



COLLEGE OF ARTS AND SCIENCES

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Quantum Mechanics 2

PHYS 5403 HOMEWORK ASSIGNMENT 4

PROBLEMS: {1, 2, 3}

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STUDENT

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Problem 1:

Consider a free gas of N non-relativistic electrons, whose single particle wavefunctions are described by plane-waves normalized by the volume of the space. The kinetic energy of the system given by:

$$K = -\frac{\hbar^2}{2m} \int d^d x \psi^\dagger(\mathbf{x}) \nabla^2 \psi(\mathbf{x})$$

where

$$\psi(\mathbf{x}) = \begin{pmatrix} \psi_\uparrow(\mathbf{x}) \\ \psi_\downarrow(\mathbf{x}) \end{pmatrix}$$

is a two component spinor, with $\psi_\sigma (\sigma = \uparrow, \downarrow)$ representing the annihilation field operator for up/down electrons, and d is the dimensionality of the space.

- (a) Write the Kinetic energy in terms of creation and annihilation operators in the momentum space, $a_{\sigma k}^\dagger$ and $a_{\sigma k}$.

In general, we can write Kinetic energy like

$$\frac{P^2}{2m} \Leftrightarrow -\frac{\hbar^2}{2m} \int \psi^\dagger(\mathbf{x}) \nabla^2 \psi(\mathbf{x}) d^d x$$

This tells us the integral must evaluate to

$$\frac{P^2}{2m} = -\frac{\hbar^2}{2m} \cdot |\mathbf{k}|^2 \Rightarrow |\mathbf{k}| = \frac{P}{\hbar} \Rightarrow \frac{P^2}{2m} = \frac{\hbar^2}{2m} \frac{P^2}{\hbar^2} \Rightarrow P^2 = P^2 \checkmark$$

This then means we can write our Kinetic energy as

$$K = \frac{\hbar^2}{2m} \sum_{\sigma} \sum_{\mathbf{k}} |\mathbf{k}|^2 a_{\sigma \mathbf{k}}^\dagger a_{\sigma \mathbf{k}}$$

- (b) Write down the momentum operator \tilde{P} in terms of $\psi^\dagger(\mathbf{x})$ and $\psi(\mathbf{x})$ field operators and then rewrite it in terms of the creation and annihilation operators in the momentum space $a_{\sigma k}^\dagger$ and $a_{\sigma k}$.

Similarly to part (a), we can write momentum in terms of field operators as

$$P = \int \psi^\dagger(\mathbf{x}) P \psi(\mathbf{x}) d^d x$$

where we use $P = \hbar |\mathbf{k}|$. This then means the momentum is then

$$P = \hbar \sum_{\sigma} \sum_{\mathbf{k}} |\mathbf{k}| a_{\sigma \mathbf{k}}^\dagger a_{\sigma \mathbf{k}}$$

Problem 1: Continued

- (c) The ground state of the system is described by the state:

$$|FS\rangle = \prod_{\alpha \leq N} c_\alpha^\dagger |0\rangle$$

where $c_\alpha \equiv a_{\sigma k}$, with the notation $\alpha \leq N$ meaning $|\mathbf{k}| \leq k_F$, with k_F the radius of the Fermi Surface (FS) and $\sigma = \uparrow, \downarrow$ for momentum states inside the FS. This state has the property that

$$\begin{aligned} a_{\sigma, k} |FS\rangle &= 0 && \text{for } |\mathbf{k}| > k_F \\ a_{\sigma, k}^\dagger |FS\rangle &= 0 && \text{for } |\mathbf{k}| < k_F \end{aligned}$$

Assuming $d = 2$ (2D electron gas), compute the total energy of the system at the ground state, $\langle K \rangle_{FS}$ and the total momentum, $\langle \mathbf{P} \rangle_{FS}$. Interpret your result.

We calculate the total energy of the system in the Ground state with

$$\langle \mathbf{k} \rangle = \langle FS | \mathbf{k} | FS \rangle$$

Evaluating the above we see

$$\langle \mathbf{k} \rangle = \frac{\hbar^2}{2m} \sum_{\sigma} \sum_{\mathbf{k}} |\mathbf{k}|^2 \langle FS | a_\sigma^\dagger a_\sigma | FS \rangle = \frac{\hbar^2}{2m} \sum_{\sigma} \sum_{\mathbf{k}} |\mathbf{k}|^2 \underbrace{\langle FS | a_\sigma^\dagger a_\sigma | FS \rangle}_{\Theta(k_F - |\mathbf{k}|)}$$

we then take the above expression and can say that

$$\langle \mathbf{k} \rangle = \frac{V}{(2\pi)^2} \frac{\hbar^2}{2m} \int_0^{2\pi} d\phi \int_0^{k_F} \kappa \cdot |\mathbf{k}|^2 dk = \frac{V\hbar^2}{4\pi m} \cdot \frac{k_F^4}{4} = \frac{V\hbar^2 k_F^4}{16\pi m}$$

where we are integrating the \mathbf{k} -Space over volume V . The expectation value of our momentum should be zero due to our free-particles having radial symmetry in our 2D case. This then means

$$\boxed{\langle \mathbf{k} \rangle = \frac{V\hbar^2 k_F^4}{16\pi m}, \langle \mathbf{p} \rangle = 0}$$

From the above it's rather straight forward to see that our expectation value of kinetic energy is only dependent upon the mass of our particle and the radius of our Fermi Surface.

Problem 1: Continued

(d) Suppose now that a uniform magnetic field \mathbf{B} is turned on. The total Hamiltonian becomes $K + \mathcal{H}_B$, where

$$\mathcal{H}_B = -\mu_B \mathbf{S} \cdot \mathbf{B}$$

where μ_B is the Zeman coupling of the electronic spin to the magnetic field and

$$\mathbf{S} = \frac{\hbar}{2} \int d^d x \psi^\dagger(\mathbf{x}) \vec{\sigma} \psi(\mathbf{x})$$

is the spin operator written in terms of field operators, with $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ as Pauli matrices. Write \mathcal{H}_B in terms of $a_{\sigma k}^\dagger$ and $a_{\sigma k}$ operators and then compute the total energy of the system (assume $d = 2$) for each spin in separate. Explain what happens with the ground state (Hint: assume B along the z -axis).

If we assume that the Magnetic Field is only in z , we can simplify if as

$$\mathcal{H}_B = -\mu_B \mathbf{S} \cdot \mathbf{B} = -\mu_B S_z B = -\mu_B B \frac{\hbar}{2} \int \gamma^+(\mathbf{x}) \sigma_z^+ \gamma(\mathbf{x}) d^2x$$

We then write our Hamiltonian in terms of creation and annihilation operators as

$$\mathcal{H}_B = -\frac{\mu_B B \hbar}{2} \sum_k \sum_\sigma a_{\sigma k}^\dagger a_{\sigma k} = -\frac{\mu_B B \hbar}{2} \sum_k a_{\uparrow k}^\dagger a_{\uparrow k} - a_{\downarrow k}^\dagger a_{\downarrow k}$$

We now calculate the total energy for each spin. For Spin up we have

$$\begin{aligned} \langle \mathcal{H} \rangle_\uparrow &= \langle K \rangle_\uparrow + \langle \mathcal{H}_B \rangle_\uparrow = \frac{V \hbar^2 k_F^4}{16 \pi m} - \frac{\mu_B B \hbar}{2} \sum_k a_{\uparrow k}^\dagger a_{\uparrow k} \\ &= \frac{V \hbar^2 k_F^4}{16 \pi m} - \frac{V \mu_B B}{8 \pi r^2} \int_0^{2\pi} d\sigma \int_0^{k_F} \langle F_S | a_{\uparrow k}^\dagger a_{\uparrow k} | F_S \rangle \kappa dk \\ &= \frac{V \hbar^2 k_F^4}{16 \pi m} - \frac{V \mu_B B}{8 \pi r^2} \left(2\pi \cdot \frac{k_F^2}{2} \right) = \frac{V \hbar^2 k_F^4}{16 \pi m} - \frac{V \mu_B B k_F^2}{8 \pi r} \\ &= \frac{V \hbar^2 k_F^2}{8 \pi r} \left(\frac{k_F^2}{2m} - \mu_B B \right) \end{aligned}$$

Where if we repeat the above for $\langle \mathcal{H} \rangle_\downarrow$ we will have $(+\mu_B B)$ instead. Namely

$$\langle \mathcal{H} \rangle_\uparrow = \frac{V \hbar^2 k_F^2}{8 \pi r} \left(\frac{k_F^2}{2m} - \mu_B B \right), \quad \langle \mathcal{H} \rangle_\downarrow = \frac{V \hbar^2 k_F^2}{8 \pi r} \left(\frac{k_F^2}{2m} + \mu_B B \right)$$

The ground state energy is essentially $\langle \mathcal{H} \rangle_\downarrow$

Problem 1: Review

Procedure:

- Use the definition of Kinetic Energy

$$-\frac{\hbar^2}{2m} \int \psi^\dagger(x) \nabla^2 \psi(x) d^d x$$

and the wave function

$$\psi_\sigma(\vec{x}) = \frac{1}{\sqrt{V}} \sum_k e^{i\vec{k}\cdot\vec{x}} a_{\sigma,k}$$

to determine what p and the kinetic energy are with the information given to us

- Use the fact that momentum in terms of field operators can be written as

$$P = \int \psi^\dagger(x) P \psi(x) d^d x$$

to find the equivalent to (a) for momentum

- To find the total energy of the system in the ground state we use

$$\langle K \rangle = \langle FS | K | FS \rangle$$

where $|FS\rangle$ is how we define the ground state of our system

- We can repeat the same for momentum but with a different operator
- Begin by writing the Hamiltonian in terms of creating and annihilation operators with

$$\mathcal{H}_B = -\frac{\mu_B B \hbar}{2} \sum_{k,\sigma} a_{\sigma,k}^\dagger a_{\sigma,k}$$

and sum over the spins ($\sigma \Rightarrow \uparrow, \downarrow$)

- Calculate the total energy with

$$\langle \mathcal{H} \rangle_{\downarrow,\uparrow} = \langle K \rangle_{\uparrow,\uparrow} + \langle \mathcal{H} \rangle_{\downarrow,\uparrow}$$

Key Concepts:

- Using the definition given to us we can represent the Kinetic energy in terms of annihilation field operators
- This is the same but with momentum instead of position
- The total momentum here should be zero due the radial symmetry of our system
- Summing over the spins we can write our Hamiltonian in terms of creation and annihilation operators. Doing this allows us to evaluate what our total energy is in the ground state

Variations:

- For any of these parts, if we are given a wave function that has different spinors then it will affect everything after
 - * We would simply do the same procedures as before but with a new wavefunction, possibly yielding new results
- This is essentially the same as part (a)
- We could be given different “eigenvalue” relationships
 - * Thus yielding different values for the expectation values
- We could be given a different Hamiltonian or Spin operator
 - * This would change the small details but the same broad procedure would apply

Problem 2:

Assume that an electron occupies a p level, which is degenerate among the three states $|n, j=1, m\rangle$, with $m = \pm 1, 0$. The electron is subjected to a perturbation $V(\mathbf{r}) = \alpha(x^2 - y^2)$.

- (a) Write the perturbation $V(\mathbf{r})$ in terms of spherical tensors of rank 2.

With our potential,

$$V(r) = \alpha(x^2 - y^2)$$

which is currently a sum of rank 1 spherical tensors. Since we are working with degenerate states, our perturbative potential must be written in terms of spherical harmonics

$$V_{m'm} = \langle n, l=1, m' | \alpha(x^2 - y^2) | n, l=1, m \rangle$$

where we are now tasked with writing X and Y in terms of spherical harmonics. The spherical harmonics for $m=\pm 1$ are,

$$Y_l^{\pm 1}(\alpha, \varphi) = \mp \left(\frac{3}{8\pi} \right)^{1/2} \sin(\alpha) e^{\pm i\alpha} \quad (*)$$

where we now calculate the spherical harmonics for our system with $(*)$ in terms of x and y . We make the definitions

$$x = r\cos(\alpha), \quad y = r\sin(\alpha)$$

Expanding $(*)$ we see that for $m=1$ we have

$$\begin{aligned} Y_1^1(\alpha, \varphi) &= - \left(\frac{3}{8\pi} \right)^{1/2} \sin(\alpha) e^{i\alpha} = - \left(\frac{3}{8\pi} \right)^{1/2} \sin(\alpha) (\cos(\alpha) + i\sin(\alpha)) \\ &= - \left(\frac{3}{8\pi} \right)^{1/2} (\cos(\alpha)\sin(\alpha) + i\sin^2(\alpha)) = - \left(\frac{3}{8\pi} \right)^{1/2} \frac{Y}{r^2} (x + iy) \end{aligned}$$

Doing the same for $m=-1$ we have

$$\begin{aligned} Y_1^{-1}(\alpha, \varphi) &= \left(\frac{3}{8\pi} \right)^{1/2} \sin(\alpha) e^{-i\alpha} = \left(\frac{3}{8\pi} \right)^{1/2} \sin(\alpha) (\cos(\alpha) - i\sin(\alpha)) \\ &= \left(\frac{3}{8\pi} \right)^{1/2} (\cos(\alpha)\sin(\alpha) - i\sin^2(\alpha)) = \left(\frac{3}{8\pi} \right)^{1/2} \frac{Y}{r^2} (x - iy) \end{aligned}$$

Problem 2: Continued

We now take the results for $Y_1^0(\alpha, \varphi)$ and $Y_1^1(\alpha, \varphi)$ that are in terms of x and y and we solve for x and y in terms of $Y_1^0(\alpha, \varphi)$ and $Y_1^1(\alpha, \varphi)$. This is of course is

$$Y_1^0 = -\frac{c}{r^2} y(x+iy) , \quad Y_1^1 = \frac{c}{r^2} y(x-iy) \quad (\text{xx})$$

Taking (xx) and solving for x and y we find

$$x = \sqrt{\frac{8\pi}{3}} r \left(\frac{Y_1^1(\alpha, \varphi) - Y_1^0(\alpha, \varphi)}{2} \right) , \quad y = \sqrt{\frac{8\pi}{3}} i r \left(\frac{Y_1^1(\alpha, \varphi) + Y_1^0(\alpha, \varphi)}{2} \right)$$

This then means x^2+y^2 is

$$\begin{aligned} x^2 - y^2 &= \frac{8\pi}{3} r^2 \left(\frac{Y_1^1(\alpha, \varphi) - Y_1^0(\alpha, \varphi)}{2} \right)^2 + \frac{8\pi}{3} r^2 \left(\frac{Y_1^1(\alpha, \varphi) + Y_1^0(\alpha, \varphi)}{2} \right)^2 \\ &= \frac{2\pi}{3} r^2 (Y_1^1)^2 - Y_1^0 Y_1^1 - Y_1^1 Y_1^0 + (Y_1^0)^2 + (Y_1^1)^2 + Y_1^0 Y_1^1 + Y_1^1 Y_1^0 + (Y_1^0)^2 \\ &= \frac{4\pi}{3} r^2 (Y_1^1)^2 + (Y_1^0)^2 \end{aligned}$$

So our perturbative potential can now be written in terms of spherical harmonics. However, since we want the potential in rank 2 tensors we use the Wigner-Eckart Theorem to determine that $m' - m = \pm 1$ or $m' - m = 0$. Further we know $j = q_z = 1 \therefore q = 2$ and thus

$$T_{\pm 2}^2 = \frac{1}{2} (x \pm iy)^2$$

We now do the same thing as before and find

$$V(r) = \frac{1}{2} (T_2^2 + T_{-2}^2)$$

- (b) Using the Wigner-Eckart theorem, write the perturbation matrix in the $|n, j = 1, m\rangle$ basis.

We use the Wigner-Eckart theorem to calculate our perturbation matrix. Using the form of the potential in (a) we find

$$\alpha \langle n, j=1, m=\pm 1 | x^2 - y^2 | n, j=1, m=\pm 1 \rangle$$

Problem 2: Continued

We now use the Wigner-Eckart Theorem to calculate the matrix elements of these spherical tensors

$$\langle \alpha', j' m' | T_j^{(k)} | \alpha, j, m \rangle = \langle j, k; m | j, k; j', m' \rangle \frac{\langle \alpha', j' | T^{(k)} | \alpha, j \rangle}{\sqrt{2j+1}}$$

We have $k=2$, $q=2$, $j=j'=1$

$$V = \frac{\alpha}{2} \langle \beta', 1, m' | T_2^2 + T_{-2}^2 | \beta, 1, m \rangle = \frac{\alpha}{2} \langle \beta', 1, m' | T_2^2 | \beta, 1, m \rangle + \frac{\alpha}{2} \langle \beta', 1, m' | T_{-2}^2 | \beta, 1, m \rangle$$

$$\langle \beta', 1, m' | T_2^2 | \beta, 1, m \rangle = \langle 1, 2; m, 2 | 1, 2; 1, m' \rangle \frac{\langle 1 | T^2 | 1 \rangle}{\sqrt{3}}$$

where we learn that $m=-m'$, since $m \in [-1, 1]$ we have the following

$$m=-1, V_{13} = \frac{\alpha}{2} \langle 1, 2; -1, 2 | 1, 2; 1, 1 \rangle c = \frac{\alpha c}{2} \sqrt{\frac{3}{5}}$$

$$m=1, V_{31} = \frac{\alpha}{2} \langle 1, 2; 1, 2 | 1, 2; 1, -1 \rangle c = \frac{\alpha c}{2} \sqrt{\frac{3}{5}}$$

This then means our perturbative matrix is

$$V = \frac{\alpha c}{2} \sqrt{\frac{3}{5}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

- (c) Find the splitting of the p energy levels in first order in perturbation theory. You don't have to solve the integrals.

To find the splitting of the p energy levels we find the second order correction to our perturbative potential. The eigenvalues of the perturbative potential are

$$(V - \lambda I) = \text{const.} \begin{pmatrix} -\lambda & 0 & 1 \\ 0 & \lambda & 0 \\ 1 & 0 & -\lambda \end{pmatrix}, \det(V - \lambda I) = \lambda^3 - \lambda = 0 \Rightarrow \lambda = 0, \pm 1$$

This then means that the original eigenvalues are

$$E_1 = -\frac{\alpha c}{2} \sqrt{\frac{3}{5}}, E_2 = 0, E_3 = \frac{\alpha c}{2} \sqrt{\frac{3}{5}}$$

To calculate the splitting of the p -energy levels is calculated in general with

$$E_m^{(n)} = \frac{|\langle \psi_m^{(n)} | \hat{H}' | \psi_n^{(n)} \rangle|^2}{E_n^{(n)} - E_m^{(n)}}$$

Problem 2: Continued

For our perturbative potential V , the first order corrections are

$$|\psi_1\rangle = (0 \ 1 \ 0)^T, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}} (1 \ 0 \ -1)^T, \quad |\psi_3\rangle = \frac{1}{\sqrt{2}} (1 \ 0 \ 1)^T$$

where the above are our eigenvectors to our perturbative potential. This finally means

$$\Delta E_m^2 = \sum_{m \neq m'} \frac{|\langle m, l, m' | V | m, l, m' \rangle|^2}{E_m^0 - E_{m'}^0}$$

- (d) Assume now that the degeneracy of the p levels is lifted by a *strong* magnetic field \mathbf{B} pointing along the z axis, with the Hamiltonian (ignore spin effects)

$$\mathcal{H}_z = \mu_B B_z m.$$

If $\mu_B B_z$, calculate the energy correction to the $|n, j=1, m\rangle$ states (in the presence of the strong field) due to the perturbation $V(\mathbf{r})$ in lowest order in perturbation theory where the result is non-zero.

By the degeneracy being lifted, we have to calculate the correction to our eigenstate energies

$$\Delta E_m^2 = \sum_{m \neq m'} \frac{|\langle m, l, m' | \hat{V} | m, l, m' \rangle|^2}{E_m^0 - E_{m'}^0}$$

where we can say $\Delta E_{-1}^2 = -\Delta E_1^2$. WI $\Delta E_1^0 = 0$ we then have

$$\Delta E_1^2 = \frac{3\alpha^2 c^2}{40\mu_B B m}, \quad \Delta E_{-1}^2 = -\frac{3\alpha^2 c^2}{40\mu_B B m}$$

Problem 2: Review

Procedure:

- – Use the mathematical formalism of writing potential in terms of spherical tensors
 - * Use the quantum numbers ($m \rightarrow$ magnetic, $l \rightarrow$ orbital, $j \rightarrow$ total) to determine the corresponding spherical harmonics
 - * Take the potential and write the components in terms of spherical harmonics
 - * Simplify and use the relationship

$$T_{\pm 2}^2 = \frac{1}{2}(x \pm iy)^2 \rightarrow T_q^{(k)}$$

to then express the potential in terms of rank 2 spherical tensors

- – Use the Wigner Eckart Theorem with the corresponding correct values (j, j', k, m, m', q) to calculate the matrix elements of our potential

$$\langle \alpha', j', m' | T_q^{(k)} | \alpha, j, m \rangle = \langle j, k; m, q | j, k; j', m' \rangle \frac{\langle \alpha', j' || T^{(k)} || \alpha, j \rangle}{\sqrt{2j+1}}.$$

- – To find the splitting of the energy levels we calculate the second order (first non zero) correction to our potential with

$$\Delta E = \sum_{m \neq m'} \frac{|\langle \psi_m | V | \psi_{m'} \rangle|^2}{E_m - E_{m'}}$$

- – Calculate the second order correction to the eigenvalue

Key Concept:

- – Using the formalism explained above we are able to express the potential given to us in terms of spherical tensors
- – Using the Wigner Eckart Theorem (Which allows us to express spherical tensor matrix elements of rank two in terms of Cloebsch Gordon coefficients) we can write our perturbative potential as a matrix
- – The splitting of p energy levels occurs where our first perturbation of our ground state energy is non zero (The second order correction in our case)
- – The first non zero perturbation occurs at the second order and this is due to the degeneracy of the p levels being lifted and our magnetic field being strong

Variations:

- – We could of course be given a different potential
 - * We would use the same formalism but this time with different spherical harmonics etc.
- – We could be asked to look at a different state
 - * This changes what our Cloebsch Gordon coefficients evaluate to in the Wigner Eckart Theorem but it is the same broad procedure
- – If we are given a different potential in (b) then this would effect what our perturbation evaluates to
 - * We would use the same procedure but with a new potential

Important Equations:

- – First order corrections (Non-Degenerate)

$$E_n^1 = \langle \psi_n^0 | \mathcal{H}' | \psi_n^0 \rangle \quad \psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | \mathcal{H}' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)} \psi_m^0$$

- Second order corrections (Non-Degenerate)

$$E_n^2 = \sum_{m \neq n} \frac{|\langle \psi_m^0 | \mathcal{H}' | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0}$$

Problem 3:

A particle with mass m is subjected to an harmonic potential

$$V(x) = \frac{1}{2}m\omega^2x^2.$$

The potential is then perturbed by an anharmonic force with potential

$$\delta V(x) = \lambda \sin(kx).$$

- (a) Find the corrected ground state ket in leading order in perturbation theory.

The Hamiltonian for this particle is

$$\hat{H} = \frac{p^2}{2m} + \frac{m\omega^2x^2}{2} + \lambda \sin(kx)$$

The ground state harmonic oscillator normalized wave function is

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) e^{-x^2/2}$$

We then calculate the first order correction to our state with

$$\psi'_n(x) = \sum_{m \neq n} \frac{\langle \psi_m^{(0)} | V | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} \psi_m^{(0)}$$

The first order correction is then

$$\begin{aligned} \psi'_0(x) &= \frac{\langle \psi_1^{(0)} | V | \psi_0^{(0)} \rangle}{E_0^{(0)} - E_1^{(0)}} \psi_1^{(0)} = \frac{1}{E_0^{(0)} - E_1^{(0)}} \frac{\lambda}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-x^2/2} H_1(x) \sin(kx) H_0(x) e^{-x^2/2} dx \psi_1^{(0)} \\ &= \frac{1}{E_0^{(0)} - E_1^{(0)}} \frac{\lambda}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-x^2} x \sin(kx) dx \psi_1^{(0)} = \frac{1}{E_0^{(0)} - E_1^{(0)}} \frac{\lambda}{\sqrt{2\pi}} \cdot e^{-k^2/4} K \sqrt{\pi} \psi_1^{(0)} \end{aligned}$$

But the problem is we need to do this for all m values. Looking at $n=2$ we see

$$\frac{\langle \psi_2^{(0)} | V | \psi_0^{(0)} \rangle}{E_0^{(0)} - E_2^{(0)}} \psi_2^{(0)} = \frac{1}{E_0^{(0)} - E_2^{(0)}} \frac{\lambda}{\sqrt{8\pi}} \int_{-\infty}^{+\infty} e^{-x^2} (4x) \sin(kx) dx \psi_2^{(0)} = 0$$

Now for $m=3$

$$\frac{\langle \psi_3^{(0)} | V | \psi_0^{(0)} \rangle}{E_0^{(0)} - E_3^{(0)}} \psi_3^{(0)} = \frac{1}{E_0^{(0)} - E_3^{(0)}} \frac{\lambda}{\sqrt{48\pi}} \int_{-\infty}^{+\infty} e^{-x^2} (6x^3 - 12x) \sin(kx) \psi_3^{(0)} = -e^{-k^2/4} k^3 \sqrt{\pi}$$

Problem 3: Continued

Examining this we see that our solution looks something of the form

$$\psi_0'(x) = \psi_0^0(x) + \lambda \sum_{m \text{ odd}} \sum_{n=0} \frac{1}{E_0^0 - E_m^0} \frac{(-1)^n}{\sqrt{2^m m!}} e^{-k^2 x^2/4} K^m \psi_m^{(0)}(x)$$

- (b) Using your result in a), calculate the expectation value of the position operator in the corrected ground state. Hint: Use the identity:

$$e^{A+B} = e^A e^B e^{-[A,B]/2}.$$

The expectation value of the position operator will look like

$$\langle x \rangle = \langle \psi_0'(x) | x | \psi_0'(x) \rangle$$

Putting this together, we find

$$\begin{aligned} \langle x \rangle &= \lambda \int_{-\infty}^{+\infty} \left(\frac{e^{-x^2/2}}{\sqrt{\pi}} + \frac{1}{E_0^0 - E_1^0} \frac{e^{-k^2 x^2/4}}{\sqrt{2}} K \frac{2x}{\sqrt{2\pi}} e^{-x^2/2} \right) (x) \left(\frac{e^{-x^2/2}}{\sqrt{\pi}} + \frac{1}{E_0^0 - E_1^0} \frac{e^{-k^2 x^2/4}}{\sqrt{2}} K \frac{2x}{\sqrt{2\pi}} e^{-x^2/2} \right) dx \\ &= \lambda \int_{-\infty}^{+\infty} \frac{e^{-x^2}}{\sqrt{\pi}} \left(\frac{2}{E_0^0 - E_1^0} \frac{e^{-k^2 x^2/4}}{\sqrt{2}} K \frac{x^2}{\sqrt{2\pi}} + e^{x^2/2} \left(1 + \frac{2}{E_0^0 - E_1^0} \frac{e^{-k^2 x^2/4}}{\sqrt{2}} K \frac{\sqrt{\pi} x}{\sqrt{2\pi}} \right) \right) dx \end{aligned}$$

Using mathematica we find

$$\langle x \rangle = -\frac{2\lambda}{\hbar\omega} e^{-\beta k^2/2} K \beta^2$$

This means the expectation value of x is then

$$\langle x \rangle = -\frac{\lambda K}{m\omega^2} e^{-\hbar k^2/4m\omega}$$

- (c) Now assume that $kx \ll 1$, such that $\delta V(x) \approx \lambda kx$. Use second order perturbation theory to calculate the corrected energy to the ground state.

The equation to calculate the second order correction is,

$$E_n^2 = \sum_{m \neq n} \frac{|\langle \psi_m^{(0)} | V | \psi_n^{(0)} \rangle|^2}{E_n^0 - E_m^0}$$

With our new potential, the second order correction for us will be,

$$E_0^2 = \lambda^2 k^2 \sum_{m \neq 0} \frac{|\langle \psi_m^0(x) | x | \psi_0^0(x) \rangle|^2}{E_0^0 - E_m^0}$$

Problem 3: Continued

This summed out is

$$E_0^2 = \lambda^2 k^2 \left(\frac{|\langle \psi_1^0(x) | x | \psi_0^0(x) \rangle|^2}{E_0^0 - E_1^0} + \frac{|\langle \psi_2^0(x) | x | \psi_0^0(x) \rangle|^2}{E_0^0 - E_2^0} + \frac{|\langle \psi_3^0(x) | x | \psi_0^0(x) \rangle|^2}{E_0^0 - E_3^0} \right)$$

Writing out what each of these states are first we have

$$\psi_0^0(x) = \frac{e^{-x^2/2}}{\sqrt{\pi/4}}, \quad \psi_1^0(x) = \frac{2x}{\sqrt{2}\sqrt{\pi/4}} e^{-x^2/2}, \quad \psi_2^0(x) = \frac{4x^2-2}{\sqrt{8}\sqrt{\pi/4}} e^{-x^2/2}, \quad \psi_3^0(x) = \frac{(8x^3-12x)}{\sqrt{48}\sqrt{\pi/4}} e^{-x^2/2}$$

Calculating the modulus square of the expectation values we find

$$\langle \psi_1^0(x) | x | \psi_0^0(x) \rangle = \int_{-\infty}^{+\infty} \frac{2x}{\sqrt{2}\sqrt{\pi/4}} e^{-x^2/2} \cdot x \cdot \frac{e^{-x^2/2}}{\sqrt{\pi/4}} dx = \frac{1}{\sqrt{2}}$$

$$\langle \psi_2^0(x) | x | \psi_0^0(x) \rangle = \int_{-\infty}^{+\infty} \frac{4x^2-2}{\sqrt{8}\sqrt{\pi/4}} e^{-x^2/2} \cdot x \cdot \frac{e^{-x^2/2}}{\sqrt{\pi/4}} dx = 0$$

$$\langle \psi_3^0(x) | x | \psi_0^0(x) \rangle = \int_{-\infty}^{+\infty} \frac{(8x^3-12x)}{\sqrt{48}\sqrt{\pi/4}} e^{-x^2/2} \cdot x \cdot \frac{e^{-x^2/2}}{\sqrt{\pi/4}} dx = 0$$

From this we can see that every term after $m=1$ will be zero. This then means our second order correction to our ground state is

$$E_0^2 = \frac{1}{2} \frac{\lambda^2 k^2}{m\omega}$$

Problem 3: Review

Procedure:

- Using the ground state normalized harmonic oscillator wave function

$$\psi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) e^{-x^2/2}$$

and our new perturbative Hamiltonian

$$\mathcal{H}' = \frac{P^2}{2m} + \frac{m}{2} \omega^2 x^2 + \lambda \sin(kx)$$

to calculate the first order correction to the ground state for non-degenerate perturbation theory

- Calculate the expectation value of position for this ground state with

$$\langle x \rangle = \langle \psi_0^1(x) | x | \psi_0^1(x) \rangle$$

where $|\psi_0^1(x)\rangle$ is the first order correction to the ground state of our harmonic oscillator

- Use second order perturbation theory to find the correction to the eigenenergies with this new perturbative potential

Key Concepts:

- Using our new Hamiltonian we are able to find the first order correction to our ground state wave function with perturbation theory formalism
- We use the corrected ground state wave function from part (a) to calculate what the most likely position of our perturbed particle now
- We use perturbation theory to find the second order correction to our eigenenergy with the new perturbative potential with our ground state wave functions

Variations:

- We of course can be given a different perturbation or ground state wave function
 - * As long as we are being asked the same question we would use the same procedure with this new change
- We could be given a different value to calculate
 - * This would just constitute using a new equation
- We could be asked for a different wave function
 - * We would then find this new wave function and then use the same procedure as before
- Because this is essentially the end of the line for what can be asked of us, we cannot have a variation to this part without changing the potential
 - * We then use the same procedure with this small change in difference