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Solution for final exam in: FYS3110 - Quantum mechanics.

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Problem 1:

1.1 The definition of S^\pm can be inverted: $S^x = (S^+ + S^-)/2$, $S^y = (S^+ - S^-)/2i$.

$$\begin{aligned}\vec{S}_1 \cdot \vec{S}_2 &= S_1^x S_2^x + S_1^y S_2^y + S_1^z S_2^z \\ &= \frac{1}{4} (S_1^+ + S_1^-) (S_2^+ + S_2^-) - \frac{1}{4} (S_1^+ - S_1^-) (S_2^+ - S_2^-) + S_1^z S_2^z \\ &= \frac{1}{2} (S_1^+ S_2^- + S_1^- S_2^+) + S_1^z S_2^z, \quad \text{q.e.d.}\end{aligned}$$

The action of the spin operators on eigenstates of S_z can be found in Griffiths p.171-172.

They are $S_-|\uparrow\rangle = \hbar|\downarrow\rangle$, $S_-|\downarrow\rangle = 0$, $S_+|\uparrow\rangle = 0$, $S_+|\downarrow\rangle = \hbar|\uparrow\rangle$, $S_z|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle$ and $S_z|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle$.

Thus for $\hbar_1 = 0$:

$$\begin{aligned}\hat{H}|\uparrow\downarrow\rangle &= \frac{J}{2\hbar^2} (S_1^+ S_2^- + S_1^- S_2^+) |\uparrow\downarrow\rangle + \frac{J}{\hbar^2} S_1^z S_2^z |\uparrow\downarrow\rangle = \frac{J}{2} |\downarrow\uparrow\rangle - \frac{J}{4} |\uparrow\downarrow\rangle \\ \hat{H}|\downarrow\uparrow\rangle &= \frac{J}{2} |\uparrow\downarrow\rangle - \frac{J}{4} |\downarrow\uparrow\rangle\end{aligned}$$

This implies that

$$\underline{\hat{H}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = -\frac{3J}{4} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad \text{q.e.d.}}$$

thus the energy eigenvalue is $\underline{E_{00} = -3J/4}$. Lets call the normalized ket $|\psi_{00}\rangle = C(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. Then normalizing gives

$$1 = \langle\psi_{00}|\psi_{00}\rangle = C^2 (\langle\uparrow\downarrow| - \langle\downarrow\uparrow|) (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = 2C^2 \implies C = 1/\sqrt{2}$$

Thus

$$\underline{|\psi_{00}\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)}$$

1.2 Rewriting $\vec{S}_1 \cdot \vec{S}_2 = [(\vec{S}_1 + \vec{S}_2)^2 - \vec{S}_1^2 - \vec{S}_2^2]/2 = \vec{S}_{\text{tot}}^2 - 3\hbar^2/4$ one sees that the energy eigenstates are the eigenstates of the total spin operator. The state used in 1.1 is the singlet state with total spin $S_{\text{tot}} = 0$, thus the remaining states are the triplet spin-1 states one can

get by combining two spin-1/2's (Griffiths page 185):

$$\begin{aligned} |\psi_{11}\rangle &= |\uparrow\uparrow\rangle \\ |\psi_{10}\rangle &= \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |\psi_{1-1}\rangle &= |\downarrow\downarrow\rangle \end{aligned}$$

all these states have the same energy $E_{11} = E_{10} = E_{1-1} = \frac{J}{4}$ which follows from $JS_{\text{tot}}(S_{\text{tot}} + 1)/2 - 3J/4 = J/4$ for $S_{\text{tot}} = 1$, or by acting with \hat{H} on the states.

1.3 For a generic state $|\psi(t)\rangle$ the expectation value is a constant of motion (time-independent) if the operator commutes with the Hamiltonian. This follows from (Griffiths page 115):

$$\frac{d\langle\psi(t)|\hat{O}|\psi(t)\rangle}{dt} = \frac{i}{\hbar} \langle\psi(t)| [\hat{H}, \hat{O}] |\psi(t)\rangle$$

Computing the commutators, one gets

$$\begin{aligned} [\hat{H}, S_1^z] &= \frac{J}{\hbar^2} [S_1^x S_2^x + S_1^y S_2^y, S_1^z] \\ &= \frac{J}{\hbar^2} ([S_1^x, S_1^z] S_2^x + [S_1^y, S_1^z] S_2^y) \\ &= \frac{J}{\hbar} ((-i)S_1^y S_2^x + iS_1^x S_2^y) \neq 0 \\ [\hat{H}, S_2^z] &= \frac{J}{\hbar} (iS_1^y S_2^x - iS_1^x S_2^y) = -[\hat{H}, S_1^z] \neq 0 \end{aligned}$$

Thus both G_1 and G_2 will depend on time. However

$$[\hat{H}, (S_1^z + S_2^z)] = 0$$

which implies that $\underline{G_3}$ will not depend on time. We also see that

$$[\hat{H}, (S_1^z - S_2^z)] \neq 0$$

thus G_4 is also time-dependent.

Therefore only G_3 will not depend on time when the initial state $|\psi(0)\rangle$ is an arbitrary state. While G_3 is a constant in t for any initial states, there are *special* initial states in which some or all of the other quantities are also constant. For instance, when the initial state is an energy eigenstates; a stationary state, all expectation values are independent of t . To find these special states, one should solve the problem exactly.

1.4 $H^0 = \frac{J}{\hbar^2} \vec{S}_1 \cdot \vec{S}_2$ and $H' = -\frac{h_1}{\hbar} S_1^z$. The lowest unperturbed energy level has energy $E_{00}^{(0)} = -\frac{3J}{4}$ and is non-degenerate. 1. order correction: $E_{00}^{(1)} = \langle \psi_{00} | H' | \psi_{00} \rangle$

$$H' | \psi_{00} \rangle = -\frac{h_1}{\hbar} S_1^z \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = -\frac{h_1}{2} \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) = -\frac{h_1}{2} | \psi_{10} \rangle$$

Therefore

$$E_{00}^1 = \langle \psi_{00} | H' | \psi_{00} \rangle = -\frac{h_1}{2} \langle \psi_{00} | \psi_{10} \rangle = 0$$

The 2. order correction is given by a sum over all states different from the ground state

$$\begin{aligned} E_{00}^{(2)} &= \frac{|\langle \psi_{11} | H' | \psi_{00} \rangle|^2}{E_{00}^0 - E_{11}^0} + \frac{|\langle \psi_{10} | H' | \psi_{00} \rangle|^2}{E_{00}^0 - E_{10}^0} + \frac{|\langle \psi_{1-1} | H' | \psi_{00} \rangle|^2}{E_{00}^0 - E_{101}^0} \\ &= \frac{|\langle \psi_{10} | H' | \psi_{00} \rangle|^2}{E_{00}^0 - E_{10}^0} = \frac{h_1^2}{4} \frac{1}{-3J/4 - J/4} \\ &= -\frac{h_1^2}{4J} \end{aligned}$$

Thus perturbation theory correct up to 2. order gives

$$\underline{E_{00} = -\frac{3J}{4} - \frac{h_1^2}{4J}}$$

1.5 The highest energy level has energy $J/4$ and is 3-fold degenerate. The action of the perturbation on the three states in 1.2 is

$$\begin{aligned} H' | \psi_{11} \rangle &= -\frac{h_1}{2} | \psi_{11} \rangle \\ H' | \psi_{10} \rangle &= -\frac{h_1}{2} | \psi_{00} \rangle \\ H' | \psi_{1-1} \rangle &= +\frac{h_1}{2} | \psi_{1-1} \rangle \end{aligned}$$

Thus we see that the three states are good states because they diagonalize the perturbation in the degenerate subspace. The energy corrections are

$$\begin{aligned} E_{11}^1 &= \langle \psi_{11} | H' | \psi_{11} \rangle = -\frac{h_1}{2} \\ E_{10}^1 &= \langle \psi_{10} | H' | \psi_{10} \rangle = 0 \\ E_{1-1}^1 &= \langle \psi_{1-1} | H' | \psi_{1-1} \rangle = \frac{h_1}{2} \end{aligned}$$

Thus to first order in perturbation theory the highest energy will be split into three:

$$\underline{E_{11} = J/4 - h_1/2, E_{10} = J/4, E_{1-1} = J/4 + h_1/2.}$$

1.6 In order to solve the system exactly we use the energy eigenstates at $h_1 = 0$ as a set of basis states. The action of the full Hamiltonian on these states are:

$$\begin{aligned}\hat{H}|\psi_{11}\rangle &= \left(\frac{J}{4} - \frac{h_1}{2}\right)|\psi_{11}\rangle \\ \hat{H}|\psi_{1-1}\rangle &= \left(\frac{J}{4} + \frac{h_1}{2}\right)|\psi_{1-1}\rangle \\ \hat{H}|\psi_{10}\rangle &= \frac{J}{4}|\psi_{10}\rangle - \frac{h_1}{2}|\psi_{00}\rangle \\ \hat{H}|\psi_{00}\rangle &= -\frac{3J}{4}|\psi_{00}\rangle - \frac{h_1}{2}|\psi_{10}\rangle\end{aligned}$$

Thus it follows that $|\psi_{1\pm 1}\rangle$ are exact eigenstates of \hat{H} with energies $E_{1\pm 1} = \frac{J}{4} \mp \frac{h_1}{2}$ in agreement with the perturbative result in 1.5. In fact, the 1. order perturbative result for these states is exact.

In the subspace spanned by $|\psi_{00}\rangle$ and $|\psi_{10}\rangle$ the Hamiltonian takes the following form:

$$\begin{pmatrix} -\frac{3J}{4} & -\frac{h_1}{2} \\ -\frac{h_1}{2} & \frac{J}{4} \end{pmatrix}$$

where $|\psi_{00}\rangle$ " = " $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|\psi_{10}\rangle$ " = " $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. (" = " means represented by). Thus we get the following condition on the eigenvalues

$$\begin{vmatrix} -\frac{3J}{4} - E & -\frac{h_1}{2} \\ -\frac{h_1}{2} & \frac{J}{4} - E \end{vmatrix} = 0$$

which is equivalent to the equation

$$E^2 + \frac{J}{2}E - \frac{3}{16}J^2 - \frac{h_1^2}{4} = 0$$

Solving this gives

$$E = -\frac{J}{4} \pm \frac{J}{2} \sqrt{1 + \left(\frac{h_1}{J}\right)^2}$$

which are the exact energy eigenvalues in the $|\psi_{00}\rangle, |\psi_{10}\rangle$ sector. In order to compare with perturbation theory we expand the square root. This gives

$$E \approx -\frac{J}{4} \pm \left(\frac{J}{2} + \frac{J}{4} \left(\frac{h_1}{J} \right)^2 + \dots \right) = \begin{cases} \frac{J}{4} + \frac{h_1^2}{4J} + \dots \\ -\frac{3J}{4} - \frac{h_1^2}{4J} + \dots \end{cases}$$

For the ground state we get agreement with the perturbation theory result in 1.4 up to $\mathcal{O}(\hbar_1^2)$. We also see that the highest energy in this sector is $J/4 + \mathcal{O}(\hbar_1)$ which agrees with the uncorrected energy level found in perturbation theory in 1.5.

Problem 2:

2.1 Particle in an infinite square well. This problem is treated in Griffiths page 32, the only difference is that the width of the potential here is $2a$. thus the energy eigenvalues are

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2} = \frac{n^2 \pi^2 \hbar^2}{8ma^2}, n = 1, 2, 3, \dots$$

The lowest energy is $E_1 = \frac{\pi^2 \hbar^2}{8ma^2}$.

2.2 With the infinite wall the wavefunction must be zero at $-a$ and a which gives the following condition on the WKB wavefunction

$$\int_{-a}^a dx P(x) = n\pi\hbar$$

where $P(x) = \sqrt{2m(E - V(x))} = \sqrt{2m(E - gx^4)}$. Writing it out we get the integral equation

$$2 \int_0^a \sqrt{2m(E - gx^4)} = n\pi\hbar$$

As $E > ga^4$ we do not encounter any problem with $P \sim 0$, thus we do not need to consider the connection formulas.

To solve this approximately we expand the square root

$$\int_0^a dx \sqrt{2mE} \sqrt{1 - \frac{gx^4}{E}} \approx \sqrt{2mE} \int_0^a dx \left(1 - \frac{gx^4}{2E}\right) = \sqrt{2mE} \left(a - \frac{ga^5}{10E}\right)$$

which inserted into the integral equation gives

$$a\sqrt{2mE} \left(1 - \frac{ga^4}{10E}\right) = \frac{n\pi\hbar}{2}$$

Dividing by $a\sqrt{2mE}$ on both sides and squaring gives

$$\left(1 - \frac{ga^4}{10E}\right)^2 = \frac{E_n}{E}$$

where E_n is the expression gotten in 2.1. Multiplying out the parenthesis on the left hand side and dropping the $(ga^4/E)^2$ -term, as is justified to first order in g , ($E \gg ga^4$), we get

$$1 - \frac{ga^4}{5E} = \frac{E_n}{E}$$

which is easily solved to give

$$E = E_n + \frac{ga^4}{5}$$

Thus to lowest order in g the correction is just a uniform shift of the energy levels.

2.3 The wave function *must* be continuous and zero outside the walls as the potential there is infinity. This implies that the wave-function should go to zero approaching the walls from the inside. The potential is symmetric around $x = 0$ so the energy eigenfunctions will have a definite symmetry, either symmetric or antisymmetric. When $g = 0$ we know that the ground state wave function is $\psi(x) = \sqrt{\frac{1}{a}} \cos(\frac{\pi}{2a}x)$ (the particle in an infinite potential well). For g large we expect the wavefunction to be more localized in the middle of the box as the particle will pay considerable potential energy if it is close to the walls. There is no particular energy penalty of having a particle in the centre of the box for any g , we thus take the wave-function to be a symmetric continuous function of x that approaches zero at the walls and stays zero outside. Two possible such symmetric polynomials of low order are

$$\psi_t(x) = \begin{cases} C_t(a - |x|) & -a \leq x \leq a \\ 0 & \text{otherwise} \end{cases}, \quad \psi_p(x) = \begin{cases} C_p(a^2 - x^2) & -a \leq x \leq a \\ 0 & \text{otherwise} \end{cases}$$

These wavefunctions have no adjustable parameters; the C 's are fixed by the normalization. Computing the expectation value $\langle \psi | H | \psi \rangle$ using one of these trial wavefunctions gives an upper bound on the ground state energy.

Lets treat the triangular case first. The normalization constant C_t is determined from

$$1 = \int_{-a}^a dx |C_t|^2 (a - |x|)^2 = 2|C_t|^2 \frac{a^3}{3} \implies 2|C_t|^2 = \frac{3}{a^3}$$

For the kinetic energy we need to differentiate ψ_t twice. Because of the discontinuities in the derivatives we get a non-zero answer

$$\frac{d^2\psi_t}{dx^2} = C_t (\delta(x + a) + \delta(x - a) - 2\delta(x))$$

and the expectation value of the kinetic energy becomes

$$\int_{-\infty}^{\infty} dx \psi_t^*(x) \frac{-\hbar^2}{2m} \frac{d^2\psi_t(x)}{dx^2} = 2|C_t|^2 \frac{\hbar^2 a}{2m}$$

the delta-functions at $x = \pm a$ do not contribute as the wave-function is zero there. For the potential energy we have

$$\int_{-\infty}^{\infty} dx \psi_t^*(x) g x^4 \psi_t(x) = 2|C_t|^2 g \int_0^a x^4 (a^2 - 2ax + x^2) = 2|C_t|^2 g a^7 \left(\frac{1}{5} - \frac{1}{3} + \frac{1}{7} \right) = 2|C_t|^2 g a^7 \frac{1}{105}$$

Putting together the potential and the kinetic energy we obtain the following upper bound on the ground state energy

$$E_{gs} \leq \underline{3 \frac{\hbar^2}{2ma^2} + \frac{3}{105} g a^4}$$

For the parabolic case we get

$$1 = |C_p|^2 \int_{-a}^a dx |\psi(x)|^2 = 2|C_p|^2 \int_0^a dx (a^2 - x^2)^2 = 2|C_p|^2 a^5 \left(1 - \frac{2}{3} + \frac{1}{5} \right) = 2|C_p|^2 a^5 \frac{8}{15}$$

which implies

$$2|C_p|^2 = \frac{15}{8a^5}$$

The first derivative of the parabolic wavefunction is also discontinuous at the walls and so the second derivative will have delta-functions at $x = \pm a$. However, exactly as in the triangular case, the wavefunction is zero at the walls, and so their contribution to the kinetic energy are zero. Therefore for the kinetic energy we get

$$\int_{-a}^a dx \psi^*(x) \frac{-\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} = 2|C_p|^2 \frac{\hbar^2}{m} \int_0^a dx (a^2 - x^2) = 2|C_p|^2 \frac{\hbar^2}{m} \frac{2a^3}{3}$$

while the potential energy term is

$$\int_{-a}^a dx \psi_p^*(x) g x^4 \psi_p(x) = 2|C|^2 g \int_0^a dx x^4 (a^4 - 2a^2 x^2 + x^4) = 2|C_p|^2 g a^9 \left(\frac{1}{5} - \frac{2}{7} + \frac{1}{9} \right) = 2|C_p|^2 g a^9 \frac{8}{315}$$

Thus we obtain for the parabolic case

$$E_{gs} \leq \underline{\frac{5}{2} \frac{\hbar^2}{2ma^2} + \frac{5}{105} g a^4}$$

We see that for small g the parabolic wave function gives a lower variational energy than the triangular wave function. In the limit $g \rightarrow 0$ we can compare the parabolic bound with the exact ground state energy found in 2.1: $E_1 = \frac{\pi^2}{4} \frac{\hbar^2}{2ma^2} = 2.467 \frac{\hbar^2}{2ma^2}$. For large g the triangular wavefunction gives the lowest energy. This is in accordance with our expectation that the wavefunction should have less weight towards the edges as g is increased.

There is not a unique answer to this subproblem. Credit will be given if the polynomial trial wavefunction is reasonable, and if the variational principle has been correctly used.