x_i, p_j] = i\hbar\delta_{ij} \tag{4}$$

and

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k \tag{5}$$

Thus, we require that

$$\Theta\mathbf{x}\Theta^{-1} = \mathbf{x}, \quad \Theta\mathbf{p}\Theta^{-1} = -\mathbf{p}, \quad \Theta\mathbf{S}\Theta^{-1} = -\mathbf{S} \tag{6}$$

Now, if the system is under the presence of an external electric field, then their interaction will be in the form of a potential that is dependent only on $\mathbf{x}$. For example, the interaction of a static electric field with charged particles result to

$$V(\mathbf{x}) = e\phi(\mathbf{x}) \tag{7}$$

where $\phi(\mathbf{x})$ is the electrostatic potential. Because of this and the fact that $\mathbf{x}$ is even under time-revesal, we can infer that

$$[\Theta, H] = 0 \tag{8}$$

As Θ and H still commute, the degeneracy is not lifted. However, if the system interacts with an external electric field, then the Hamiltonian can have terms that contain $\mathbf{S}\cdot\mathbf{B}$ and

$\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}$ where $B = \nabla \times \mathbf{A}$. Since p and S are odd under time reversal, we can infer that

$$[\Theta, H] \neq 0 \tag{9}$$

Since Θ and H no longer commute, the argument for obtaining at least a two-fold degeneracy in a time-reversal invariant system with half-integer j is not valid any more. The states $\Theta |n\rangle$ and $|n\rangle$ can have different energies, lifting the degeneracy.

II. Van der Waals Interaction

Prove that the interaction between two polarizable hydrogen-like atoms in their ground state leads to a r^{-6} potential in perturbation theory.

Solution:
The total Hamiltonian in this scenario is

$$H = H_0 + V = (H_{0_1} + H_{0_2}) + V \tag{10}$$

where the unperturbed Hamiltonians H_{0_1} and H_{0_2} for both atoms and their interaction V is given by

$$H_{0_{1[2]}} = -\frac{\hbar^2}{2m}\nabla^2_{1[2]} - \frac{e^2}{r_{1[2]}}, \quad V = \frac{e^2}{r} + \frac{e^2}{|\mathbf{r} + \mathbf{r}_2 - \mathbf{r}_1|} - \frac{e^2}{|\mathbf{r} + \mathbf{r}_2|} - \frac{e^2}{|\mathbf{r} - \mathbf{r}_1|} \tag{11}$$

Note that $\mathbf{r} = r\hat{\boldsymbol{k}}$. H_0 here is the product of the ground state wave functions

$$\begin{gathered} U_0^{(0)}(\mathbf{r}_1, \mathbf{r}_2) = U_{100}^{(0)}(\mathbf{r}_1)\, U_{100}^{(0)}(\mathbf{r}_2) \\ \langle \mathbf{r}_1, \mathbf{r}_2 | 0^{(0)} \rangle = \langle \mathbf{r}_1 | 100 \rangle \langle \mathbf{r}_2 | 100 \rangle \end{gathered} \tag{12}$$

Note that

$$\frac{1}{|\mathbf{r} + \mathbf{r}_2|} = \frac{1}{\sqrt{|\mathbf{r}|^2 + |\mathbf{r}_2|^2 + 2\mathbf{r}_2 \cdot \mathbf{r}}} = \frac{1}{\sqrt{r^2 + r_2^2 + 2z_2 r}} = \frac{1}{r}\frac{1}{\sqrt{1 + \left(\frac{r_2}{r}\right)^2 + 2\frac{z_2}{r}}} \tag{13}$$

and

$$\frac{1}{|\mathbf{r} - \mathbf{r}_1|} = \frac{1}{\sqrt{|\mathbf{r}|^2 + |\mathbf{r}_1|^2 - 2\mathbf{r}_1 \cdot \mathbf{r}}} = \frac{1}{\sqrt{r^2 + r_1^2 - 2z_1 r}} = \frac{1}{r}\frac{1}{\sqrt{1 + \left(\frac{r_1}{r}\right)^2 - 2\frac{z_1}{r}}} \tag{14}$$

If we assume that $r >> a_0 \approx |\mathbf{r}_1| \approx |\mathbf{r}_2|$, then we obtain

$$\begin{aligned} \frac{1}{|\mathbf{r} + \mathbf{r}_2 - \mathbf{r}_1|} &= \frac{1}{\sqrt{|\mathbf{r}|^2 + |\mathbf{r}_2 - \mathbf{r}_1|^2 + 2(\mathbf{r}_2 - \mathbf{r}_1) \cdot \mathbf{r}}} \\ &= \frac{1}{\sqrt{r^2 + |\mathbf{r}_2 - \mathbf{r}_1|^2 + 2(z_2 - z_1)r}} \\ &\approx \frac{1}{\sqrt{r^2}} \\ \frac{1}{|\mathbf{r} + \mathbf{r}_2 - \mathbf{r}_1|} &\approx \frac{1}{r} \end{aligned} \tag{15}$$

The binomial expansion, which is valid in this case, is given by

$$(1+x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \dots \tag{16}$$

which, for $n = -1/2$, becomes

$$(1+x)^(-1/2) = 1 - \frac{1}{2}x + \frac{3}{8}x^2 + \dots \tag{17}$$

Thus, Eq. (13) becomes

$$\begin{aligned}
\frac{1}{|\mathbf{r}+\mathbf{r}_2|} &= \frac{1}{r}\left[1 + \left(\frac{r_2}{r}\right)^2 + 2\frac{z_2}{r}\right]^{-1/2} \\
&= \frac{1}{r}\left[1 - \frac{1}{2}\left(\frac{r_2}{r}\right)^2 - \frac{z_2}{r} + \frac{3}{8}\left(\left(\frac{r_2}{r}\right)^2 + 2\frac{z_2}{r}\right)^2 + \dots\right] \\
&= \frac{1}{r}\left[1 - \frac{1}{2}\left(\frac{r_2}{r}\right)^2 - \frac{z_2}{r} + \frac{3}{8}\cdot 4\left(\frac{z_2}{r}\right)^2 + \dots\right] \\
\frac{1}{|\mathbf{r}+\mathbf{r}_2|} &\approx \frac{1}{r}\left[1 - \frac{1}{2}\left(\frac{r_2}{r}\right)^2 - \frac{z_2}{r} + \frac{3}{2}\left(\frac{z_2}{r}\right)^2\right]
\end{aligned} \tag{18}$$

where we kept terms only up to the order R^{-3}. In the same manner, Eq. (14) leads to

$$\begin{aligned}
\frac{1}{|\mathbf{r}-\mathbf{r}_1|} &= \frac{1}{r}\left[1 + \left(\frac{r_1}{r}\right)^2 - 2\frac{z_1}{r}\right]^{-1/2} \\
&= \frac{1}{r}\left[1 - \frac{1}{2}\left(\frac{r_1}{r}\right)^2 + \frac{z_1}{r} + \frac{3}{8}\left(\left(\frac{r_1}{r}\right)^2 - 2\frac{z_1}{r}\right)^2 + \dots\right] \\
&= \frac{1}{r}\left[1 - \frac{1}{2}\left(\frac{r_1}{r}\right)^2 + \frac{z_1}{r} + \frac{3}{8}\cdot 4\left(\frac{z_1}{r}\right)^2 + \dots\right] \\
\frac{1}{|\mathbf{r}-\mathbf{r}_1|} &\approx \frac{1}{r}\left[1 - \frac{1}{2}\left(\frac{r_1}{r}\right)^2 + \frac{z_1}{r} + \frac{3}{2}\left(\frac{z_2}{r}\right)^2\right]
\end{aligned} \tag{19}$$

Substituting these equations to V, we have

$$\begin{aligned}
V &\approx \frac{e^2}{r} + \frac{e^2}{r} - \frac{e^2}{r}\left[1 - \frac{1}{2}\left(\frac{r_2}{r}\right)^2 - \frac{z_2}{r} + \frac{3}{2}\left(\frac{z_2}{r}\right)^2\right] - \frac{e^2}{r}\left[1 - \frac{1}{2}\left(\frac{r_1}{r}\right)^2 + \frac{z_1}{r} + \frac{3}{2}\left(\frac{z_2}{r}\right)^2\right] \\
&\approx \frac{e^2}{r^3}\left[2r^2 - \left(r^2 - \frac{1}{2}r_2^2 - z_2 r + \frac{3}{2}z_2^2\right) - \left(r^2 - \frac{1}{2}r_1^2 + z_1 r + \frac{3}{2}z_1^2\right)\right] \\
&\approx \frac{e^2}{r^3}\left[\frac{1}{2}\left(r_2^2 + r_1^2\right) + r\left(z_2 - z_1\right) - \frac{3}{2}\left(z_2^2 + z_1^2\right)\right] \\
V &\approx \frac{e^2}{r^3}\left[\frac{1}{2}\left(x_2^2 + y_2^2 + z_2^2 + x_1^2 + y_1^2 + z_1^2\right) + r\left(z_2 - z_1\right) - \frac{3}{2}\left(z_2^2 + z_1^2\right)\right]
\end{aligned} \tag{20}$$

Now, note that with $|\mathbf{r}_1| \approx |\mathbf{r}_2|$, we can infer that $x_1 \approx x_2$. Thus, we obtain

$$x_2^2 + x_1^2 \approx x_1^2 + x_1^2 = 2x_1^2 = 2x_1 x_1 \approx 2x_1 x_2 \tag{21}$$

This also applies to other coordinates. Also, note that$z_2 - z_1 \approx 0$. Applying these relations to V, we get

$$\begin{aligned} V &\approx \frac{e^2}{r^3}\left[\frac{1}{2}\left(x_2^2 + x_1^2 + y_2^2 + y_1^2\right) - \left(z_2^2 + z_1^2\right)\right] \\ &\approx \frac{e^2}{r^3}\left[\frac{1}{2}\left(2x_1x_2 + 2y_1y_2\right) - 2z_1z_2\right] \\ V &\approx \frac{e^2}{r^3}\left(x_1x_2 + 2y_1y_2 - 2z_1z_2\right) \end{aligned} \tag{22}$$

Using this, we calculate the first order correction to be

$$E^{(1)} \approx \langle 0^{(0)}|V|0^{(0)}\rangle = \frac{e^2}{r^3}\langle 0^{(0)}|x_1x_2 + 2y_1y_2 - 2z_1z_2|0^{(0)}\rangle = 0 \tag{23}$$

since

$$\langle 0^{(0)}|x_1x_2|0^{(0)}\rangle = \int d\mathbf{r}_1 \int d\mathbf{r}_2 U_{100}^{(0)}\left(\mathbf{r}_1\right) U_{100}^{(0)}\left(\mathbf{r}_2\right)\left(x_1x_2\right) = 0 \tag{24}$$

as $U_0^{(0)}$ is even while V is an odd function for each coordinate. On the other hand, the second order correction leads to

$$E^{(2)} \approx \sum_{k\neq 0}\frac{|\langle k^{(0)}|V|0^{(0)}\rangle|^2}{E_0 - E_k} =\approx \frac{e^4}{r^6}\sum_{k\neq 0}\frac{|\langle k^{(0)}|x_1x_2 + 2y_1y_2 - 2z_1z_2|0^{(0)}\rangle|^2}{E_0 - E_k} \tag{25}$$

Since $E_k > E_0$ as E_0 is the ground state energy, we can infer that the denominator is negative. From the form of the numerator, we can also infer that it is positive. Thus, we see that the interaction varies as $-1/r^6$. This weak attractive interaction between two ground state atoms is the Van der Waals interaction.

III. Perturbed Harmonic Oscillator

Let a particle be in a harmonic potential of natural frequency ω. It is perturbed by a weak constant force $f > 0$. (Use parity to simplify matrix element calculations as needed.)

(a) Obtain the shift in the ground state energy up to second order.

Solution:
The unperturbed Hamiltonian for this scenario is

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 \tag{26}$$

The unperturbed allowed energies are

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \tag{27}$$

while the perturbation is of the form

$$V = fx \tag{28}$$

It would be useful later on to note that from $a\,|n\rangle = \sqrt{n}\,|n-1\rangle$ and $a^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle$, along with $[a, a^\dagger] = 1$, we can obtain the following relations:

$$\langle n|\,a^\dagger \pm a\,|n\rangle = \langle n|\,a^\dagger\,|n\rangle \pm \langle n|\,a\,|n\rangle = \sqrt{n+1}\,\cancelto{0}{\langle n|n+1\rangle} \pm \sqrt{n}\,\cancelto{0}{\langle n|n-1\rangle} = 0 \tag{29}$$

$$\langle n|\,a^2\,|n\rangle = \sqrt{n}\,\langle n|a|n-1\rangle = \sqrt{n(n-1)}\,\cancelto{0}{\langle n|n-2\rangle} = 0 \tag{30}$$

$$\langle n|\left(a^\dagger\right)^2|n\rangle = \sqrt{n+1}\,\langle n|a^\dagger|n-1\rangle = \sqrt{(n+1)(n-1)}\,\cancelto{0}{\langle n|n+2\rangle} = 0 \tag{31}$$

$$\langle n|\,a^\dagger a\,|n\rangle = \sqrt{n}\,\langle n|a^\dagger|n-1\rangle = \sqrt{n^2}\,\cancelto{1}{\langle n|n\rangle} = n \tag{32}$$

$$\langle n|\,aa^\dagger\,|n\rangle = \langle n|\,1 + a^\dagger a\,|n\rangle = \cancelto{1}{\langle n|n\rangle} + \langle n|a^\dagger a|n\rangle = 1 + n \tag{33}$$

Also, note that x and p are related to the annihilation and creation operators by

$$x = \sqrt{\frac{\hbar}{2m\omega}}\left(a^\dagger + a\right), \qquad p = -i\sqrt{\frac{m\omega\hbar}{2}}\left(a^\dagger - a\right) \tag{34}$$

Then, the first order correction to the energies is

$$\begin{aligned}
E_n^{(1)} &= \langle n|V|n\rangle \\
&= \langle n|fx|n\rangle \\
&= f\,\langle n|\sqrt{\frac{\hbar}{2m\omega}}\left(a^\dagger + a\right)|n\rangle \\
&= f\sqrt{\frac{\hbar}{2m\omega}}\,\langle n|a^\dagger + a|n\rangle \\
E_n^{(1)} &= 0
\end{aligned} \tag{35}$$

by making use of Eq. (29). As for the second order correction, we can calculate this using

$$E_n^{(2)} = \sum_{m\neq n} \frac{|\,\langle m|V|n\rangle\,|^2}{E_n - E_m} \tag{36}$$

Note that

$$\begin{aligned}
\langle m|V|n\rangle &= f\,\langle m|x|n\rangle \\
&= f\sqrt{\frac{\hbar}{2m\omega}}\,\langle m|a^\dagger + a|n\rangle \\
&= f\sqrt{\frac{\hbar}{2m\omega}}\left(\langle m|a^\dagger|n\rangle + \langle m|a|n\rangle\right) \\
\langle m|V|n\rangle &= f\sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n+1}\,\langle m|n+1\rangle + \sqrt{n}\,\langle m|n-1\rangle\right)
\end{aligned} \tag{37}$$

in which we can infer that

$$\langle m|V|n\rangle = \begin{cases} f\sqrt{\frac{(n+1)\hbar}{2m\omega}}, & m = n+1 \\ f\sqrt{\frac{n\hbar}{2m\omega}}, & m = n-1 \\ 0, & \text{other values of } m \end{cases} \tag{38}$$

Also, we have

$$E_n - E_{n+1} = \left(n + \frac{1}{2}\right)\hbar\omega - \left(n + 1 + \frac{1}{2}\right)\hbar\omega = -\hbar\omega \tag{39}$$

and

$$E_n - E_{n-1} = \left(n + \frac{1}{2}\right)\hbar\omega - \left(n - 1 + \frac{1}{2}\right)\hbar\omega = \hbar\omega \tag{40}$$

Thus, $E_n^{(2)}$ is calculated to be

$$\begin{aligned} E_n^{(2)} &= \frac{|\langle n+1|V|n\rangle|^2}{E_n - E_{n+1}} + \frac{|\langle n-1|V|n\rangle|^2}{E_n - E_{n-1}} \\ &= -\frac{1}{\hbar\omega}\left(f\sqrt{\frac{(n+1)\hbar}{2m\omega}}\right)^2 + \frac{1}{\hbar\omega}\left(f\sqrt{\frac{n\hbar}{2m\omega}}\right)^2 \\ &= \frac{f^2}{2m\omega^2}(n - n - 1) \\ E_n^{(2)} &= -\frac{f^2}{2m\omega^2} \end{aligned} \tag{41}$$

(b) Complete the square in the Hamiltonian to obtain the exact ground state energy.

Solution:
The total Hamiltonian is

$$H = H_0 + V = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 + fx = \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 + \frac{2f}{m\omega^2}x\right) \tag{42}$$

By completing the square:

$$\left(\frac{b}{2a}\right)^2 = \left(\frac{2f}{2m\omega^2}\right)^2 = \frac{f^2}{m^2\omega^4} \tag{43}$$

The Hamiltonian becomes

$$\begin{aligned} H &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x^2 + \frac{2f}{m\omega^2}x + \frac{f^2}{m^2\omega^4} - \frac{f^2}{m^2\omega^4}\right) \\ &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2\left(x - \frac{f}{m\omega^2}\right)^2 - \frac{f^2}{2m\omega^2} \end{aligned} \tag{44}$$

This means that the Hamiltonian is shifted by some constant term. To keep this shift, we apply a change of variables $x' = x - \frac{f}{m\omega^2}$ and let this be our new position operator. Letting $\langle n|$ act on both sides of $H|n\rangle = E_n|n\rangle$, we have

$$\begin{aligned} \langle n|H|n\rangle &= \langle n|E_n|n\rangle \\ \langle n|\frac{p^2}{2m} + \frac{1}{2}m\omega^2x'^2 - \frac{f^2}{2m\omega^2}|n\rangle &= E_n \cancelto{1}{\langle n|n\rangle} \end{aligned} \tag{45}$$

Substituting in Eq. (34) into E_n (just note that $x \to x'$), we get

$$E_n = \frac{1}{2m}\langle n|\left(-i\sqrt{\frac{m\omega\hbar}{2}}\left(a^\dagger + a\right)\right)^2|n\rangle + \frac{1}{2}m\omega^2\langle n|\left(\sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)\right)^2|n\rangle - \frac{f^2}{2m\omega^2}\cancelto{1}{\langle n|n\rangle} \tag{46}$$

Expanding this,

$$\begin{aligned} E_n = &-\frac{1}{2m}\left(\frac{m\omega\hbar}{2}\right)\langle n|\left(a^\dagger\right)^2 + a^2 + a^\dagger a + aa^\dagger|n\rangle \\ &+\frac{1}{2}m\omega^2\left(\frac{\hbar}{2m\omega}\right)\langle n|\left(a^\dagger\right)^2 + a^2 - a^\dagger a - aa^\dagger|n\rangle - \frac{f^2}{2m\omega^2} \end{aligned} \tag{47}$$

Applying Eqs. (29) - (33), E_n becomes

$$\begin{aligned} E_n &= -\frac{\hbar\omega}{4}[-n-(1+n)] + \frac{\hbar\omega}{4}(n+1+n) - \frac{f^2}{2m\omega^2} \\ &= \frac{\hbar\omega}{4}2(2n+1) - \frac{f^2}{2m\omega^2} \\ E_n &= \frac{\hbar\omega}{2}(2n+1) - \frac{f^2}{2m\omega^2} \end{aligned} \tag{48}$$

Therefore, the exact ground state energy is

$$E_0 = \frac{\hbar\omega}{2} - \frac{f^2}{2m\omega^2} \tag{49}$$

IV. Delta Function Perturbation

A particle is in an infinite square well of width a. Let there be a repulsive delta perturbation $\alpha\delta(x-a/2)$ located at the center of the well. Calculate the correction to the ground state energy up to second-order perturbation theory.

Solution:
The allowed energies of a particle in an infinite square well is

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{50}$$

It is given that we introduce a perturbation V where

$$V = \alpha\delta(x-\frac{a}{2}) \tag{51}$$

at the center of the well. Note that the unperturbed wave functions for this scenario are given by

$$\langle x|n^{(0)}\rangle = \psi_n^{(0)}(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right) \tag{52}$$

Then, we can calculate the first-order correction to the energies to be

$$\begin{aligned} E_n^{(1)} &= \langle n^{(0)}|V|n^{(0)}\rangle \\ &= \langle n^{(0)}|\alpha\delta(x-\frac{a}{2})|n^{(0)}\rangle \\ &= \alpha\int_0^\infty \left(\psi_n^{(0)}\right)^* \delta(x-\frac{a}{2})\psi_n^{(0)}\mathrm{d}x \\ &= \alpha\int_0^\infty \frac{2}{a}\sin^2\left(\frac{n\pi}{a}x\right)\delta(x-\frac{a}{2})\mathrm{d}x \\ E_n^{(1)} &= \alpha\frac{2}{a}\sin^2\left(\frac{n\pi}{2}\right) \end{aligned} \tag{53}$$

We can infer from this that

$$E_n^{(1)} = \begin{cases} 0, & n \text{ is even} \\ \alpha\frac{2}{a}, & n \text{ is odd} \end{cases} \tag{54}$$

As for the second-order correction, we can calculate this using

$$E_n^{(2)} = \sum_{k\neq n} \frac{|\langle k^{(0)}|V|n^{(0)}\rangle|^2}{E_n - E_k} \tag{55}$$

Note that

$$\begin{aligned} \langle k^{(0)}|V|n^{(0)}\rangle &= \langle k^{(0)}|\alpha\delta(x-\frac{a}{2})|n^{(0)}\rangle \\ &= \alpha\int_0^\infty \left(\psi_k^{(0)}\right)^* \delta(x-\frac{a}{2})\psi_n^{(0)}\mathrm{d}x \\ &= \alpha\int_0^\infty \frac{2}{a}\sin\left(\frac{k\pi}{a}x\right)\sin\left(\frac{n\pi}{a}x\right)\delta(x-\frac{a}{2})\mathrm{d}x \\ \langle k^{(0)}|V|n^{(0)}\rangle &= \alpha\frac{2}{a}\sin\left(\frac{k\pi}{2}\right)\sin\left(\frac{n\pi}{2}\right) \end{aligned} \tag{56}$$

in which we can infer that

$$|\langle k^{(0)}|V|n^{(0)}\rangle|^2 = \begin{cases} \alpha^2\frac{4}{a^2}, & n, m \text{ are both odd} \\ 0, & \text{other values of } m, n \end{cases} \tag{57}$$

Also, note that

$$E_n - E_k = \frac{n^2\pi^2\hbar^2}{2ma^2} - \frac{k^2\pi^2\hbar^2}{2ma^2} = (n^2-k^2)\frac{\pi^2\hbar^2}{2ma^2} \tag{58}$$

Thus, substituting these relations to Eq. (55), we obtain

$$E_n^{(2)} = \alpha^2\frac{4}{a^2}\cdot\frac{2ma^2}{\pi^2\hbar^2}\sum_{k\neq n}\frac{1}{n^2-k^2} \tag{59}$$

Now, by partial fraction decomposition, we have

$$\frac{1}{n^2-k^2} = \frac{A}{n-k} + \frac{B}{n+k} \tag{60}$$

which we can rearrange to

$$1 = A(n-k) + B(n+k) \tag{61}$$

From this, we can get the following system of equations:

$$1 = An + Bn \tag{62}$$
$$0 = Ak - Bk \tag{63}$$

which we can infer the relation

$$A = \frac{1}{2n} = B. \tag{64}$$

Applying this to Eq. (60) and the fact that n and k must be both odd, we get

$$\begin{aligned}\frac{1}{n^2-k^2} &= \frac{1}{2n}\left[\frac{1}{n-k}+\frac{1}{n+k}\right]\\ &= \frac{1}{2n}\left[\frac{1}{2i+1-(2j+1)}+\frac{1}{2i+1+2j+1}\right]\\ &= \frac{1}{2n}\left[\frac{1}{2(i-j)}+\frac{1}{2(i+j+1)}\right]\\ \frac{1}{n^2-k^2} &= \frac{1}{4n}\left[\frac{1}{i-j}+\frac{1}{i+j+1}\right]\end{aligned} \tag{65}$$

where $n=2i+1$ and $k=2j+1$.Note that the condition $k\neq n$ is equivalent to $i\neq j$. Splitting the sum into two parts (one with $k<n$ terms and another with $k>n$ terms), we have

$$\sum_{k\neq n}\frac{1}{n^2-k^2} = \frac{1}{4n}\left[\sum_{j=0}^{i-1}\left(\frac{1}{i-j}+\frac{1}{i+j+1}\right)+\sum_{j>i}\left(\frac{1}{i-j}+\frac{1}{i+j+1}\right)\right] \tag{66}$$

By rearranging the indices, note that we can get

$$\sum_{j=0}^{i-1}\frac{1}{i-j}=\sum_{l=1}^{i}\frac{1}{l}, \quad \sum_{j=i+1}^{2i}\frac{1}{i-j}=-\sum_{l=1}^{i}\frac{1}{l} \tag{67}$$

We see that these terms cancel out and Eq. (66) becomes

$$\begin{aligned}\sum_{k\neq n}\frac{1}{n^2-k^2} &= \frac{1}{4n}\left[\sum_{j=0}^{i-1}\frac{1}{i+j+1}+\sum_{j\geq 2i+1}\left(\frac{1}{i-j}+\frac{1}{i+j+1}\right)+\sum_{j=i+1}^{2i}\frac{1}{i+j+1}\right]\\ &= \frac{1}{4n}\left[\left(\sum_{j=0}^{i-1}\frac{1}{i+j+1}+\sum_{j=i+1}^{2i}\frac{1}{i+j+1}+\sum_{j\geq 2i+1}\frac{1}{i+j+1}\right)+\sum_{j\geq 2i+1}\frac{1}{i-j}\right]\\ &= \frac{1}{4n}\left[\left(\sum_{j\geq 0}\frac{1}{i+j+1}-\frac{1}{2i+1}\right)+\sum_{j\geq 2i+1}\frac{1}{i-j}\right]\\ &= \frac{1}{4n}\left[\sum_{l\geq i+1}\frac{1}{l}-\frac{1}{n}-\sum_{l\geq i+1}\frac{1}{l}\right]\\ \sum_{k\neq n}\frac{1}{n^2-k^2} &= -\frac{1}{4n^2}\end{aligned} \tag{68}$$

Therefore, $E_n^{(2)}$ becomes

$$E_n^{(2)} = \frac{8\alpha^2 m}{\pi^2\hbar^2}\cdot -\frac{1}{4n^2} = -\frac{2\alpha^2 m}{n^2\pi^2\hbar^2} \tag{69}$$