

UNIVERSITY OF OSLO

Faculty of Mathematics and Natural Sciences

Exam in: FYS3110 – Quantum mechanics

Date and time: Nov. 26 at 09:00 (4 hours)

Remember to put your candidate number on your answer sheets (not your name).

Problem 1

1a) (6 points) What is a quantum state? In your answer, explain how a quantum state is different from a classical state and how it is represented mathematically.

Solution:

A quantum state

- is the description of the system/object at a specific instant in time.
- contains information about all the probabilities for different measurement outcomes for all possible types of measurements that can be performed on the system/object.
- is represented mathematically as a normalized complex vector; a ket.

The first point is also true for a classical state, –it is also the description of a system/object at a specific time. In contrast, the other two points are different for a classical state. A classical state is defined in terms of a set of definite measurement values. Thus there are no probabilities encoded in a classical state. (There can be uncertainties/probabilities as to which classical state the system/object is in, but not in the classical state itself.) Mathematically a classical state is represented as a point in a set, not as a complex vector. (Thus there is no meaning attached to adding classical states together.)

Grading:

To get max score on this subproblem correct and not misleading answers must be given to 1) what a quantum state is, 2) how it is represented mathematically and 3) how it is different from at classical state.

1b) (6 points) In organic chemistry there is a rule known as Hückel's rule. It states that ring molecules with $N = 4n + 2$ electrons are particularly stable ($n \geq 0$ is an integer). Explain in words why Hückel's rule holds by assuming that the electrons are non-interacting non-relativistic particles constrained to move on a circle.

Solution:

A free non-relativistic particle has an energy which is proportional to k^2 . The periodic nature of the circle causes k to be quantized in appropriate units, the minimum value being $k = 0$. Now consider building up the many-body wave function by filling in the one-particle states. The lowest energy state has $k = 0$ and can according to the Pauli principle

be filled with at most 2 electrons (because of spin). Then for the next particle, we must fill it into either the $k = 1$ or the $k = -1$ levels as they are degenerate. The total energy per particle will therefore make a jump. This ensures stability of the $N = 2$ molecule. Then filling more electrons into one-particle states, we see that the Pauli principle allows for a total of 4 electrons in the $|k| = 1$ levels. The next electron must be put into the $|k| = 2$ levels, which again causes a jump in the energy per particle. Thus $N = 6$ electrons is the next stable configuration. Going further, each $|k|$ level takes 4 electrons before the energy per particle increase substantially. Thus we expect particularly stable molecules to exist when $N = 4n + 2$ where $n \geq 0$, as these corresponds to "filled shells". This is Hückels rule. Note that this is the same reasoning as in the explanation of why noble elements are stable.

An alternative way to get the single-particle energy levels is to recognize that the Hamiltonian for a particle moving in a circle (in the xy-plane) is proportional to L_z^2 which has quantum numbers $m^2\hbar^2$, where m is an integer $m \geq 0$. Then two electrons can be filled in $m = 0$ before there is a jump in energy per particle, and then 4 electrons can be filled in the $m = \pm 1$ levels, etc.

Grading:

No equations are necessary to get full score here. For full score the answer must be a convincing explanation containing correct statements about non-relativistic one-particle energies on a circle, and the "aufbau" of the molecule; the sequence of filling electrons into these and the restrictions following from the Pauli principle. The particular stability of "filled shells" or equivalently filled $|k|$ levels should also be mentioned.

Problem 2

2a) (2 points) Two kets $|A\rangle$ and $|B\rangle$ are specified in terms of an orthonormal basis set $\{|0\rangle, |1\rangle, |2\rangle\}$ as

$$\begin{aligned}|A\rangle &= i|0\rangle + |1\rangle - i|2\rangle \\ |B\rangle &= -i|0\rangle + |1\rangle + 3i|2\rangle\end{aligned}$$

Calculate the inner product $\langle A|B\rangle$. Alternatives: -8,-6,-5,-4,-3,-2,-1,0,1,2,3,4,5,6,8,

Solution:

The bra $\langle A|$ is

$$\langle A| = -i\langle 0| + \langle 1| + i\langle 2|$$

So that

$$\langle A|B\rangle = (-i\langle 0| + \langle 1| + i\langle 2|)(-i|0\rangle + |1\rangle + 3i|2\rangle) = -1\langle 0|0\rangle + \langle 1|1\rangle - 3\langle 2|2\rangle = \underline{-3}$$

2b) (2 points) Two hermitian operators $\hat{A}$ and $\hat{B}$ commute: $[\hat{A}, \hat{B}] = 0$. Which of the following statements is certainly true: Alternatives: $\hat{A}$ and $\hat{B}$ have both positive eigenvalues, the eigenstates of $\hat{A}$ are eigenstates of $\hat{B}$, $\hat{A}$ and $\hat{B}$ are symmetry operators, one can construct eigenstates of $\hat{A}$ that are also eigenstates of $\hat{B}$, the ground state expectation value of $\hat{A}$ (and of $\hat{B}$) is conserved (does not change in time), $\hat{A}$ (and $\hat{B}$) has a degenerate energy spectrum, $\hat{A}$ and $\hat{B}$ are unitary operators.

Solution:

The correct answer is one can construct eigenstates of $\hat{A}$ that are also eigenstates of $\hat{B}$.

2c) (2 points) What is the result of the operation:

$$(L_z L_x + i L_z L_y) Y_1^0(\theta, \phi)$$

where L_x, L_y and L_z are linear differential operators representing the respective angular momentum components, and $Y_1^0(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \cos \theta$. Alternatives: $0, -\hbar^2 \sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi}, \hbar^2 \sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi}, -\hbar^2 \sqrt{\frac{3}{4\pi}} \sin \theta e^{i\phi}, \hbar^2 \sqrt{\frac{3}{4\pi}} \sin \theta e^{i\phi}, -\hbar^2 \sqrt{\frac{3}{8\pi}} \sin \theta e^{-i\phi}, \hbar^2 \sqrt{\frac{3}{8\pi}} \sin \theta e^{-i\phi}, -\hbar^2 \sqrt{\frac{3}{4\pi}} \sin \theta e^{-i\phi}, \hbar^2 \sqrt{\frac{3}{4\pi}} \sin \theta e^{-i\phi}, \hbar^2 \sqrt{\frac{3}{2\pi}} \cos \theta, \hbar^2 \sqrt{\frac{3}{4\pi}} \cos \theta$

Solution:

We can write $L_z L_x + i L_z L_y = L_z (L_x + i L_y) = L_z L_+$ where L_+ raises the m quantum number by one and multiplies with the factor $\hbar \sqrt{l(l+1) - m(m+1)}$ (B & DD. eq (8.68)). Therefore

$$\begin{aligned} L_z (L_x + i L_y) Y_1^0(\theta, \phi) &= \hbar \sqrt{2} L_z Y_1^{+1}(\theta, \phi) = +\hbar^2 \sqrt{2} Y_1^{+1}(\theta, \phi) = -\hbar^2 \sqrt{2} \sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi} \\ &= -\hbar^2 \sqrt{\frac{3}{4\pi}} \sin \theta e^{i\phi} \end{aligned}$$

where we also used $L_z Y_1^{+1} = +\hbar Y_1^{+1}$ (B & DD eq (8.30)), and $Y_1^{+1} = -\sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi}$.

2d) (2 points) A hydrogen atom is in a highly excited state with large n and $l = n - 1$, so that its wave function is proportional to $r^{n-1} e^{-r/(na_0)} Y_{n-1}^m(\theta, \phi)$. Let $p(r)$ be the *radial probability density* for finding the electron at a distance r from the origin. It is normalized according to $\int_0^\infty p(r) dr = 1$. How does the position r_m at which $p(r_m)$ is a *maximum* behave as a function of n ? Alternatives: $n^{-2}, n^{-3/2}, n^{-1}, n^{-1/2}, n^0, n^{1/2}, n^1, n^{3/2}, n^2, n^{5/2}, n^3$

Solution:

With the given wavefunction, the radial probability density becomes

$$p(r) \propto r^{2(n-1)} e^{-2r/(na_0)} r^2 = r^{2n} e^{-2r/(na_0)}$$

The maximum of this is gotten by differentiating w.r.t. r and setting equal to zero

$$\frac{d}{dr} \left(r^{2n} e^{-2r/(na_0)} \right) = \left(2nr^{2n-1} - \frac{2}{na_0} r^{2n} \right) e^{-2r/(na_0)} = 0 \implies \underline{r_m = n^2 a_0}$$

Thus the correct alternative is n^2 .

2e) (2 points) Two spin-2 particles form a bound state with maximal total spin and total spin 0 in the z-direction. What is the probability of measuring each of the two spins to have spin 0 in the z-direction in this bound state. Select the closest alternative Alternatives: 0,0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8,0.9,1

Solution:

The maximal spin when combining two spin-2's is 4. Thus the bound state is $|4, 0\rangle$. Using the Clebsch-Gordan table 2×2 , we see that

$$\begin{aligned} |4, 0\rangle = & \sqrt{\frac{1}{70}}|2, +2\rangle \otimes |2, -2\rangle + \sqrt{\frac{8}{35}}|2, +1\rangle \otimes |2, -1\rangle + \sqrt{\frac{18}{35}}|2, 0\rangle \otimes |2, 0\rangle \\ & + \sqrt{\frac{8}{35}}|2, -1\rangle \otimes |2, +1\rangle + \sqrt{\frac{1}{70}}|2, -2\rangle \otimes |2, +2\rangle \end{aligned}$$

The probability is

$$P = |\langle 2, 0 | \otimes \langle 2, 0 | | 4, 0 \rangle|^2 = \frac{18}{35} \approx 0.51$$

Thus the closest alternative is: 0.5

2f) (2 points) A hydrogen atom is in a highly excited state with large principal quantum number n and maximal value of its angular momentum. How does the life-time of this state behave as a function of n when n is large? You may consider electric dipole spontaneous transitions only, and furthermore that the dipole transition matrix element behaves as n^2 for large n . Alternatives: $n^{-5}, n^{-4}, n^{-3}, n^{-2}, n^{-1}, n^0, n^1, n^2, n^3, n^4, n^5$

Solution:

The transition rate out of this state due to spontaneous electric dipole transitions

$$R \propto \omega^3 |D|^2$$

where ω is the energy difference between the initial and final state divided by $\hbar$, and D is the dipole transition matrix element. The initial state has quantum numbers n and $l = n - 1$ as that corresponds to the maximum angular momentum. In electric dipole transitions $\Delta l = \pm 1$, thus for spontaneous decay where the energy decreases the only possibility for the final state is a state with $l' = n - 2$ which must correspond to $n' = n - 1$. The energy difference between the initial and final states is

$$\hbar\omega = \frac{E_1}{n^2} - \frac{E_1}{(n-1)^2} = E_1 \left(\frac{(n-1)^2 - n^2}{n^2(n-1)^2} \right) = -E_1 \frac{2n-1}{n^2(n-1)^2} \sim -E_1 \frac{2}{n^3}$$

where we have taken the limit of large n . Now using the assumption that the matrix element $D \sim n^2$. i.e. $|D|^2 \sim n^4$, we find that

$$R \propto \left(\frac{1}{n^3} \right)^3 n^4 = \frac{1}{n^5}$$

The lifetime is the inverse of the transition rate, thus it behaves as $\underline{n^5}$ for n large. This can be very long, of the order milliseconds, when $n \sim 100$, for these so-called circular Rydberg states.

Problem 3

Consider a particle with mass m moving in one dimension, subject to an attractive delta-function potential, so that the Hamiltonian operator in the coordinate representation is

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - \alpha \delta(x)$$

where the delta-function strength α is a positive quantity with units of energy times length. In this problem we will treat H using the variational method using a family of normalized Gaussian trial wave functions

$$\psi_L(x) = \left(\frac{2}{\pi L^2} \right)^{1/4} e^{-x^2/L^2}$$

where L is a real and positive variational parameter with units of length.

3a) (6 points) Show that the expectation value of the kinetic energy in the trial wave-function $\psi_L(x)$ is $\hbar^2/(2mL^2)$.

Solution:

$$E_k = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \psi_L^*(x) \frac{\partial^2}{\partial x^2} \psi_L(x) = \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \left(\frac{\partial}{\partial x} \psi_L(x) \right)^2$$

where we used partial integration, and observed that $\psi_L(x)$ is real and that the surface terms vanish at infinity. Carrying out the differentiation, we get

$$\frac{\partial}{\partial x} \psi_L(x) = -\left(\frac{2}{\pi L^2} \right)^{1/4} \frac{2x}{L^2} e^{-x^2/L^2}$$

Inserting this into the expression for the kinetic energy, we get

$$E_k = \frac{\hbar^2}{2m} \left(\frac{2}{\pi L^2} \right)^{1/2} \frac{2}{L^2} \int_{-\infty}^{\infty} dx \frac{2x^2}{L^2} e^{-2x^2/L^2} = \frac{\hbar^2}{2m} \left(\frac{2}{\pi L^2} \right)^{1/2} \frac{2}{L^2} \left(\frac{L^2}{2} \right)^{1/2} \int_{-\infty}^{\infty} dx' x'^2 e^{-x'^2}$$

where we changed variables to $x' = x\sqrt{2/L^2}$ in the last step. The value of the integral is $\sqrt{\pi}/2$ (B & DD. (2.173) or Rottmann integral 50)). Thus

$$E_k = \frac{\hbar^2}{2m} \left(\frac{2}{\pi L^2} \right)^{1/2} \frac{2}{L^2} \left(\frac{L^2}{2} \right)^{1/2} \frac{\sqrt{\pi}}{2} = \frac{\hbar^2}{2mL^2}$$

Grading:

For full score on this subproblem, the calculation must be completely free of errors.

3b) (6 points) Find the best (lowest) upper bound on the ground state energy of H using the trial wave functions $\psi_L(x)$.

Solution:

To calculate the trial energy we also need the potential energy. It is

$$-\alpha \int_{-\infty}^{\infty} dx \psi_L^*(x) \delta(x) \psi_L(x) = -\alpha \psi_L^2(0) = -\alpha \left(\frac{2}{\pi L^2} \right)^{1/2} = -\alpha \sqrt{\frac{2}{\pi}} \frac{1}{L}$$

and so the full trial energy is

$$E_{tr} = \frac{\hbar^2}{2mL^2} - \alpha \sqrt{\frac{2}{\pi}} \frac{1}{L}$$

This should be minimized. Differentiating w.r.t. L and setting equal to zero, we get

$$-\frac{\hbar^2}{2m} \frac{2}{L^3} + \alpha \sqrt{\frac{2}{\pi}} \frac{1}{L^2} = 0 \implies \frac{1}{L} = \frac{\alpha m}{\hbar^2} \sqrt{\frac{2}{\pi}}$$

Inserting this into the trial energy, we get the lowest upper bound on the ground state energy:

$$E_{tr,min} = \frac{\hbar^2}{2m} \frac{\alpha^2 m^2}{\hbar^4} \frac{2}{\pi} - \alpha \frac{\alpha m}{\hbar^2} \frac{2}{\pi} = -\frac{\alpha^2 m}{\pi \hbar^2}$$

Grading:

For full score on this subproblem, the variational energy must be correct. Then it must also be minimized correctly w.r.t. L and the minimum of the variational energy must be correct.

Problem 4

Two indistinguishable fermions, each with spin-1/2 and mass m move non-relativistically in a one-dimensional harmonic oscillator potential of angular frequency ω . The fermions interact via a spin-dependent interaction

$$V = -\frac{J}{\hbar^2} a \delta(\hat{x}_1 - \hat{x}_2) \vec{S}_1 \cdot \vec{S}_2$$

where $\hat{x}_i$ and $\vec{S}_i$ are the coordinate and spin operators of fermion i . J is a positive constant with units of energy and a is a positive constant with units of length.

4a) (6 points) Treat V as a perturbation, and use first order perturbation theory to calculate the first order perturbative correction to the ground state energy of this system. Identify also the dimensionless parameter that must be small for perturbation theory to be valid.

Solution:

The ground state of the unperturbed system is to place both fermions in the ground state of the harmonic oscillator and make a singlet spin configuration to ensure a proper fermion wave function. Thus

$$|g.s^0\rangle = \frac{1}{\sqrt{2}}|0\rangle \otimes |0\rangle \otimes (|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle)$$

This is the unique ground state, and so the first order perturbative correction to the ground state is

$$\begin{aligned} E^1 &= \langle g.s^0 | V | g.s^0 \rangle = -\frac{Ja}{\hbar^2} \langle 0 | \otimes \langle 0 | \delta(\hat{x}_1 - \hat{x}_2) | 0 \rangle \otimes | 0 \rangle \\ &\quad \times \frac{1}{2} (\langle \uparrow | \otimes \langle \downarrow | - \langle \downarrow | \otimes \langle \uparrow |) \vec{S}_1 \cdot \vec{S}_2 (|\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle) \end{aligned}$$

The first matrix element can be calculated by inserting complete sets of states

$$\langle 0 | \otimes \langle 0 | \delta(\hat{x}_1 - \hat{x}_2) | 0 \rangle \otimes | 0 \rangle = \int_{-\infty}^{\infty} dx'_1 dx'_2 dx_1 dx_2 \langle 0 | x'_1 \rangle \langle 0 | x'_2 \rangle \langle x'_1 | \otimes \langle x'_2 | \delta(\hat{x}_1 - \hat{x}_2) | x_1 \rangle \otimes | x_2 \rangle \langle x_1 | 0 \rangle \langle x_2 | 0 \rangle$$

Now

$$\langle x'_1 | \otimes \langle x'_2 | \delta(\hat{x}_1 - \hat{x}_2) | x_1 \rangle \otimes | x_2 \rangle = \delta(x_1 - x_2) \delta(x'_1 - x_1) \delta(x'_2 - x_2)$$

Integrating over the primed quantities, we therefore get

$$\langle 0 | \otimes \langle 0 | \delta(\hat{x}_1 - \hat{x}_2) | 0 \rangle \otimes | 0 \rangle = \int_{-\infty}^{\infty} dx_1 dx_2 \delta(x_1 - x_2) |\langle x_1 | 0 \rangle|^2 |\langle x_2 | 0 \rangle|^2$$

Now we insert the explicit expression for the ground state wave function of the harmonic oscillator

$$\langle x | 0 \rangle = \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-\frac{m\omega}{2\hbar} x^2}$$

and get

$$\begin{aligned} \langle 0 | \otimes \langle 0 | \delta(\hat{x}_1 - \hat{x}_2) | 0 \rangle \otimes | 0 \rangle &= \frac{m\omega}{\pi\hbar} \int_{-\infty}^{\infty} dx_1 dx_2 \delta(x_1 - x_2) e^{-\frac{m\omega}{\hbar} x_1^2} e^{-\frac{m\omega}{\hbar} x_2^2} \\ &= \frac{m\omega}{\pi\hbar} \int_{-\infty}^{\infty} dx_1 e^{-\frac{2m\omega}{\hbar} x_1^2} = \frac{m\omega}{\pi\hbar} \sqrt{\frac{\hbar\pi}{2m\omega}} = \sqrt{\frac{m\omega}{2\pi\hbar}} \end{aligned}$$

For the second matrix element we can rewrite

$$\vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2} (S^2 - 3\hbar^2/2)$$

and use the fact that the ground state is a spin singlet: $S^2 = 0$. We therefore get

$$\frac{1}{2} (\langle \uparrow | \otimes \langle \downarrow | - \langle \downarrow | \otimes \langle \uparrow |) \vec{S}_1 \cdot \vec{S}_2 (| \uparrow \rangle \otimes | \downarrow \rangle - | \downarrow \rangle \otimes | \uparrow \rangle) = -\frac{3\hbar^2}{4}$$

Together this gives the answer

$$E^1 = Ja \frac{3}{4} \sqrt{\frac{m\omega}{2\pi\hbar}}$$

The unperturbed ground state energy is $\hbar\omega$. Thus the energy correct to first order in perturbation theory is

$$E \approx \hbar\omega \left(1 + \frac{3Ja}{4\hbar\omega} \sqrt{\frac{m\omega}{2\pi\hbar}} \right) = \hbar\omega \left(1 + \frac{3}{8\sqrt{\pi}} \frac{Ja}{\hbar\omega} \sqrt{\frac{2m\omega}{\hbar}} \right) = \hbar\omega \left(1 + \frac{3}{8\sqrt{\pi}} \frac{J}{\hbar\omega} \frac{a}{\sqrt{\frac{\hbar}{2m\omega}}} \right)$$

So the perturbation parameter that should be small for perturbation theory to be valid is

$$\frac{J}{\hbar\omega} \frac{a}{\sqrt{\frac{\hbar}{2m\omega}}}$$

which we recognize as the product of the energy ratio $J/(\hbar\omega)$ and the length ratio $a/\sqrt{\frac{\hbar}{2m\omega}}$, where $\hbar\omega$ is the characteristic oscillator energy, and $\sqrt{\frac{\hbar}{2m\omega}}$ is the characteristic oscillator length. Thus if Ja is small compared to these, first order perturbation theory will be a good approximation.

It is also possible to write the ground state as

$$\Psi = \psi_0(x_1)\psi_0(x_2)\chi_s$$

where ψ_0 is the ground state wave function for the 1D harmonic oscillator and χ_s is representing the singlet state of two spin-1/2s. Then the energy shift is given by

$$\begin{aligned} \Delta E &= -\frac{Ja}{\hbar^2} \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 |\psi_0(x_1)|^2 |\psi_0(x_2)|^2 \delta(x_1 - x_2) \frac{-3\hbar^2}{4} \\ &= \frac{3Ja}{4} \int_{-\infty}^{\infty} dx_1 |\psi_0(x_1)|^4 = \frac{3Ja}{4} \frac{m\omega}{\pi\hbar} \int_{-\infty}^{\infty} dx_1 e^{-\frac{2m\omega}{\hbar}x_1^2} = Ja \frac{3}{4} \sqrt{\frac{m\omega}{2\pi\hbar}} \end{aligned}$$

where we have used the expectation value of the spin-interaction in the singlet state as calculated above.

Grading:

To get full score on this problem, the answer must be correct including the identification of the small parameter. Partial scores will be given based on how close the reasoning in the answer comes to fully solve the problem. In particular, a partial credit of 1 point will be given for writing down the correct formula for the non-degenerate perturbative first order

energy correction, and up to 2 points for correctly identifying the ground state.

Problem 5

A Hamiltonian for a particle of mass m moving in two dimensions is given as

$$\hat{H} = \frac{1}{2m} \left(\hat{p}_x - \frac{\hbar}{l^2} \hat{y} \right)^2 + \frac{1}{2m} \hat{p}_y^2$$

where $\hat{p}_x, \hat{p}_y$ are the momentum operators in the x and y -directions respectively, and $\hat{y}$ is the position operator in the y -direction. l is a positive constant with units of length.

In the two first subproblems below consider $\hat{H}$ to be a perturbed version of the following Hamiltonian

$$\hat{H}^0 = \frac{1}{2m} \hat{p}_x^2 + \frac{1}{2m} \hat{p}_y^2 + \frac{1}{2m} \left(\frac{\hbar}{l^2} \right)^2 \hat{y}^2$$

5a) (3 points) What are the energy eigenstates and corresponding energies of $\hat{H}^0$?

Solution:

Let us rewrite $\hat{H}^0$ slightly

$$\hat{H}^0 = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{m}{2} \left(\frac{\hbar}{ml^2} \right)^2 \hat{y}^2$$

so that we can recognize the harmonic oscillator potential $\frac{1}{2}m\omega^2\hat{y}^2$ in the y -direction. Thus $\omega \equiv \hbar/(ml^2)$. The eigenstates of $\hat{H}^0$ thus separate into plane waves in the x -direction and harmonic oscillator occupation number states in the y -direction. Therefore the eigenstates can be written

$$|k\rangle \otimes |n\rangle$$

where $|k\rangle$ are plane waves with wave vector k and $|n\rangle$ are harmonic oscillator occupation number states. Their energies are

$$E_{k,n} = \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{ml^2} (n + 1/2)$$

Grading:

Full score will be given if the answer makes it clear that the eigenstates are combinations (products) of one-dimensional harmonic oscillator states and plane wave states, and that the expression for the energy is correct.

5b) (6 points) Calculate the energy levels of $\hat{H}$ correct to first order in perturbation theory using $\hat{H}^0$ as the unperturbed Hamiltonian.

Solution:

We first determine if the unperturbed problem is degenerate. The level (k, n) is degenerate if there exists another set of quantum numbers (k', n') such that

$$E_{k,n} = E_{k',n'} \implies \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{ml^2} (n + 1/2) = \frac{\hbar^2 k'^2}{2m} + \frac{\hbar^2}{ml^2} (n' + 1/2).$$

It is clear that there is at least one such set, namely $(k' = -k, n' = n)$. And there can also be other solutions dependent on the exact value of l . Thus we need to use degenerate perturbation theory.

Comparing $\hat{H}$ and $\hat{H}^0$ we see that the perturbation is

$$\hat{H}^1 = -\frac{1}{m} \frac{\hbar}{l^2} \hat{y} \hat{p}_x = -\frac{\hbar}{ml^2} \sqrt{\frac{\hbar}{2m\omega}} (a^\dagger + a) \hat{p}_x = -\frac{\hbar}{ml\sqrt{2}} (a^\dagger + a) \hat{p}_x$$

where we have written the coordinate operator $\hat{y}$ in terms on raising and lowering operators and used $\omega = \frac{\hbar}{ml^2}$. Applying $\hat{H}^1$ to the unperturbed eigenkets, we get

$$\hat{H}^1 |k\rangle \otimes |n\rangle = -\frac{\hbar}{ml\sqrt{2}} \hbar k (\sqrt{n+1} |k\rangle \otimes |n+1\rangle + \sqrt{n} |k\rangle \otimes |n-1\rangle)$$

and therefore the full perturbation matrix between degenerate states is

$$\langle k' | \otimes \langle n' | \hat{H}^1 |k\rangle \otimes |n\rangle = -\frac{\hbar}{ml\sqrt{2}} \hbar k (\sqrt{n+1} \delta_{n',n+1} + \sqrt{n} \delta_{n',n-1}) \delta_{k,k'}$$

Thus the perturbation matrix is diagonal in k . Now for a given value of k , different values of n are not degenerate. Thus the perturbation matrix is 0 in the degenerate subspace. Therefore, the first order perturbative correction to the energy levels is 0.

Grading:

For full score on this subproblem the answer must be correct and be obtained using non-degenerate perturbation theory. Partial credit of 2 points will be given for finding the correct form of the perturbation.

In the last subproblem solve $\hat{H}$ exactly (not with perturbation theory).

5c) (3 points) Start by writing down the equation that $\chi_k(y)$ must satisfy for the function $\chi_k(y)e^{ikx}$ to be an exact energy eigenfunction of $\hat{H}$ with eigenenergy E . Then find the exact energy levels of $\hat{H}$.

Solution:

$$\begin{aligned}
\hat{H}\chi_k(y)e^{ikx} &= E\chi_k(y)e^{ikx} \\
\left[\frac{1}{2m} \left(\frac{\hbar}{i} \frac{\partial}{\partial x} - \frac{\hbar}{l^2} y \right)^2 + \frac{1}{2m} \left(\frac{\hbar}{i} \frac{\partial}{\partial y} \right)^2 \right] \chi_k(y)e^{ikx} &= E\chi_k(y)e^{ikx} \\
\left[\frac{1}{2m} \left(\hbar k - \frac{\hbar}{l^2} y \right)^2 - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} \right] \chi_k(y) &= E\chi_k(y) \\
\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{m}{2} \left(\frac{\hbar}{ml^2} \right)^2 (y - l^2 k)^2 \right] \chi_k(y) &= E\chi_k(y)
\end{aligned}$$

We see that the left hand side has the form of a displaced harmonic oscillator. Changing variables to $y' = y - l^2 k$ we get an ordinary harmonic oscillator with $\omega = \frac{\hbar}{ml^2}$. Therefore the exact energy levels of $\hat{H}$ is given by

$$E_n = \frac{\hbar^2}{ml^2} \left(n + \frac{1}{2} \right)$$

Note that k does not enter the exact energies! This means that each energy level is infinitely degenerate as k can take an infinite number of values.

Although it was not asked about, it is interesting to compare this result to perturbation theory. We see that the difference is a term of order k^2 , while the perturbation is linear in k . Therefore second order degenerate perturbation theory must give the exact answer. This is because it is the only order of perturbation theory that gives contributions of the order k^2 , which is what is needed to cancel the k^2 contributions from $\hat{H}^0$.

It is useful to see this by explicit computation. Using the non-perturbative formula for the second order correction to the energy level (k, n) , we have

$$E_{k,n}^2 = \sum_{k', n' \neq k, n} \frac{|\langle k', n' | H^1 | k, n \rangle|^2}{E_{k,n} - E_{k', n'}}$$

This is of course questionable as we are dealing with degenerate states here. Nevertheless we can use it when the unperturbed states are good states (which they are since they diagonalize the perturbation matrix; it is zero) provided we leave out the degenerate states from the sum. Inserting the matrix element found in the previous subproblem, and carrying out the sum over k' , we get

$$E_{k,n}^2 = \left(\frac{\hbar}{ml\sqrt{2}} \hbar k \right)^2 \sum_{n' \neq n} \frac{(n+1)\delta_{n', n+1} + n\delta_{n', n-1}}{\hbar\omega(n - n')} = \frac{\hbar^4 k^2}{2m^2 l^2 \hbar\omega} \left(\frac{n+1}{-1} + \frac{n}{+1} \right)$$

Now we use $\omega = \frac{\hbar}{ml^2}$. Then

$$E_{k,n}^2 = -\frac{\hbar^4 k^2 ml^2}{2m^2 l^2 \hbar^2} = -\frac{\hbar^2 k^2}{2m}$$

which is precisely what is needed to get the exact result.

Grading:

To reconcile the exact solution with perturbation theory is not required as it was not asked about. 1 point will be given for obtaining the correct equation for χ , an additional 2 points will be awarded for recognizing the shifted harmonic oscillator and getting the correct answer.

THE END