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Solution to resit exam
FY2045 Quantum Mechanics I

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Problem 1 Multiple choice problems

a) The rule for addition two angular momenta with quantum numbers j_1 and j_2 is that the total angular momentum quantum number j can take the values

$$j = j_1 + j_2, j_1 + j_2 - 1, \ldots, |j_1 - j_2|.$$

With $j_1 = 4$ and $j_2 = 3/2$, we therefore get

$$j = \frac{11}{2}, \frac{9}{2}, \frac{7}{2}, \frac{5}{2}.$$

Hence, alternative **C** is the correct answer.

b) We require

$$\begin{aligned}\langle\psi|\psi\rangle &= 1 \\ &= |A|^2[\langle 2|2\rangle + 2^2\langle 4|4\rangle + \langle 6|6\rangle] = |A|^2[1+4+1] = 6|A|^2.\end{aligned}$$

Choosing A positive and real, we therefore get $A = 1/\sqrt{6}$, which is option **E**.

c) The energy expectation value is

$$\begin{aligned}\langle\psi|\hat{H}|\psi\rangle &= \frac{1}{6}\left[\langle 2|\hat{H}|2\rangle + 2^2\langle 4|\hat{H}|4\rangle + \langle 6|\hat{H}|6\rangle\right] \\ &= \frac{\hbar\omega}{6}\left[2 + \frac{1}{2} + 4\left(4 + \frac{1}{2}\right) + 6 + \frac{1}{2}\right] = \hbar\omega\left[4 + \frac{1}{2}\right] \\ &= \frac{9}{2}\hbar\omega.\end{aligned}$$

Hence, **E** is the correct answer.

d) Taking the complex conjugate of the prefactors, we get

$$\langle\psi| = \frac{1}{3}\left[(1-2i)\langle 1| + 2i\langle 2|\right],$$

which is option **D**.

e) The ground state of a symmetric potential should be symmetric and have zero notes, excluding options **C**, **D** and **E**.

Since the potential with $n = 3$ increases faster than the potential with $n = 1$ when $x > 1$, the wavefunction should decrease more rapidly for $n = 3$ compared to $n = 1$. Comparing ψ_A and ψ_B with ψ_0, we see that this is the case for ψ_A. Therefore, ψ_A is the best option for a trial wavefunction for the ground state, making **A** the correct answer.

f) We consider each statement:

A: If $\langle n|\psi\rangle$ is nonzero only for $n = 1$, we must have $|\psi\rangle = |1\rangle$. Therefore, since $|1\rangle$ is an energy eigenstate, ψ is also an energy eigenstate, making this statement **true**.

B: A state vector can be written as a superposition of **any** complete set of basis vectors, not only position basis vectors. Hence, this statement if **false.**

C: Though the Heisenberg uncertainty principle only sets restrictions on the product of the variance of p_x and x, we can always calculate their expectation values, which in fact are needed to calculate the variance. Hence, this is statement **not true.**

D: The outcome of a measurement of the energy will leave the system in an energy eigenstate with energy equal to the outcome of the measurement. When the state before the measurement is a superposition of energy eigenstates with **different** eigenenergies, the states of the system before and after the measurement necessarily have to be different, making this statement is **false**.

E: For a Hermitian Hamiltonian, probability is conserved, and hence the normalization is always $\langle\psi|\psi\rangle = 1$. Since this is independent of time, this statement is **false**.

Conclusion: Option **A** is correct.

g) Since the Hamiltonian is diagonal, we directly read off the energy eigenvalues as $E_\pm = \pm\hbar\omega$, with corresponding eigenspinors

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

A general solution to the Schrödinger equation is therefore $\chi = a_+\chi_+ e^{-iE_+t/\hbar} + a_-\chi_- e^{-iE_-t/\hbar}$. At $t = 0$, the given state can be written as a superposition of the two energy eigenstates with coefficients $a_\pm = 1/\sqrt{2}$, meaning that at times $t > 0$ we have

$$\chi(t) = \frac{1}{\sqrt{2}}\chi_+ e^{-iE_+t/\hbar} + \frac{1}{\sqrt{2}}\chi_- e^{-iE_-t/\hbar} = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix}. \tag{1}$$

Alternative **D** is the correct answer.

h) We consider each statement.

A: Even though the particle is in the eigenstate of S_x with eigenvalue $\hbar/2$ at $t = 0$, S_x and H do not commute, making the expectation value of S_x time-dependent. We will therefore not always measure $S_x = \hbar/2$. This is clear also from the answer in **e)**, where the spin state is proportional to the eigenspinor of S_x with eigenvalue $+\hbar/2$ only at certain times. **Not true.**

B: We insert $t = \frac{\pi}{4\omega}$ into the time-dependent state found in **e)**, Eq. (1),

$$\chi\left(\frac{\pi}{4\omega}\right) = \frac{e^{-i\pi/4}}{\sqrt{2}}\begin{pmatrix} 1 \\ e^{i\pi/2} \end{pmatrix} = \frac{e^{-i\pi/4}}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}. \tag{2}$$

Operating on this state with $S_y = \frac{\hbar}{2}\sigma_y$, we get

$$S_y\chi\left(\frac{\pi}{4\omega}\right) = \frac{\hbar}{2}\frac{e^{-i\pi/4}}{\sqrt{2}}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 \\ i \end{pmatrix} = \frac{\hbar}{2}\frac{e^{-i\pi/4}}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} = \frac{\hbar}{2}\chi\left(\frac{\pi}{4\omega}\right).$$

Hence, we see that $\chi(t)$ at $t = \frac{\pi}{4\omega}$ is an eigenstate of S_y with eigenvalue $\hbar/2$, making the statement **true.**

C: At certain times the state in Eq. (1) will be an eigenstate of S_y, e.g. at $t = \pi/4\omega$ as found above. If we measure at exactly these times, we will know the outcome of a measurement of the spin along the y direction. Hence, this is **not true.**

D: We found above that $\chi(t)$ at $t = \pi/4\omega$ is an eigenvector of S_y with eigenvalue $\hbar/2$. Since the operators for S_y and S_x do not commute, the an eigenstate of S_y cannot simultaneously be an eigenstate of S_x, and this statement is, therefore, **not true**.

E: The energy eigenstates are simultaneous eigenstates of H and S_z, and a measurement of the energy would therefore also determine the component of the spin along z. Hence we do not lose all information about the spin state when measuring the energy. **Not true.**

Conclusion: Option **B** is the correct answer.

i) The momentum eigenstates are delta-function normalized,

$$\langle p_2 | p_1 \rangle = \delta(p_2 - p_1).$$

Hence, we get

$$\langle p_2 | \hat{p} | p_1 \rangle = p_1 \langle p_2 | p_1 \rangle = p_1 \delta(p_2 - p_1) = p_2 \delta(p_2 - p_1),$$

where we can move p_1 outside the bracket since it is a number, not an operator. Hence, the correct answer is alternative **E**.

Problem 2 Short answer questions

a) Physical observables should be real quantities. Since Hermitian operators have real eigenvalues, a physical observable f must be represented by a Hermitian operator $\hat{f} = \hat{f}^\dagger$:

$$f = \langle f | \hat{f} | f \rangle = \langle f | \hat{f}^\dagger | f \rangle = [\langle f | \hat{f} | f \rangle]^* = f^*.$$

b) Bosons states must be symmetric under exchange of identical particles, which allows many identical bosons to occupy the same single-particle state. Fermion states must be completely antisymmetric under exchange of identical particles, which means that identical fermions cannot occupy the same single-particle state (Pauli exclusion principle). In three dimensions bosons have integer spin, while fermions have half-integer spin.

c) Superposition of different energy eigenstates can give time-dependent wavefunctions due to the different energies in the exponentials. For instance,

$$\Psi = \psi_1 e^{-iE_1 t/\hbar} + \psi_2 e^{-iE_2 t/\hbar}$$

gives

$$|\Psi|^2 = |\psi_1|^2 + |\psi_2|^2 + 2\,\mathrm{Re}\{\psi_1 \psi_2^*\} \cos\left(\frac{E_1 - E_2}{\hbar} t\right),$$

which has a time-dependent term. Only one term or a superposition of degenerate energy eigenstates gives no time-dependence.

Problem 3 Normalization condition

Since the state is normalized, we have $\langle \psi | \psi \rangle = 1$. The position eigenstates form a complete basis set, meaning that we have the completeness relation

$$1 = \int_{-\infty}^{\infty} dx \; |x\rangle\langle x|.$$

By inserting a completeness relation, we get

$$
\begin{aligned}
1 = \langle\psi|\psi\rangle &= \int_{-\infty}^{\infty} dx\ \langle\psi|x\rangle\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx\ [\langle x|\psi\rangle]^*\langle x|\psi\rangle = \int_{-\infty}^{\infty} dx\ \psi(x)^*\psi(x) \\
&= \int_{-\infty}^{\infty} dx\ |\psi(x)|^2.
\end{aligned}
$$

Hence, the wavefunction $\psi(x)$ is also normalized.

Problem 4 Identical particles in a box

a) From the formula sheet we have

$$dW = PdV,$$

where W, P and V are the work, pressure and volume, respectively. Since only L_x can change, we have

$$dV = L_y L_z dL_x,$$

and, therefore,

$$dW = PL_y L_z dL_x = F_x dL_x,$$

where we have used the fact that the pressure in the x direction is defined as the force F_x per unit area.

Finally, the work done on the piston by the particle is equal to the reduction in the particles energy,

$$dW = -dE.$$

Hence,

$$F_x = -\frac{dE}{dL_x},$$

which we could also have used directly. We then get, for a general energy state $E_{n_x n_y n_z}$

$$F_x^{n_x n_y n_x} = -\frac{dE_{n_x n_y n_z}}{dL_x} = -\frac{\hbar^2}{2m}\frac{d}{dL_x}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right) = \frac{\hbar^2\pi^2 n_x^2}{mL_x^3}.$$

Hence, for the ground state ($n_x = n_y = n_z = 1$) we get

$$\underline{\underline{F_x = \frac{\hbar^2\pi^2}{mL_x^3}.}}$$

b) We first need to find the ground state of the system when the box contains 8 identical non-interacting particles. Since the particles have spin $\frac{3}{2}$, each energy eigenstate labeled by (n_x, n_y, n_z) can be occupied with four particles with $m_z = \pm\frac{3}{2}, \pm\frac{1}{2}$. The lowest energy eigenstates are

n_x	n_y	n_z	$\frac{2mL^2}{\hbar^2\pi^2} E_{n_x n_y n_z}$	Order
1	1	1	9/4	1
2	1	1	3	2
1	2	1	21/4	4
1	1	2	21/4	4
3	1	1	17/4	3

We only need the two lowest states, with four particles in each, giving the total force

$$F_x = 4F_x^{111} + 4F_x^{211} = \frac{\hbar^2\pi^2}{mL_x^3}[4 + 16] \overset{L_x=2L}{=} \underline{\underline{\frac{5\hbar^2\pi^2}{2mL^3}}}.$$

Problem 5 Spin $\frac{1}{2}$

a) Since $\hat{H}_0 \propto \hat{S}_z$, $\hat{H}_0$ and $\hat{S}_z$ commute and the eigenstates of $\hat{S}_z$ are also eigenstates of $\hat{H}_0$. Therefore, we get

$$\hat{H}_0|\uparrow\rangle = -\frac{2\mu_B B_0}{\hbar}\hat{S}_z|\uparrow\rangle = -\mu_B B_0|\uparrow\rangle \equiv -\epsilon|\uparrow\rangle, \tag{3a}$$

and

$$\hat{H}_0|\downarrow\rangle = \epsilon|\downarrow\rangle. \tag{3b}$$

Hence, the energy eigenstates of the system are the spin-up and -down states $|\uparrow\rangle$ and $|\downarrow\rangle$, with eigenenergies $-\epsilon$ and ϵ, respectively.

b) The expectation values are

$$\begin{aligned}\langle S_z\rangle = \langle\chi|\hat{S}_z|\chi\rangle &= \frac{\hbar}{2}\Big(\langle\uparrow|\cos\alpha + \langle\downarrow|e^{-i\phi}\sin\alpha\Big)\Big(\cos\alpha|\uparrow\rangle - e^{i\phi}\sin\alpha|\downarrow\rangle\Big) \\ &= \frac{\hbar}{2}\left[\cos^2\alpha - \sin^2\alpha\right] = \underline{\underline{\frac{\hbar}{2}\left[2\cos^2\alpha - 1\right]}}, \end{aligned} \tag{4}$$

$$\langle H_0\rangle = -\frac{2\mu_B B_0}{\hbar}\langle S_z\rangle = -\mu_B B_0\left[2\cos^2\alpha - 1\right] = \underline{\underline{-\epsilon\left[2\cos^2\alpha - 1\right]}}. \tag{5}$$

$|\chi\rangle$ is an energy eigenstate when it is proportional to only $|\uparrow\rangle$ or $|\downarrow\rangle$, meaning for $\alpha = \frac{\pi}{2}\cdot n$ with $n \in \mathbb{Z}$ and any $\phi \in \mathbb{R}$.

c) To simplify the calculations we write the state as

$$|\psi(t)\rangle = \frac{e^{i\mu_B B_0 t/\hbar}}{\sqrt{2}} \left[|\uparrow\rangle + e^{i\phi'}|\downarrow\rangle\right], \tag{6}$$

where

$$\phi' \equiv \phi - 2i\mu_B B_0 t/\hbar. \tag{7}$$

Expressing the $\hat{S}_{x/y}$ in terms of the ladder operators, we get

$$\hat{S}_x = \frac{\hat{S}_+ + \hat{S}_-}{2}, \tag{8a}$$

$$\hat{S}_y = \frac{\hat{S}_+ - \hat{S}_-}{2i}. \tag{8b}$$

The expectation values are then readily calculated:

$$\begin{aligned}
\langle S_x\rangle(t) &= \frac{1}{4}\left(\langle\uparrow| + \langle\downarrow|e^{-i\phi'}\right)[\hat{S}_+ + \hat{S}_-]\left(|\uparrow\rangle + e^{i\phi'}|\downarrow\rangle\right) \\
&= \frac{1}{4}\left(\langle\uparrow| + \langle\downarrow|e^{-i\phi'}\right)\left(\hbar|\downarrow\rangle + \hbar e^{i\phi'}|\uparrow\rangle\right) \\
&= \frac{\hbar}{4}\left[e^{i\phi'} + e^{-i\phi'}\right] = \frac{\hbar}{2}\cos\phi' \\
&= \underline{\underline{\frac{\hbar}{2}\cos\left(\phi - \frac{2\mu_B B_0 t}{\hbar}\right)}}, &(9a) \\
\langle S_y\rangle(t) &= \frac{\hbar}{4i}\left[e^{i\phi'} - e^{-i\phi'}\right] \\
&= \underline{\underline{\frac{\hbar}{2}\sin\left(\phi - \frac{2\mu_B B_0 t}{\hbar}\right)}}, &(9b) \\
\langle S_z\rangle(t) &= \frac{\hbar}{4}\left(\langle\uparrow| + \langle\downarrow|e^{-i\phi'}\right)\left(|\uparrow\rangle - e^{i\phi}|\downarrow\rangle\right) = \frac{\hbar}{4}[1-1] = \underline{\underline{0}}. &(9c)
\end{aligned}$$

The oscillating expectation values of the x and y components of the spin spin describes Larmor precession in a static magnetic field.

Problem 6 Perturbation theory

a) When $\lambda = 0$, $\hat{H}$ and $\hat{H}_0$ are identical, and the expansion in powers of λ should be equal to the exact solutions of the unperturbed system, giving

$$|\psi_n^{(0)}\rangle = |\phi_n\rangle,$$

$$E_n^{(0)} = \epsilon_n.$$

b) We need the matrix element

$$\langle\downarrow|\hat{U}|\uparrow\rangle = \frac{\lambda 2\kappa}{\hbar}\langle\downarrow|\hat{S}_x|\uparrow\rangle = \lambda\kappa \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \lambda\kappa. \tag{10}$$

Hence

$$|\chi_-^{(1)}\rangle = \frac{\langle\downarrow|\hat{U}|\uparrow\rangle}{E_\uparrow - E_\downarrow}|\downarrow\rangle = \underline{\underline{-\frac{\lambda\kappa}{2\epsilon}|\downarrow\rangle}}, \tag{11}$$

$$E_-^{(2)} = \frac{|\langle\downarrow|\hat{U}|\uparrow\rangle|^2}{E_\uparrow - E_\downarrow} = \underline{\underline{-\frac{\lambda^2\kappa^2}{2\epsilon}}}, \tag{12}$$

and the ground state to first order in λ is

$$\underline{\underline{|\chi_-\rangle = |\uparrow\rangle - \frac{\lambda\kappa}{2\epsilon}|\downarrow\rangle}}, \tag{13}$$

and eigenenergy to second order in λ is

$$\underline{\underline{E_- = -\epsilon - \frac{\lambda^2\kappa^2}{2\epsilon}}}. \tag{14}$$

c) We rewrite the Hamiltonian

$$\begin{aligned} \hat{H} &= -\frac{2}{\hbar}\sqrt{\epsilon^2+\lambda^2\kappa^2}\left[\frac{\epsilon}{\sqrt{\epsilon^2+\lambda^2\kappa^2}}\hat{S}_z - \frac{\lambda\kappa}{\sqrt{\epsilon^2+\lambda^2\kappa^2}}\hat{S}_x\right] \\ &= -\frac{2}{\hbar}\xi\hat{\mathbf{S}}\cdot\hat{n}, \end{aligned} \tag{15}$$

where

$$\xi = \sqrt{\epsilon^2+\lambda^2\kappa^2}, \tag{16}$$

$$\hat{n} = -\frac{\lambda\kappa}{\xi}\hat{e}_x + \frac{\epsilon}{\xi}\hat{e}_z. \tag{17}$$

Using $\hat{n}$ as the spin quantization axis, defining the operator $\hat{S}_n = \hat{\mathbf{S}}\cdot\hat{n}$ with eigenstates

$$\hat{S}_n|\pm\rangle = \pm\frac{\hbar}{2}|\pm\rangle, \tag{18}$$

we find

$$\hat{H}|\pm\rangle = -\frac{2}{\hbar}\xi\hat{S}_n|\pm\rangle = \mp\xi|\pm\rangle. \tag{19}$$

Therefore, the eigenenergies are

$$E_\mp = \mp\xi. \tag{20}$$

For small λ, we get

$$E_- = -\sqrt{\epsilon^2+\lambda^2\kappa^2} \approx -\epsilon - \frac{\lambda^2\kappa^2}{2\epsilon} + \dots, \tag{21}$$

which agrees with our result from perturbation theory.