UNIVERSITETET I OSLO

Det matematisk-naturvitenskapelige fakultet

Take home exam in: FYS3110 - Quantum mechanics.

Due: October 17. 2016 at 12:00 in the box marked FYS3110 in the Physics front office.

Pages: 3

Remember to put your <u>candidate number</u>, not your name, on your answer sheets.

Some subproblems have more than one question, be sure to answer them all.

Problem 1

This problem is about spin-1/2 systems. For a single spin-1/2, orthonormal eigenstates of the spin squared operator $\hat{S}^2 \equiv \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2$ and the spin z-component \hat{S}_z are denoted $|\uparrow\rangle \equiv |s| = 1/2, m_s = 1/2$ and $|\downarrow\rangle \equiv |s| = 1/2, m_s = -1/2$, such that $\hat{S}^2|\uparrow\rangle = \hbar^2 \frac{1}{2} \left(\frac{1}{2} + 1\right) |\uparrow\rangle$, $\hat{S}_z|\uparrow\rangle = +\frac{\hbar}{2} |\uparrow\rangle$ and $\hat{S}^2|\downarrow\rangle = \hbar^2 \frac{1}{2} \left(\frac{1}{2} + 1\right) |\downarrow\rangle$, $\hat{S}_z|\downarrow\rangle = -\frac{\hbar}{2} |\downarrow\rangle$. You may use without further explanation the commutation relations $[\hat{S}^x, \hat{S}^y] = i\hbar \hat{S}^z$, $[\hat{S}^y, \hat{S}^z] = i\hbar \hat{S}^x$ and $[\hat{S}^z, \hat{S}^x] = i\hbar \hat{S}^y$. Define also $\hat{S}^{\pm} = \hat{S}^x \pm i\hat{S}^y$.

- **1.1** Use the commutation relations above to show that $\hat{S}^+|\downarrow\rangle$ is an eigenstate of \hat{S}^z . What is its eigenvalue?
- **1.2** Express $\hat{S}^{-}\hat{S}^{+}$ in terms of the operators \hat{S}^{z} , \hat{S}^{2} and appropriate constants. Use this expression to compute the norm of the states: $|\psi_{1}\rangle = \hat{S}^{+}|\downarrow\rangle$ and $|\psi_{2}\rangle = \hat{S}^{+}|\uparrow\rangle$.

In the following you can assume that the phase of the states are chosen such that the relations $\hat{S}^+|\downarrow\rangle = \hbar|\uparrow\rangle$ and $\hat{S}^-|\uparrow\rangle = \hbar|\downarrow\rangle$ hold.

1.3 Consider the state $|\phi\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle + e^{i\theta}|\downarrow\rangle\right)$ where θ is real, and compute the "uncertainty" product $\sigma_{sx}^2 \sigma_{sy}^2$ where $\sigma_{sx}^2 = \langle \phi | \left(\hat{S}^x - \langle \phi | \hat{S}^x | \phi \rangle\right)^2 |\phi\rangle$ and $\sigma_{sy}^2 = \langle \phi | \left(\hat{S}^y - \langle \phi | \hat{S}^y | \phi \rangle\right)^2 |\phi\rangle$. Find the values of θ for which $\sigma_{sx}^2 \sigma_{sy}^2 = 0$. Is the Heisenberg uncertainty relation violated for these values of θ ? (do not just answer yes or no, do a computation!)

Now consider a system of three interacting spin degrees of freedom with the following Hamiltonian

$$H = \frac{J}{\hbar^2} \left(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1 \right)$$

where J is a positive number with units of energy. The spin operators are $\vec{S}_1 \equiv \vec{S} \otimes I \otimes I$, $\vec{S}_2 \equiv I \otimes \vec{S} \otimes I$, $\vec{S}_3 \equiv I \otimes I \otimes \vec{S}$, and $\vec{S} = (S^x, S^y, S^z)$ where S^α is the spin-1/2 operator in direction α . I is the identity operator. We have omitted the hat on operators to simplify the notation. A general state of this three-spin system is a linear combination of product states $|m_{s_1}m_{s_2}m_{s_3}\rangle \equiv |m_{s_1}\rangle \otimes |m_{s_2}\rangle \otimes |m_{s_3}\rangle$ where m_{s_i} is the spin-z quantum number of spin number i, either up $(+\frac{1}{2})$ or down $(-\frac{1}{2})$. For instance, the product state $|\uparrow\downarrow\uparrow\rangle = |\uparrow\rangle \otimes |\downarrow\rangle \otimes |\uparrow\rangle$ is a state where spin number 1 is in the state $|\uparrow\rangle$, spin number 2 in state $|\downarrow\rangle$ and spin number 3 is in the state $|\uparrow\rangle$.

1.4 Express $\vec{S}_1 \cdot \vec{S}_2$ in terms of $S_1^+, S_1^-, S_2^+, S_2^-, S_1^z$ and S_2^z . Use it, and similar expressions, to compute $H|\uparrow\downarrow\downarrow\rangle$.

Define the total spin operators as follows

$$\vec{S}_{tot} \equiv \vec{S}_1 + \vec{S}_2 + \vec{S}_3$$
, and $S_{tot}^2 \equiv \vec{S}_{tot} \cdot \vec{S}_{tot}$.

- **1.5** Compute the commutator $[H, S_{tot}^z]$ and write down the 8 eigenstates of S_{tot}^z and their corresponding eigenvalues.
- **1.6** Find the energy eigenvalues of H. (Hint: Express H in terms of S_{tot}^2)
- 1.7 Write down all the normalized eigenstates of S_{tot}^2 which have total spin quantum number $s_{tot} = 1/2$, i.e. having eigenvalue $\hbar^2 \frac{1}{2} \left(\frac{1}{2} + 1 \right)$ (Hint: You may use the Clebsch-Gordan tables on page 190 in Griffiths (Table 8. Chapter 4). First combine two of the spins, then combine the result with the third spin).
- **1.8** Assume that at time t=0 the spin system is in the state $|\uparrow\downarrow\downarrow\rangle$. Find an analytic expression for the probability of finding the system in the same state $|\uparrow\downarrow\downarrow\rangle$ at a later time t. Make a plot of this probability as a function of time.

Problem 2

Consider the operator $e^{-\hat{H}s}$ where s is a real positive number with units of inverse energy and \hat{H} is the Hamiltonian. (NB! there is no imaginary unit in the exponent).

2.1 Assume that you know the Hamiltonian \hat{H} , but not its ground state $|E_0\rangle$. However, assume that you do have a way to compute $|\psi(s)\rangle \equiv e^{-\hat{H}s}|\psi\rangle$ efficiently for any s and $|\psi\rangle$. This situation is not unrealistic as matrix-vector multiplications are much faster than solving for the eigenvectors. How can you use this to calculate (approximately) the ground state expectation value $\langle E_0|\hat{O}|E_0\rangle$ of a given hermitian operator \hat{O} ? How does the error depend on s? What is/are the requirement(s) on $|\psi\rangle$ for this to work?