Quantumphysics 2

Exam July 2, 2010. Tentamenhal, 9.00-12.00.

◇ *Write your name and student number on each sheet you use.*
◇ *The exam has 5 problems. The number of points for each exercise is an indication about the time you are supposed to spend to solve it.*
◇ *Read the problems carefully and give complete and readable answers.*
◇ *No books or personal notes are allowed.*

Problem 1 (22 pts)

i) Prove that $\hat{J}^2 = \hat{J}_-\hat{J}_+ + \hat{J}_z^2 + \hbar\hat{J}_z$ (5 pts)

Answer: We use ladder operators to rewrite J_x and J_y. Then, we have

$$J_x^2 + J_y^2 + J_z^2 = \frac{J_+J_- + J_-J_+}{2} + J_z^2.$$

Using the commutator $[J_+, J_-] = J_+J_- - J_-J_+ = 2\hbar J_z$, we have

$$J^2 = \hbar J_z + J_-J_+ + J_z^2.$$

ii) Consider a particle with spin s=1/2. Derive the Pauli matrices $\hat{\sigma}_{x,y,z}$. What is the relation between these matrices and the $\hat{S}_{x,y,z}$ operators?
Hint: Work in the basis with $\hat{S}_z$ diagonal. Use ladder operators. (4 pts)

Answer: In this basis, it is elementary to see that

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}\sigma_z.$$

Using the ladder operators, we can easily build the matrix for S_x and S_y and consequently derive σ_x and σ_y.

iii) What is the action of the angular momentum operators $\hat{J}^2$ and $\hat{J}_z$ on Y_l^m functions? Evaluate $\int d\Omega (Y_l^m)^* Y_{l'}^{m'}$ (2 pts)

Answer:

$$J^2|j, m_j\rangle = \hbar^2 j(j+1)|j, m_j\rangle \quad J_z|j, m_j\rangle = m_j\hbar|j, m_j\rangle$$

$$\int d\Omega (Y_l^m)^* Y_{l'}^{m'} = \delta_{ll'}\delta_{mm'}$$

iv) Prove that the degeneracy of the H-atom energy levels E_n is n^2 (excluding the spin degeneracy). (2 pts)

Answer: The degeneracy $\mathcal{D}$ is

$$\mathcal{D} = \sum_{l=0}^{n-1}(2l+1) = n^2.$$

Extra: Including spin, we have to take into account the Pauli's principle, so we can accommodate 2 electrons per energy level. Thus $\mathcal{D} = 2n^2$.

v) Write down the quantum mechanical angular momentum operator in a coordinate representation. `(2 pts)`

Answer: $\hat{L} = -i\hbar\vec{r} \times \vec{\nabla}$

vi) Evaluate the commutators $[\hat{L}_x, \hat{L}_y]$ and $[\hat{L}_z, \hat{L}_y]$. Using these outcomes, evaluate $[\hat{L}_z\hat{L}_x, \hat{L}_y]$. `(4 pts)`

Answer: The first two commutators give respectively $i\hbar L_z$ and $-i\hbar L_x$. Therefore

$$[\hat{L}_z\hat{L}_x, \hat{L}_y] = L_z[L_x, L_y] + [L_z, L_y]L_x = i\hbar(L_z^2 - L_x^2)$$

vii) An unperturbed system has only two eigenfunctions $|1\rangle = xe^{-x^2}$ and $|2\rangle = x^3e^{-x^2}$ which are non-degenerate. Suppose there is a perturbing potential of the form αx. Argue (*i.e. do not calculate!*) why this perturbation does not lead to a first or second order correction to either the energy or the wavefunctions. `(3 pts)`

Answer: All the integrals involved in the perturbation calculations are vanishing because we are integrating an odd function on a even domain. So the perturbation does not change the energetic levels.

Problem 2 `(16 pts)`

Consider the wavefunction of the $|211\rangle$ level of the hydrogen atom

$$\phi_{211} = \frac{1}{\sqrt{3}(2a_0)^{3/2}}\frac{r}{a_0}\mathrm{e}^{-r/2a_0}Y_1^1,$$

with $Y_1^1 = -\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin(\theta)\mathrm{e}^{i\phi}$.

i) Show that ϕ_{211} is normalized. Hint: $\int_0^\infty dr r^m \mathrm{e}^{-xr} = m!x^{-(m+1)}$. `(6 pts)`

Answer:

$$\int\int\int \phi_{211}^{*}\phi_{211}dV = \int_0^{\infty}\int_0^{\pi}\int_0^{2\pi} \frac{1}{3(2a_0)^3}\frac{r^2}{a_0^2}\mathrm{e}^{-r/a_0}Y_1^{1*}Y_1^{1}r^2\sin(\theta)drd\theta d\phi =$$

$$\frac{1}{24}\int_0^{\infty}\rho^4 e^{\rho}d\rho \quad \times \quad \frac{3}{8\pi}\int_0^{\pi}\int_0^{2\pi}\sin^3(\theta)d\theta d\phi$$

The integral over $\rho = r/a_0$ using repeated partial integration gives 1, the second gives $\frac{3}{4}\int_0^{\pi}\sin^3(\theta)d\theta = -\frac{3}{4}\int_0^{\pi}(1-\cos^2(\theta))d\cos(\theta) = 1$

ii) What are the possible outcomes of a measurement of L_x on this state? With what probabilities will these values occur?
Hint: Diagonalize L_x and rewrite Y_1^1 in the new basis. `(7 pts)`

Answer: Eigenvectors-eigenvalues combinations are: $1/\sqrt{2}(1,0,-1)$ with $0\hbar$, $1/2(1,-\sqrt{2},1)$ with $-\hbar$ and $1/2(1,\sqrt{2},1)$ with $\hbar$. Initial state is $\psi = (1,0,0)$, so with $c_m = \langle\psi|\phi_m\rangle$ with ϕ_m the previous three normalized basis states we get $P = 1/2$ for $0\hbar$ and $P = 1/4$ for $\pm\hbar$.

iii) Would an optical transition from this state to the state $|321\rangle$ be allowed by a dipole transition? Why/why not? `(3 pts)`

Answer: Yes, since it adheres to the selection rules $\Delta L = 1$, $\Delta m = 0$.

Problem 3 `(15 pts)`

A two-level system is described by the following hamiltonian

$$\hat{H} = \frac{\hbar\omega}{2}\Big(-|0\rangle\langle 0| + |1\rangle\langle 1|\Big),$$

where $|0\rangle$ and $|1\rangle$ are the orthogonal eigenstates associated with the two energy levels ($E_0 < E_1$).

i) Write $\hat{H}$ in matrix representation. `(1 pt)`

Answer:

$$\hat{H} = \frac{\hbar\omega}{2}\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

ii) What are the eigenvalues of this Hamilton operator? `(1 pt)`

Answer: The matrix is already diagonalized, so the eigenvalues are on the diagonal, so $\pm\hbar\omega/2$.

Let's now introduce the operator $\hat{a}$ and its self-adjoint $\hat{a}^\dagger$. They act on the two levels as follows:

$$\hat{a}|0\rangle = 0 \quad \hat{a}|1\rangle = |0\rangle \quad \hat{a}^\dagger|0\rangle = |1\rangle \quad \hat{a}^\dagger|1\rangle = 0.$$

iii) Write the matrix of $\hat{a}$ and $\hat{a}^\dagger$ in the basis of the eigenvectors of the hamiltonian. `(2 pts)`

Answer:

$$\hat{a}^\dagger = \begin{pmatrix} \langle 0|a^\dagger|0\rangle & \langle 0|a^\dagger|1\rangle \\ \langle 1|a^\dagger|0\rangle & \langle 1|a^\dagger|1\rangle \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad \hat{a} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

iv) Prove that $\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = \mathbb{1}$, where $\mathbb{1}$ is the identity matrix. `(2 pts)`

Answer:

$$\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1}$$

We define now the operator $\hat{N} = \hat{a}^\dagger\hat{a}$ (*number operator*) and the operator $\hat{Q} = \hat{a}^\dagger - \hat{a}$.

v) Give the matrix representation for $\hat{Q}$ and find the eigenvalues and eigenvectors. `(3 pts)`

Answer:

$$Q = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \qquad q_1 = i \quad q_2 = -i.$$

$$|q_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} i \\ 1 \end{pmatrix} \qquad |q_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -i \\ 1 \end{pmatrix}$$

vi) Prove that the operators $\hat{N}$ represents a quantity that is conserved in time, and the the operator $\hat{Q}$ represents a quantity that is not conserved in time. `(2 pts)`

Answer: Since $[N, H] = 0$ but $[Q, H] \neq 0$, N is conserved but Q is not.

vii) Suppose that the system is in the eigenstate $|q_1\rangle$ at time $t = 0$. Evaluate *explicitly* $\langle Q\rangle$ for times $t > 0$. `(4 pts)`

Answer:

$$|q_1(t)\rangle = e^{-iHt/\hbar}|q_1\rangle = \frac{e^{-iHt/\hbar}}{\sqrt{2}}\left(i\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right) = \frac{1}{\sqrt{2}}\left[ie^{i\omega t/2}|0\rangle + e^{-i\omega t/2}|1\rangle\right].$$

With this outcome, we have

$$\langle Q\rangle = i\cos(\omega t)$$

Problem 4 (12 pts)

The density operator that describes a beam of electrons, in the basis where S_z is diagonal, has these elements:

$$\rho_{11} = 1/3 \qquad \rho_{12} = (1+i)/3.$$

i) What are the values of ρ_{22} and ρ_{21}?
Using this, give the matrix representation of the density operator. (5 pts)

Answer: Since $\mathrm{Tr}\rho = 1$, we achieve that $\rho_{22} = 2/3$. Then, since ρ has to be hermitian, we find that $\rho_{21} = (1-i)/3$. Thus,

$$\rho \doteq \begin{pmatrix} 1/3 & (1+i)/3 \\ (1-i)/3 & 2/3 \end{pmatrix}$$

ii) A state is a pure state if and only if $\rho^2 = \rho$. Is ρ describing a pure state? (2 pts)

Answer: Since with this density matrix we have $\rho = \rho^2$, the system is in a pure state.

iii) Consider the matrices of S_x and S_y you found in Problem 1 ii). Evaluate the expectation values $\langle S_x \rangle$ and $\langle S_y \rangle$. (5 pts)

Answer: A fundamental property of the density operator is that $\langle A \rangle = \mathrm{Tr}(\rho A)$. Therefore

$$\langle S_x \rangle = \mathrm{Tr}(\rho S_x) = Tr\left[\begin{pmatrix} 1/3 & (1+i)/3 \\ (1-i)/3 & 2/3 \end{pmatrix}\begin{pmatrix} 0 & \hbar/2 \\ \hbar/2 & 0 \end{pmatrix}\right] = \hbar/3$$

$$\langle S_y \rangle = \mathrm{Tr}(\rho S_x) = Tr\left[\begin{pmatrix} 1/3 & (1+i)/3 \\ (1-i)/3 & 2/3 \end{pmatrix}\begin{pmatrix} 0 & -i\hbar/2 \\ i\hbar/2 & 0 \end{pmatrix}\right] = -\hbar/3$$

Problem 5 (25 pts)

An electron and a hole in a semiconductor have spin 1/2. The Hamilton operator for them is given by

$$\hat{H}_0 = 2\gamma \hat{S}^e \cdot \hat{S}^h.$$

The superscript e and h stand for electron and hole, $\hat{S}$ are spin operators, and γ is the spin-spin interaction strength. The eigenstates of the system are then a non-degenerate singlet state, and a triply degenerate triplet state. The singlet state is given by

$$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \tag{1}$$

with energy $-\Delta$ ($\Delta > 0$) and the triplet states are given by

$$\begin{array}{c} |\downarrow\downarrow\rangle \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |\uparrow\uparrow\rangle \end{array} \tag{2}$$

all three with energy 0. The first arrow in the "ket's" stand for the electron spin, the second for the hole spin.
We call the normalized basis of these four states $\{\phi_i\}$.

i) Is γ negative or positive? Why? `(2 pts)`

Answer: γ is positive since the singlet state has lowest energy (*i.e.* the electron and hole spins energetically prefer not to be parallel aligned.

Now consider this system in the presence of a magnetic field B in the z direction. This leads to a additional term in the Hamilton operator of the form: $\hat{V} = \mu_b B(g_e \hat{S}_z^e + g_h \hat{S}_z^h)$, where μ_b is the Bohr magneton, and g_e, g_h are the g-factors for the electron and hole, respectively. .

ii) Write down the action of the additional term $\hat{V}$ on the basis wavefunctions $\{\phi_i\}$ of $\hat{H}_0$. A useful definition here is $\alpha = \mu_b B(g_e - g_h)/2$ and $\beta = \mu_b B(g_e + g_h)/2$ `(5 pts)`

Answer: $\mathrm{V}|S\rangle = \alpha|T_0\rangle$, $\mathrm{V}|T_0\rangle = \alpha|S\rangle$, $\mathrm{V}|T_{-1}\rangle = -\beta|T_{-1}\rangle$ and $\mathrm{V}|T_{+1}\rangle = \beta|T_{+1}\rangle$.

iii) Give the matrix representation of the Hamilton operator $\hat{H} = \hat{H}_0 + \hat{V}$ using $\{\phi_i\}$ as basis. `(3 pts)`

Answer: $$\begin{pmatrix} -\Delta & 0 & \alpha & 0 \\ 0 & -\beta & 0 & 0 \\ \alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & \beta \end{pmatrix}$$

iv) Show that the diagonalization of this matrix gives the four eigenvalues $\pm\beta$ and $\frac{-\Delta \pm \sqrt{\Delta^2 + 4\alpha^2}}{2}$. `(5 pts)`

Answer: The two eigenvalues $\pm\beta$ can be read directly from the matrix. What is left is to find the eigenvalues of $\begin{pmatrix} -\Delta & \alpha \\ \alpha & 0 \end{pmatrix}$ which yields the two other values $\lambda_\pm$.

v) Give the corresponding four eigenvectors for the Hamilton operator $\hat{H}$. `(6 pts)`

Answer: Using the basis $|S\rangle$, $|T_{-1}\rangle$, $|T_0\rangle$, $|T_{+1}\rangle$, the eigenvectors-eigenvalues pairs are $(0, 1, 0, 0)$ with $-\beta$, $(0, 0, 0, 1)$ with β, $(1, 0, \alpha/\lambda_+, 0)$ with λ_+ and $(1, 0, \alpha/\lambda_-, 0)$ with λ_-.

vi) Assume that $|\alpha| << |\Delta|$, give an approximation for the wavefunctions (valid to order α/Δ) and eigenvalues (valid to order α^2/Δ).(3 pts)

Answer: $(0,1,0,0)$ with $-\beta$, $(0,0,0,1)$ with β, $(1,0,-\alpha/\Delta,0)$ with $-\Delta-\frac{\alpha^2}{\Delta}$ and $(\alpha/\Delta,0,1,0)$ with $\frac{\alpha^2}{\Delta}$

vii) How do the four energy levels scale with the magnetic field? (1 pts)

Answer: Singlet and $m=0$ of the triplet scale quadratic in B, the other two linear in B.