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BACHELOR IN PHYSICS

Quantum Physics II
Final exam – January 14th, 2022
(Time: 3 hours)

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1 [1.5 points]. In a Hilbert space, $|1\rangle$ and $|2\rangle$ are pure states, orthogonal to each other. Consider in the basis $\{|1\rangle, |2\rangle\}$ the matrix

$$\varrho = \frac{1}{4}\begin{pmatrix} 1 & i\sqrt{3} \\ -i\sqrt{3} & 3 \end{pmatrix},$$

Is it a density matrix? Is it a pure state? If so, write its expression as a superposition of states $|1\rangle$ and $|2\rangle$.

The matrix ϱ is selfadjoint (0.25), has unit trace (0.25) and satisfies $\varrho^2 = \varrho$ (0.25). It is also positive semidefinite since, for arbitrary $|\chi\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$, one has

$$\langle\chi|\varrho|\chi\rangle = \frac{1}{4}\left[|a|^2 + 3|b|^2 + i\sqrt{3}(a^\star b - ab^\star)\right] = \frac{1}{4}\left|a - i\sqrt{3}b\right|^2 \geq 0$$

(0.25). Hence ϱ is a density matrix and a pure state.

Any pure state $|\psi\rangle = c_1|1\rangle + c_2|2\rangle$ can be written as a density matrix

$$\varrho_\psi = \begin{pmatrix} c_1 c_1^\star & c_1 c_2^\star \\ c_2 c_1^\star & c_2 c_2^\star \end{pmatrix}.$$

In particular, for the pure state given by ϱ above, we have

$$\varrho = \frac{1}{2}|1\rangle - \frac{i\sqrt{3}}{2}|2\rangle,$$

modulo an arbitrary global phase (0.5).

2 [3 points]. A system is formed by two particles with spin $s_1 = 3/2$ and $s_2 = 1/2$ in a uniform magnetic field $\mathbf{B} = (0, 0, B)$. Its Hamiltonian is

$$H = - \left(\gamma_1 \mathbf{S}_1 + \gamma_2 \mathbf{S}_2 \right) \cdot \mathbf{B} \,,$$

where $\mathbf{S}_1$ and $\mathbf{S}_2$ are the spin operators of the particles and $\gamma_1 \neq \gamma_2$ their gyromagnetic ratios. At ime $t = 0$ the square $\mathbf{S}^2$ of the total spin $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ and its third components $S_z = S_{1z} + S_{2z}$ are measured, with results $6\hbar^2$ and $-\hbar$.

(a) Write the state of the system $|\psi(0)\rangle$ immediately after the measurement.

(b) Find the state $|\psi(t)\rangle$ at time t.

(c) Assume that $\gamma_2 = 2\gamma_1$. If $\mathbf{S}^2$ is measured at time $t_{\mathrm{m}} = \pi/(B\gamma_1)$, what values can be obtained and with what probabilities?

(a) $6\hbar^2 = S(S+1)\hbar^2$ corresponds to total spin number $S = 2$. In turn, $-\hbar = M\hbar$ corresponds to total spin third component number $M = -1$. In the spin basis $|S,\, M\rangle := |\frac{3}{2},\, \frac{1}{2},\, S,\, M\rangle$, the initial state is thus (0.5)

$$|\psi(0)\rangle = |S = 2,\, M = -1\rangle \,.$$

(b) The Hamiltonian is diagonal in the basis $|m_1,\, m_2\rangle := |\frac{3}{2},\, \frac{1}{2},\, m_1,\, m_2\rangle$,

$$H = -(\gamma_1 \, S_{1z} + \gamma_2 \, S_{2z}) \, B \,, \qquad \begin{cases} \text{eigenvectors:} & |m_1, m_2\rangle \,, \\ \text{eigenvalues:} & E_{m_1, m_2} = -\hbar \, (\gamma_1 m_1 + \gamma_2 m_2) B \end{cases}$$

(0.5). To find the time evolution of $|\psi(0)\rangle$, it is convenient to write it in terms of states $|m_1,\, m_2\rangle$. Using the Clebsch-Gordan coefficients tables, we have

$$|\psi(0)\rangle = |S = 2,\, M = -1\rangle = \sqrt{\frac{3}{4}} \, \left|m_1 = -\tfrac{1}{2},\, m_2 = -\tfrac{1}{2}\right\rangle + \sqrt{\frac{1}{4}} \, \left|m_1 = -\tfrac{3}{2},\, m_2 = \tfrac{1}{2}\right\rangle$$

(0.5). Since $\left|m_1 = -\tfrac{1}{2},\, m_2 = -\tfrac{1}{2}\right\rangle$ and $\left|m_1 = -\tfrac{3}{2},\, m_2 = \tfrac{1}{2}\right\rangle$ have energies $\hbar(\gamma_1 + \gamma_2)B/2$ and $\hbar(3\gamma_1 - \gamma_2)B/2$, it follows that (0.5)

$$|\psi(t)\rangle = \sqrt{\frac{3}{4}} \, e^{-\mathrm{i}(\gamma_1 + \gamma_2)Bt/2} \, \left|m_1 = -\tfrac{1}{2},\, m_2 = -\tfrac{1}{2}\right\rangle + \sqrt{\frac{1}{4}} \, e^{-\mathrm{i}(3\gamma_1 - \gamma_2)Bt/2} \, \left|m_1 = -\tfrac{3}{2},\, m_2 = \tfrac{1}{2}\right\rangle \,.$$

(c) At time $t = t_{\mathrm{m}} = \pi/(B\gamma_1)$ and for $\gamma_2 = 2\gamma_1$, the state is

$$|\psi(t_{\mathrm{m}}; \gamma_2 = 2\gamma_1)\rangle = \sqrt{\frac{3}{4}} \, e^{-3\mathrm{i}\pi/2} \, \left|m_1 = -\tfrac{1}{2},\, m_2 = -\tfrac{1}{2}\right\rangle + \sqrt{\frac{1}{4}} \, e^{-\mathrm{i}\pi/2} \, \left|m_1 = -\tfrac{3}{2},\, m_2 = \tfrac{1}{2}\right\rangle \,.$$

Using again the tables of Clebsch-Gordan coefficients to go back to the basis $|S, M\rangle$, we have

$$|\psi(t_{\mathrm{m}}; \gamma_2 = 2\gamma_1)\rangle = \mathrm{i} \sqrt{\frac{3}{4}} \left[\sqrt{\frac{3}{4}} \, |S = 2,\, M = -1\rangle + \sqrt{\frac{1}{4}} \, |S = 1,\, M = -1\rangle \right]$$

$$- \mathrm{i}\sqrt{\frac{1}{4}} \left[\sqrt{\frac{1}{4}} \, |S = 2,\, M = -1\rangle - \sqrt{\frac{3}{4}} \, |S = 1,\, M = -1\rangle \right]$$

$$= \frac{\mathrm{i}}{2} \, |S = 2,\, M = -1\rangle + \frac{\mathrm{i}\sqrt{3}}{2} \, |S = 1,\, M = -1\rangle$$

(0.5). A measurement of $\mathbf{S}^2$ at this time may only give (0.5)

$$6\hbar^2 \text{ with probability } \frac{1}{4}; \qquad 2\hbar^2 \text{ with probability } \frac{3}{4}.$$

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3 [0.5+1.5 points]. The energy levels and wave functions of an electron in a Hydrogen atom in a constant magnetic field B oriented in the positive z direction are given by

$$E^{(0)}_{n\,m_\ell\,m_s} = -\frac{1}{4\pi\epsilon_0}\frac{Z^2 e^2}{2a_0 n^2} + \hbar\omega\,(m_\ell + 2m_s), \qquad |n,\,\ell,\,m_\ell,\,m_s\rangle, \qquad \omega = \frac{eB}{2m}. \qquad (1)$$

Assume that $\hbar\omega \ll e^2/4\pi\epsilon_0 a_0$. Consider a system formed by two electrons in such a potential that do not interact with each other.

(a) Find the system ground state, its energy and its degeneracy.

(b) Determine the first order correction in perturbation theory to the ground state energy due to an electron interaction

$$H_I = \frac{\alpha^2}{\hbar^2}\frac{e^2}{4\pi\epsilon_0\,|\mathbf{x}_1 - \mathbf{x}_2|}\,\mathbf{S}_1\cdot\mathbf{S}_2\,.$$

Here $\alpha \approx 1/137$ is the fine structure constant and $\mathbf{S}_1$ and $\mathbf{S}_2$ are the electrons spin operators.

HINT. The Hydrogen atom ground state wave function for a nucleus with charge Ze is

$$\psi_{100}(\mathbf{x}) = \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} e^{-Zr/a_0}, \qquad r := |\mathbf{x}|, \qquad a_0 = \text{Bohr radius}\,.$$

The following integral may be useful

$$\int_{\mathbf{R^3}} d^3\mathbf{y}_1 \int_{\mathbf{R^3}} d^3\mathbf{y}_2\,\frac{e^{-(|\mathbf{y}_1|+|\mathbf{y}_2|)}}{|\mathbf{y}_1 - \mathbf{y}_2|} = 20\pi^2\,.$$

(a) (0.5) In the ground state, both electrons have $n = 1$, $\ell = 0$, $m_\ell = 0$ (and $s = \frac{1}{2}$). One of them has $m_s = -1/2$, and the other one has $m_s = 1/2$. According to Pauli's exclusion principle, the ground state is then

$$|\psi_0(1,2)\rangle = \frac{1}{\sqrt{2}}\left[|1,0,0,\tfrac{1}{2}\rangle_1\,|1,0,0,-\tfrac{1}{2}\rangle_2 - |1,0,0,\tfrac{1}{2}\rangle_2\,|1,0,0,-\tfrac{1}{2}\rangle_1\right]$$

$$= \frac{1}{\sqrt{2}}\,|1,0,0\rangle_1\,|1,0,0\rangle_2 \otimes \left[|m_{s1} = \tfrac{1}{2},\, m_{s2} = -\tfrac{1}{2}\rangle - |m_{s1} = -\tfrac{1}{2},\, m_{s2} = \tfrac{1}{2}\rangle\right].$$

It is nondegenerate and has energy

$$E^{(0)}_0 = -\frac{Z^2 e^2}{4\pi\epsilon_0 a_0}\,.$$

(b) Change now from the spin basis $|m_{s1}, m_{s2}\rangle$ associated to $\{\mathbf{S}_1^2, \mathbf{S}_2^2, S_{1z}, S_{2z}\}$ to the basis $|S, M\rangle$ associated to $\{\mathbf{S}_1^2, \mathbf{S}_2^2, \mathbf{S}^2, S_z\}$, with $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$. Since

$$\left| S{=}0,\, M{=}0 \right\rangle = \frac{1}{\sqrt{2}} \left[\left| m_{s1} = \tfrac{1}{2},\, m_{s2} = -\tfrac{1}{2} \right\rangle - \left| m_{s1} = -\tfrac{1}{2},\, m_{s2} = \tfrac{1}{2} \right\rangle \right],$$

the ground state can be written as (0.5)

$$|\psi_0(1,2)\rangle = \left| \psi_{100}(1)\, \psi_{100}(2) \right\rangle \otimes \left| S{=}0,\, M{=}0 \right\rangle.$$

Noting that $\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{2} \left(\mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2 \right)$, the first order correction to the ground state energy due to the perturbation H_I is given by

$$E_0^{(1)} = \left\langle \psi_0(1,2) \,|\, H_I \,|\, \psi_0(1,2) \right\rangle$$

$$= \frac{\alpha^2 e^2}{4\pi\epsilon_0 \hbar^2} \left[\int d^3\mathbf{x}_1 \int d^3\mathbf{x}_2 \, \frac{\psi_{100}(\mathbf{x}_1)^2 \, \psi_{100}(\mathbf{x}_2)^2}{|\mathbf{x}_1 - \mathbf{x}_2|} \right] \left\langle S{=}0,\, M{=}0 \,\Big|\, \tfrac{1}{2} \left(\mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2 \right) \,\Big|\, S{=}0,\, M{=}0 \right\rangle$$

$$(2)$$

To compute the orbital integral, use $\psi_{100}(\mathbf{x})$ above and make the change $\mathbf{x} = \dfrac{a_0}{2Z}\, \mathbf{y}$. This gives

$$\int d^3\mathbf{x}_1 \int d^3\mathbf{x}_2 \, \frac{\psi_{100}(\mathbf{x}_1)^2 \, \psi_{100}(\mathbf{x}_2)^2}{|\mathbf{x}_1 - \mathbf{x}_2|} = \frac{Z}{32\pi^2 a_0} \int d^3\mathbf{y}_1 \int d^3\mathbf{y}_2 \, \frac{e^{-(|\mathbf{y}_1| + |\mathbf{y}_2|)}}{|\mathbf{y}_1 - \mathbf{y}_2|} = \frac{5Z}{8a_0}$$

The spin part (0.5) in eq. (2) is calculated using

$$\left\langle S,\, M \,\Big|\, \tfrac{1}{2} \left(\mathbf{S}^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2 \right) \,\Big|\, S,\, M \right\rangle = \frac{\hbar^2}{2} \left[S(S+1) - s_1(s_1+1) - s_2(s_2+1) \right].$$

For $s_1 = s_2 = \frac{1}{2}$ and $S = 0$, this gives $-\frac{3}{4}\hbar^2$. Altogether (0.5),

$$E_0^{(1)} = -\frac{15\,\alpha^2}{32} \frac{Ze^2}{4\pi\epsilon_0 a_0} = \frac{15\,\alpha^2}{32\,Z} E_0^{(0)} \approx \frac{10^{-5}}{Z} E_0^{(0)}.$$

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4 [2 points]. Consider a system formed by four non-interacting electrons in the Hydrogen atom like potential of exercise 3, so that the one-particle states and energy levels are given by eq. (1) and H_I is neglected. What is the ground state energy of the system and its degeneracy?

The energy of the ground state is obtained by filling one-particle eigenstates in accordance with Pauli's exclusion principle while keeping the total energy at its minimum. Two electrons will be allocated in the states $\left| 1, 0, 0, \frac{1}{2} \right\rangle$ and $\left| 1, 0, 0, -\frac{1}{2} \right\rangle$, and will have energies (0.5)

$$E_0 = -\frac{Z^2 e^2}{8\pi\epsilon_0 a_0} - \hbar\omega, \qquad E_1 = -\frac{Z^2 e^2}{8\pi\epsilon_0 a_0} + \hbar\omega.$$

The other two will go into states with $n = 2$. The table

ℓ	m_ℓ	m_s	$m_\ell + 2m_s$
0	0	$-1/2$	-1
1	-1	$-1/2$	-2
1	0	$-1/2$	-1
1	1	$-1/2$	0

collects all one-particles states with $n = 2$ and $m_2 = -\frac{1}{2}$. We have restricted ourselves to $m_2 = -\frac{1}{2}$ since states with $n = 2$ and $m_s = \frac{1}{2}$ have $m_\ell + 2m_s \geq 0$ and the table already contains three levels with negative $m_\ell + 2m_s$. The third electron will then be in a state $\left|2, 1, -1, -\frac{1}{2}\right\rangle$ (0.5) with energy

$$E_3 = -\frac{1}{4} \frac{Z^2 e^2}{8\pi\epsilon_0 a_0} - 2\hbar\omega \,.$$

Finally the fourth electron will be either in a state $\left|2, 0, 0, -\frac{1}{2}\right\rangle$ or $\left|2, 1, 0, -\frac{1}{2}\right\rangle$ (0.5) and will have energy

$$E_4 = -\frac{1}{4} \frac{Z^2 e^2}{8\pi\epsilon_0 a_0} - \hbar\omega \,.$$

All in all, the ground state has degeneracy two (0.5) and energy

$$E_T = E_1 + E_2 + E_3 + E_4 = -\frac{5}{2} \frac{Z^2 e^2}{8\pi\epsilon_0 a_0} - 3\hbar\omega \,.$$

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5 [1.5 points]. The Hamiltonian for a particle with spin $\frac{1}{2}$ in a magnetic field $\mathbf{B}$ is

$$H = -\gamma\, \mathbf{S} \cdot \mathbf{B}$$

where $\gamma > 0$ is the particle gyromagnetic ratio. Assume that $\mathbf{B}$ has the form $\mathbf{B} = (B_x, 0, B_z)$, with $B_x, B_z > 0$ constant. If $|+\rangle$ and $|-\rangle$ denote the eigenstates of S_z. Use the variational method to find an upper bound to the ground state energy taking as trial wave function

$$|\psi(\theta)\rangle = \cos\theta\, |+\rangle + \sin\theta\, |-\rangle \,, \qquad 0 \leq \theta \leq \pi.$$

Noting $\mathbf{S} = (\hbar/2)\, \boldsymbol{\sigma}$ and

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y := \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad |+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

the Hamiltonian and the trial wave function are written as (0.25)

$$H = -\frac{\gamma\hbar}{2} \begin{pmatrix} B_z & B_x \\ B_x & -B_z \end{pmatrix}, \qquad |\psi(\theta)\rangle = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, \qquad \langle\psi(\theta)|\psi(\theta)\rangle = 1 \,.$$

The variational energy function is then

$$E(\theta) = \frac{\langle\psi(\theta)|H|\psi(\theta)\rangle}{\langle\psi(\theta)|\psi(\theta)\rangle} = -\frac{\gamma\hbar}{2} \left[B_x \sin(2\theta) + B_z \cos(2\theta) \right]$$

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(0.75). In its domain $[0, \pi]$, $E(\theta)$ is a smooth oscillating function with extrema at (0.25)

$$\frac{dE(\theta)}{d\theta}\bigg|_{\theta=\theta_\mathrm{m}} = -\gamma\hbar \left[B_x \cos(2\theta_\mathrm{m}) - B_z \sin(2\theta_\mathrm{m}) \right] = 0 \quad \Rightarrow \quad \tan(2\theta_\mathrm{m}) = \frac{B_x}{B_z} \,.$$

Since B_x, B_z are both positive, $2\theta_\mathrm{m}$ must be either in $(0, \pi/2)$ or $(\pi, 3\pi/2)$. For $2\theta_\mathrm{m}$ in $(0, \pi/2)$, both $\sin(2\theta_\mathrm{m})$ and $\cos(2\theta_\mathrm{m})$ are positive, so that $E(\theta_\mathrm{m})$ is negative. For $2\theta_\mathrm{m}$ in $(\pi/2, 3\pi/2)$, it is the other way around; both the sine and the cosine take negative values and $E(\theta_\mathrm{m})$ is positive. Hence $2\theta_\mathrm{m}$ in $(0, \pi/2)$ is a minimum and $2\theta_\mathrm{m}$ in $(\pi/2, 3\pi/2)$ is a maximum (0.25).

Alternatively one may study the sign of the second derivative at $\theta = \theta_\mathrm{m}$. Using that

$$\frac{d^2 E(\theta)}{d\theta^2}\bigg|_{\theta=\theta_\mathrm{m}} = 2\gamma\hbar \left[B_x \sin(2\theta_\mathrm{m}) + B_z \cos(2\theta_\mathrm{m}) \right] = 2\gamma\hbar\, B_z \cos(2\theta_\mathrm{m}) \left(\frac{B_x^2}{B_z^2} + 1 \right),$$

it is clear that the second derivative has at $2\theta_\mathrm{m}$ the same sign as $\cos(2\theta_\mathrm{m})$. Hence $2\theta_\mathrm{m}$ in $(0, \pi/2)$ is a minimum, and $2\theta_\mathrm{m}$ in $(\pi/2, 3\pi/2)$ is a maximum.

The variational method then gives the bound

$$E(\theta_\mathrm{m}) = -\frac{\gamma\hbar}{2} \cos(2\theta_\mathrm{m}) B_z \left(1 + \frac{B_x^2}{B_z^2} \right) = -\frac{\gamma\hbar}{2} B_z \sqrt{1 + \frac{B_x^2}{B_z^2}} = -\frac{\gamma\hbar}{2} |\mathbf{B}| \,,$$

(0.5) where use has been made of

$$\cos^2 \alpha = \frac{1}{1 + \tan^2 \alpha} \,.$$