Solution to Problem Set No. 6: 
Time Independent Perturbation Theory

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1 The Anharmonic Oscillator

1.1

As a first step we invert the definitions of creation and annihilation operators to express \( \hat{X} \), \( \hat{P} \) in terms of \( (\hat{a}, \hat{a}^\dagger) \)

\[
\hat{X} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}^\dagger + \hat{a})
\]

(1)

\[
\hat{P} = i\sqrt{\frac{m\hbar\omega}{2}} (\hat{a}^\dagger - \hat{a})
\]

(2)

Hence

\[
\hat{V} = \lambda \hat{X}^4
\]

(3)

\[
= \frac{\lambda\hbar^2}{4m^2\omega^2} (\hat{a}^\dagger + \hat{a})^4
\]

(4)

Since the first order wave function mix is proportional to the expectation value \( \langle n|\hat{V}|m \rangle \), we see from the form of \( \hat{V} \) that for \( |m\rangle \) to mix with \( |n\rangle \), one need

\[
n - 4 \leq m \leq n + 4
\]

(5)

1.2

We now expand (4) out and write all terms in normal ordering:

\[
\hat{V} = \frac{\lambda\hbar^2}{4m^2\omega^2} \left[ \hat{a}^{4\dagger} + 4\hat{a}^{3\dagger}\hat{a} + 6\hat{a}^{2\dagger}\hat{a}^2 + 4\hat{a}^{3\dagger}\hat{a}^3 + \hat{a}^{4\dagger} + 6\hat{a}^{2\dagger} + 12\hat{a}^\dagger\hat{a} + 6\hat{a}^2 + 3 \right]
\]

(6)

The matrix element \( \langle n|\hat{V}|0 \rangle \) can be read off as

\[
\langle 0|\hat{V}|0 \rangle = 3 \frac{\lambda\hbar^2}{4m^2\omega^2}
\]

(7)

\[
\langle 2|\hat{V}|0 \rangle = 6\sqrt{2} \frac{\lambda\hbar^2}{4m^2\omega^2}
\]

(8)

\[
\langle 4|\hat{V}|0 \rangle = \sqrt{24} \frac{\lambda\hbar^2}{4m^2\omega^2}
\]

(9)
\[ \Delta E_n^{(1)} = \langle n|\hat{V}|n \rangle = \frac{\lambda h^2}{4m^2\omega^2} [3 + 12n + 6n(n - 1)] \] (10)

\[ |n^{(1)}\rangle = \sum_{m \neq n} \frac{\langle n|\hat{V}|m \rangle}{E_n - E_m} |m\rangle \] (11)
\[ = \frac{\lambda h}{4m^2\omega^3} \left( \frac{\sqrt{n(n-1)(n-2)(n-3)}}{4} |n-4\rangle + (2n-1)\sqrt{n(n-1)} |n-2\rangle 
- (2n+5)\sqrt{(n+1)(n+2)} |n+2\rangle - \frac{\sqrt{(n+1)(n+2)(n+3)(n+4)}}{4} |n+4\rangle \right) \] (12)

(for \( n < 4 \) just ignore the negative eigenkets)

\[ \Delta E_0^{(1)} = \langle 0|\hat{V}|0 \rangle = \frac{3\lambda h}{4m^2\omega^3} \] (13)
\[ \Delta E_0^{(2)} = \sum_{m \neq 0} \frac{|\langle m|\hat{V}|0 \rangle|^2}{E_0^{(0)} - E_m^{(0)}} = -\frac{21\lambda^2 h^3}{8m^4\omega^5} \] (14)

2 Charged Particle in a Magnetic Field

2.1 Assuming that the eigen wave function can be factorized into \( \Psi = 1/\sqrt{L}e^{iky}\phi(x) \) and plug it into the unperturbed Schrödinger equation \( H_0\Psi = E\Psi \) we can show that
\[ e^{iky} \left[ \hat{P}^2_x + \left( k\hbar - \frac{eB}{c} x \right)^2 \right] \phi_n(x) = 2MEe^{iky}\phi_n(x) \] (15)

We can factor \( e^{iky} \) out and rewrite the full eigen equation as
\[ \left[ \hat{P}^2_x + \left( k\hbar - \frac{eB}{c} X \right)^2 \right] \phi_n = 2M \phi_n \] (16)

We see that if we make a shift
\[ x \rightarrow x' = x - \frac{k\hbar c}{eB} \] (17)
\[ = x - kl^2 \] (18)

then since it is just a shift on \( x \), \( P_X \) stays invariant. So we can cast the whole eigen equation in terms of \( x' \):
\[ \left[ \hat{P}^2_{x'} + \frac{\hbar^2}{l^2} x'^2 \right] \phi_n = 2M \phi_n \] (19)
Hence the eigen function $\phi_n$ must be a function of $x' = x - kl^2$. Also note that this equation is just the equation of the 1D simple harmonic oscillator. We can directly write down its solution in terms of Hermite polynomials:

$$\phi_n(x') = [4^n(n!)^2\pi\hbar l^2]^{-1/4} H_n \left( \frac{x'}{l} \right) e^{-x'^2/2l^2} \tag{20}$$

The whole solution is thus

$$\Psi_{n,k}(x,y) = \frac{1}{\sqrt{L}} e^{iky} \phi_n(x - kl^2) \tag{21}$$

The unperturbed energies are just the eigen energy of a simple harmonic oscillator

$$E_{n,k} = \frac{\hbar eB}{Mc} (n + \frac{1}{2}) \tag{22}$$

$$= \hbar \omega_c (n + \frac{1}{2}) \tag{23}$$

We see that the $\Psi(x,y)$ is also a eigen function of $\hat{P}_y$. If we demand periodic boundary condition in the y direction, then we can show that $k = 2\pi m/L$, where $m$ is an integer. The constraint from magnetic flux is more subtle. In order to do this we first consider the case where the length of strip $W$ is finite and then take $W \to \infty$. We know that the symmetric point $x - kl^2$ of the wave function has to lie inside the region $-W/2 < x < W/2$, so

$$|kl^2| < \frac{W}{2} \tag{24}$$

$$\left| \frac{2\pi hc}{eBL} m \right| < \frac{W}{2} \tag{25}$$

$$|m| < \frac{eBW L}{4\pi hc} = \frac{N_\phi}{2} \tag{26}$$

Since $m$ can only take integer values, the allowed values of $m$ is thus

$$-\frac{N_\phi - 1}{2} < m < \frac{N_\phi - 1}{2} \tag{27}$$

2.2

Since $[\hat{H}, \hat{P}_y] = 0$, the y-momentum is conserved and the inner products of different $k$ eigenstates vanish by orthogonality. If $\tilde{V}(x)$ is an operator only depending on $x$, we can factor out the $x$ and $y$ inner products and show that $\langle n', k' | \tilde{V} | n, k \rangle$ of different $k$ vanish. More explicitly:

$$\langle n', k' | \tilde{V}(x) | n, k \rangle = \langle k' | \otimes \langle \phi_{n',k'} | \tilde{V}(x) ( | k \rangle \otimes | \phi_{n,k} \rangle) \tag{28}$$

$$= \langle k' | k \rangle \langle \phi_{n',k'} | \tilde{V}(x) | \phi_{n,k} \rangle \tag{29}$$

$$= \delta_{k,k'} \langle n', k' | \tilde{V}(x) | n, k \rangle \tag{30}$$

2.3

We skip the $y$ integrals here since the wave functions in y direction are othonomal.

$$V_{00}(k) = \frac{V_0}{\sqrt{\pi \hbar l^2}} \int_{-\infty}^{\infty} dx e^{-\frac{(x-kl)^2}{\alpha^2}} e^{-\frac{x^2}{2a^2}} \tag{31}$$

$$= \frac{V_0}{\sqrt{\hbar}} \left( \frac{l^2}{2a^2} + 1 \right)^{-\frac{1}{2}} e^{-\frac{k^2l^2}{2a^2} + l} \tag{32}$$
\[ V_{11}(k) = \frac{V_0}{\sqrt{4\pi\hbar^2}} \int_{-\infty}^{\infty} dx \frac{4x^2}{l^2} e^{-\frac{(x-kl)^2}{l^2}} e^{-\frac{x^2}{2a^2}} \]
\[ = \sqrt{8}V_0 \frac{a^3(l^2 + 2a^2(2k^2 + 1))}{(2a^2 + l^2)^{\frac{3}{2}}} e^{-\frac{k^2l^2}{2a^2 + l^2}} \] (33)

\[ V_{01}(k) = V_{10}(k) = \frac{V_0}{\sqrt{2\pi\hbar^2}} \int_{-\infty}^{\infty} dx \frac{2x}{l} e^{-\frac{(x-kl)^2}{l^2}} e^{-\frac{x^2}{2a^2}} \]
\[ = \sqrt{8}V_0 \frac{a^3k}{\sqrt{\hbar}} \frac{1}{(2a^2 + l^2)^{\frac{3}{2}}} e^{-\frac{k^2l^2}{2a^2 + l^2}} \] (34)

2.4

According to first order perturbation theory, the energy shift is proportional to the expectation value of the perturbative potential in the unperturbed eigenstates of which we just computed above.

\[ \Delta E_0(k) = V_{00}(k) = \frac{V_0}{\sqrt{\hbar}} \left( \frac{l^2}{2a^2} + 1 \right)^{-\frac{3}{2}} e^{-\frac{k^2l^2}{2a^2 + l^2}} \] (37)

\[ \Delta E_1(k) = V_{11}(k) = \frac{\sqrt{8}V_0 a^3(l^2 + 2a^2(2k^2 + 1))}{\sqrt{\hbar}} \frac{1}{(2a^2 + l^2)^{\frac{3}{2}}} e^{-\frac{k^2l^2}{2a^2 + l^2}} \] (38)

We plot the \( k \)-dependence of the energy difference below: (assuming \( V_0 = \hbar = a = l = 1 \))

We see that in the case of ground states, each \( k \) corresponds to a different shift \( \Delta E_0(k) \), so the degeneracies are completely removed. However in the first excited states, there is a region in which there are two different \( k \)'s corresponding to the same energy shift. We still have a two-fold degeneracies in first excited states in this region.

2.5

To the first order, the perturbed wave function is given by

\[ \Psi_n^{(1)} = \Psi_n^{(0)} + \sum_{m \neq n} \frac{\langle n|V|m \rangle}{E_n^{(0)} - E_m^{(0)}} \Psi_m^{(0)} \] (39)
Using our previous results we explicitly write down the perturbed wave functions for \( n = 0 \) and \( n = 1 \):

\[
\Psi_{0,k}^{(1)} = \frac{1}{\sqrt{L}} e^{iky} \left[ \phi_0(x - kl^2) - \frac{V_{10}(k)}{\hbar\omega_c} \phi_1(x - kl^2) \right]
\]

\[
\Psi_{1,k}^{(1)} = \frac{1}{\sqrt{L}} e^{iky} \left[ \phi_1(x - kl^2) + \frac{V_{10}(k)}{\hbar\omega_c} \phi_0(x - kl^2) \right]
\]

(40)

(41)

Where we ignored the contribution from all the higher energy levels.

Now we want to compute the total current

\[
\vec{J} = \frac{\hbar}{2mi} \int_{-\infty}^{\infty} dx \int_{-L/2}^{L/2} dy \vec{j}_{n,k}(x,y)
\]

(42)

where \( \vec{j}_{n,k}(x,y) \) is the current density

\[
\vec{j}_{n,k}(x,y) = \Psi_{n,k}(x,y)^* \vec{\nabla} \Psi_{n,k}(x,y) - \Psi_{n,k}(x,y) \vec{\nabla}^* \Psi_{n,k}(x,y)^*
\]

(43)

We immediately see that \( j_x \) is zero since \( \phi(x) \) is real everywhere even after the perturbation as we already know that wave functions of different \( k \) do not mix. The other component of current can be worked out to be

\[
j_y(x,y) = \frac{\hbar}{mL} |\phi_0^{(1)}(x - kl^2)|^2
\]

(44)

After integrating we obtain the total current as a function of \( (n,k) \):

\[
\vec{J}_{n,k} = \frac{\hbar}{m} \hat{y}
\]

(45)

The current is linear to \( k \). This is because we are working with eigenstates of \( \hat{P}_y \) and that the perturbation \( V \) does not depend on \( y \) so it preserves the \( y \)-symmetry.

2.6

If we look at the figure of the first order shift of the energy, we see that there is a region where \( \Delta E_0 > \Delta E_1 \). In this region if we tune \( V_0 \) large enough we can actually see that the two perturbed energy levels starting cross each other. We can calculate the required \( V_0 \) to be

\[
V_0(k) = \frac{\hbar\omega_c}{\Delta E_0(k) - \Delta E_1(k)}
\]

\[
= \sqrt{\frac{\hbar^3}{8\omega_c^2} \frac{(l^2 + 2a^2)^{5/2}}{a^3(l^2 + 4a^2k^2)} e^{2a^2x^2}}
\]

(46)

(47)

We also see that \( \Delta E_0 - \Delta E_1 \) has maximum at \( k = 0 \), so the mixing first occurs at \( k = 0 \) as one gradually increases \( V_0 \).

To resolve the degeneracy we turn to almost degenerate perturbation theory and treat the two nearly degenerate states exactly while keeping states of other \( k \) perturbatively. This means that we need to solve for the matrix equation

\[
\begin{pmatrix}
E_0^{(0)}(k) + V_{00}(k) & V_{01}(k) \\
V_{10}(k) & E_1^{(0)}(k) + V_{11}(k)
\end{pmatrix}
\begin{pmatrix}
\Psi
\end{pmatrix}
= E
\begin{pmatrix}
\Psi
\end{pmatrix}
\]

(48)
Defining $E^{(1)}_n = E^{(0)}_n + V_{nn}$ we write the eigenvalues as

$$E_{\pm}(k) = \frac{E^{(1)}_0(k) + E^{(1)}_1(k)}{2} \pm \sqrt{\left(\frac{E^{(1)}_0(k) - E^{(1)}_1(k)}{2}\right)^2 + V^{2}_{10}(k)}$$

(49)

Here since $V_{10}(k) \neq 0$, the energies will at least be split by $V_{10}(k)$. We see that the energy level actually repels each other as we tune up $V_0$, and we can infer that there won’t be any level crossing in the perturbative expansion.

### 3 Model of a Hydrogen-like Atom

#### 3.1

Since $\hat{W}(r)$ is a function only of $r$, it commutes with the total angular momentum operator $\hat{L}^2$ and the $z$-direction angular momentum operator $\hat{L}_z$. The matrix elements of $W$ can be decomposed into

$$\langle n', l', m' | \hat{W} | n, l, m \rangle = \langle n' | \hat{W}(r) | n \rangle \langle l', m' | l \rangle \langle m \rangle$$

(50)

$$= \delta_{l, l'} \delta_{m, m'} \langle n', l', m' | \hat{W} | n, l, m \rangle$$

(51)

#### 3.2

The perturbative potential $W(r)$ is

$$W(r) = \begin{cases} V_0 + e^2/r , & r \leq d \\ 0 , & r > d \end{cases}$$

(52)

We now calculate the matrix elements of $\hat{W}$:

$$\langle 1, 0, 0 | \hat{W} | 1, 0, 0 \rangle = \frac{4}{a_0^3} \int_0^d r^2 dr \left( V_0 + \frac{e^2}{r} \right) e^{-2r/a_0}$$

$$= \frac{1}{a_0^3} \left( e^{2\left[ a_0 - (a_0 + 2d)e^{-2d/a_0} \right]} + V_0 [a_0^2 - (a_0^2 + 2a_0d + 2d^2)e^{-2d/a_0}] \right)$$

(53)

$$\langle 2, 0, 0 | \hat{W} | 2, 0, 0 \rangle = \frac{1}{8a_0^3} \int_0^d r^2 dr \left( V_0 + \frac{e^2}{r} \right) \left( 2 - \frac{r}{a_0} \right)^2 e^{-r/a_0}$$

$$= \frac{1}{8a_0^4} \left( e^{2\left[ 2a_0^3 - (2a_0^3 + 2a_0^2d + a_0d^2 + d^3)e^{-d/a_0} \right]} + V_0 [8a_0^4 - (8a_0^4 + 8a_0^3d + 4a_0^2d^2 + d^3)e^{-d/a_0}] \right)$$

(54)

$$\langle 2, 1, 0 | \hat{W} | 2, 1, 0 \rangle = \frac{1}{24a_0^4} \int_0^d r^2 dr \left( V_0 + \frac{e^2}{r} \right) \frac{r^2}{a_0^2} e^{-r/a_0}$$

$$= \frac{1}{24a_0^4} \left( e^{2\left[ 6a_0^3 - (6a_0^3 + 6a_0^2d + 3a_0d^2 + d^3)e^{-d/a_0} \right]} + V_0 [24a_0^4 - (24a_0^4 + 24a_0^3d + 12a_0^2d^2 + 4a_0d^3 + d^4)e^{-d/a_0}] \right)$$

(55)

$$\langle 2, 1, 0 | \hat{W} | 2, 1, 0 \rangle$$

$$= \frac{1}{24a_0^4} \left( e^{2\left[ 6a_0^3 - (6a_0^3 + 6a_0^2d + 3a_0d^2 + d^3)e^{-d/a_0} \right]} + V_0 [24a_0^4 - (24a_0^4 + 24a_0^3d + 12a_0^2d^2 + 4a_0d^3 + d^4)e^{-d/a_0}] \right)$$

(56)
\[
\langle 2, 0, 0 | \hat{W} | 1, 0, 0 \rangle = \frac{1}{\sqrt{2a_0^2}} \int_0^\frac{e^2}{r} \left( V_0 + \frac{e^2}{r} \right) \left( 2 - \frac{r}{a_0} \right) e^{-3r/2a_0} dr
\]
\[
= \frac{\sqrt{2}}{27a_0^3} \left( e^2 [4a_0^2 - (4a_0^2 + 6a_0d + 9d^2)e^{-3d/2a_0}] + 9V_0d^3e^{-3d/2a_0} \right)
\]
\[
(2, 1, \pm 1 | \hat{W} | 2, 1, \pm 1) = \langle 2, 1, 0 | \hat{W} | 2, 1, 0 \rangle
\]

3.3

The shift in the ground state energy is just the matrix element \( \langle 1, 0, 0 | \hat{W} | 1, 0, 0 \rangle \) as we just calculated
\[
\Delta E^{(1)}_{1,0,0} = \frac{1}{a_0^2} \left( e^2 [a_0 - (a_0 + 2d)e^{-2d/a_0}] + V_0[a_0^2 - (a_0^2 + 2a_0d + 2d^2)e^{-2d/a_0}] \right)
\]

3.4

As seen from (56), (58) and (61), it is clear that this perturbation \( W(r) \) lifts the degeneracies between the \( |2, 0, 0\rangle \) and \( |2, 1, 0\rangle \) eigenstates while fail to resolve the 3-fold degeneracy of quantum number \( m \) among \( |2, 1, m\rangle \) states. The energy difference is given by
\[
\Delta E = \frac{e^{-d/a_0}}{12a_0^4} [e^2 d^2(3a_0 - d) + V_0d^3(2a_0 - d)]
\]

This follows from that the radial wave functions are completely determined by quantum number \( l \) in hydrogen atom solutions. As the perturbation does not have angular dependence this feature will continue to hold.