Homework sheet 4 – Due 03/16/2025

Problem 1: Expectation values and time evolution for two spins. [4 + 3 + 3 = 10 points]

Consider two spin 1/2 particles with four basis states $\{|\uparrow,\uparrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\downarrow,\downarrow\rangle\}$. Let the system be in the following states

$$|\psi\rangle = \frac{1}{2}|\uparrow,\uparrow\rangle + \frac{1}{2}|\uparrow,\downarrow\rangle + \frac{1}{\sqrt{2}}|\downarrow,\downarrow\rangle. \tag{1}$$

a) Single qubit measurements:

i) First, we measure $\hat{S}_z^{(1)}$. Determine the probability to measure $-\hbar/2$. What is the state after the measurement?

ii) Immediately after measuring $\hat{S}_z^{(1)}$ and having obtained $-\hbar/2$, we measure $\hat{S}_x^{(1)}$. Which results are possible and what are the probabilities?

iii) Now $\hat{S}_z^{(1)}$ and $\hat{S}_z^{(2)}$ are measured simultaneously. Determine the probability to obtain equal or opposite values.

b) Calculate $\langle\hat{\vec{S}}^{(1)}\rangle, \langle\hat{\vec{S}}^{(2)}\rangle$ where $\langle\dots\rangle$ are quantum-mechanical expectation values with respect to $|\psi\rangle$. Demonstrate that the vectors of expectation values have a norm below $\hbar/2$. Interpret the result. Which type of states would imply vectors of expectation values with norm equal to $\hbar/2$.

c) Now consider time evolution with the Hamiltonian

$$H = -\omega_1\hat{S}_z^{(1)} - \omega_2\hat{S}_z^{(2)}. \tag{2}$$

Calculate $|\psi(t)\rangle$ with $|\psi(0)\rangle = |\psi\rangle$ as given above.

Problem 2: Two-qubit gates and entanglement [2+3+5= 10 points]

Consider two spin-1/2 particles with spin operators $\hat{\vec{S}}^{(1)}, \hat{\vec{S}}^{(2)}$.

a) Using the basis $\{|\uparrow,\uparrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\downarrow,\downarrow\rangle\}$, determine the matrix form of the time evolution operator $U(t) = e^{-iHt/\hbar}$ for

$$H = \frac{J}{\hbar^2}\hat{\vec{S}}^{(1)}\cdot\hat{\vec{S}}^{(2)} + \frac{J}{4} \tag{3}$$

Comment: *The resulting $U(t)$ is a gate which is closely related to the fSim-gate, a native continuous two-qubit gate for some platforms of quantum computers, e.g. in Google's superconducting quantum chips [link].*

b) Assume that the system is prepared in one of the four product states $|\uparrow,\uparrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$. For each of those four initial states, answer the following questions

- Does $U(t)$ create entangled states?
- If $U(t)$ does create entanglement, write out the state.

c) We next define a measure of entanglement in the $m_1 + m_2 = 0$ sector of states. Such states can most generically be represented as $|\psi\rangle = \cos(\theta)|\uparrow,\downarrow\rangle + \sin(\theta)e^{i\phi}|\downarrow,\uparrow\rangle$.

i) Relate θ, ϕ to the state obtained by applying the unitary from the previous section, $U(t)$, to $|\uparrow,\downarrow\rangle$. Which θ correspond to Bell-pairs?

ii) Using the basis states $\{|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle\}$, write out the density matrix $\rho = |\psi\rangle\langle\psi|$.

iii) Determine the reduced density matrix at site 1. It is defined as

$$\rho_1 = \sum_{m_2=\uparrow,\downarrow} ({}_2\langle m_2|)\ \rho\ (|m_2\rangle_2). \tag{4}$$

Write ρ_1 as a matrix.
Hint: *For clarity we added a subscript $_2$ to indicate that $|m_2\rangle_2$ lives in the Hilbert space of the second qubit. In this calculation it is useful to return to a less compact notation $|m_1, m_2\rangle = |m_1\rangle_1 \otimes |m_2\rangle_2$ to see that partial inner products are taken as $({}_2\langle\tilde{m}_2|)\,|m_1, m_2\rangle = |m_1\rangle_1\, \langle\tilde{m}_2|m_2\rangle_2 = \delta_{m_2,\tilde{m}_2}\,|m_1\rangle_1$*

iv) For which θ is the entanglement entropy

$$S_{\text{entanglement}}(\theta) = -\text{tr}\left[\rho_1 \ln \rho_1\right] \tag{5}$$

maximal? For which θ is it minimal? Compare to the angles θ correspoding to Bell pairs (subexercise i) and to angles corresponding to product states. Sketch the entanglement entropy as a function of θ.

Problem 3: Heisenberg trimer. [3 + 3 + 4 = 10 points]

a) Consider a system of three spin-1/2 particles $\hat{\vec{S}}^{(1)}, \hat{\vec{S}}^{(2)}, \hat{\vec{S}}^{(3)}$.

i) Demonstrate that the total Hilbert space decomposes as

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = \frac{1}{2} \oplus \frac{1}{2} \oplus \frac{3}{2}. \tag{6}$$

Hint: *First take the direct product of the Hilbert spaces of the first and second spin. For $\otimes$ and $\oplus$ you may use the same rules of distributivity and associativity as for regular multiplication and addition on $\mathbb{R}$.*

ii) Consider the Hamiltonian

$$H = \frac{J}{\hbar^2}\left[\hat{\vec{S}}^{(1)} \cdot \hat{\vec{S}}^{(2)} + \hat{\vec{S}}^{(2)} \cdot \hat{\vec{S}}^{(3)} + \hat{\vec{S}}^{(3)} \cdot \hat{\vec{S}}^{(1)}\right]. \tag{7}$$

Write it in terms of $\hat{\vec{S}} = \sum_{i=1}^{3} \hat{\vec{S}}^{(i)}$. Check that $\hat{\vec{S}}^2, \hat{S}_z$ are observables compatible with the Hamiltonian and use part i) to determine the spectrum of the system.

b) Explicitly construct the eigenstates in the three sectors $1/2, 1/2, 3/2$ on the right hand side of Eq. (6). As in the lecture course, start from the highest weight state. For $j = 1/2$, $m = 1/2$ states, choose eigenstates which are have equal probability of being in each of the three states $|\downarrow\uparrow\uparrow\rangle, |\uparrow\downarrow\uparrow\rangle, |\uparrow\uparrow\downarrow\rangle$ (and analogously for $j = 1/2, m = -1/2$.)

c) Consider three spin ring-exchange term

$$H_{\text{ring}} = \frac{\tilde{J}}{\hbar^3}\hat{\vec{S}}^{(1)} \cdot (\hat{\vec{S}}^{(2)} \times \hat{\vec{S}}^{(3)}). \tag{8}$$

i) Convince yourself that $\hat{\vec{S}}$ commutes with H_{ring}. *(It is sufficient to prove it for $\hat{S}_z$ and infer the result for other components of $\hat{\vec{S}}$ by isotropy arguments.)*

ii) Calculate the energy corrections to first order in $\tilde{J}$.