Problem Set 4 215A-Quantum Mechanics, Fall 2017

Due: Friday, November 10, 2017 by 5pm
Put homework in mailbox labelled 215A on 1st floor of Broida (by elevators).

Problem 1
Sakurai Problems: 3.9, 3.10, 3.11, 3.12

2: Three-site Antiferromagnet

This problem requires familiarity with angular momentum operators with \( j > 1/2 \), as well as addition of angular momentum - neither of which I covered in class. So, please read Sections 3.5 and 3.8 in Sakurai, which should give you the background to do this problem.

Consider a three-site Heisenberg anti-ferromagnet with Hamiltonian

\[
H = J(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1),
\]

where \( \vec{S}_j \) denote spin operators with spin-S. Here the spin \( S \) can be integer or half-integer and the exchange coupling \( J > 0 \).

a.) How many states are there in the Hilbert space for the three spins?

b.) What is the ground state energy, \( E(S) \), for arbitrary integer and half-integer spin? [Hint, rewrite the Hamiltonian in terms of the total spin, \( \vec{S}_{\text{tot}} = \vec{S}_1 + \vec{S}_2 + \vec{S}_3 \).]

c.) What is the ground state degeneracy, \( N(S) \), for arbitrary integer and half-integer spin \( S \)?

d.) Treating the spins as classical vectors with magnitude \( S \), evaluate the classical ground state energy \( E_{cl} \) and verify that the ratio \( E(S)/E_{cl} \rightarrow 1 \) as \( S \rightarrow \infty \).

3: Density Matrices for a spin-1/2 particle

(a) Let \( |\uparrow\rangle, |\downarrow\rangle \) label, as usual, the two basis states of a spin-1/2 particle, \( \vec{S} = (\hbar/2)\vec{\sigma} \). Consider two different density matrices: (i) A pure state density matrix corresponding to a quantum state with equal amplitude to be spin-up and spin-down, (ii) A density matrix describing a mixture of the two basis states, \( |\uparrow\rangle, |\downarrow\rangle \), with equal probability. Show that these two situations lead to the same value for \( \langle \hat{\sigma}_z \rangle \) but different values for \( \langle \hat{\sigma}_x \rangle \).

(b) Consider the density matrix for a spin-1/2 particle with magnetic moment \( \mu \) in a magnetic field, with Hamiltonian,

\[
\hat{H} = -\frac{1}{2} g\mu \vec{B} \cdot \vec{\sigma},
\]

where \( g \) is a constant. Using the equation of motion for the density operator \( \hat{\rho} \), find the motion of the polarization vector, \( \vec{P} = \langle \vec{\sigma} \rangle = \text{Tr}[\hat{\rho}(t)\vec{\sigma}] \), and compare it with the classical equation of motion of a spinning magnetic dipole in a magnetic field.

4: Schmidt-Decomposition and Reduced Density Matrices

Consider a bipartite quantum system built from a direct product Hilbert space of the two parts, \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \). Let \( |a_i\rangle_A \) with \( i = 1, 2, ..., n \) label a complete orthonormal basis of states in Hilbert space \( A \), and likewise for Hilbert space \( B \): \( |b_j\rangle_B \), with \( j = 1, 2, ..., N \geq n \). The most general quantum state in the full Hilbert space can be expressed as,

\[
|\Phi\rangle = \sum_{i=1}^{n} \sum_{j=1}^{N} c_{ij} |a_i\rangle_A \otimes |b_j\rangle_B,
\]
with complex coefficients, $c_{ij}$.

A theorem proven on the wikipedia page, http://en.wikipedia.org/wiki/Schmidt_decomposition, states that there always exist orthonormal sets, $|\psi_i\rangle_A, |\phi_j\rangle_B$ with $i, j = 1, 2, ... n$ such that the general state $|\Phi\rangle$ can be re-expressed in a Schmidt-decomposed form:

$$|\Phi\rangle = \sum_{i=1}^{n} v_i |\psi_i\rangle_A \otimes |\phi_i\rangle_B,$$

with the normalization condition, $\sum_{i=1}^{n} |v_i|^2 = 1$.

(a) Using this Schmidt form, obtain expressions for the reduced density matrices,

$$\tilde{\rho}_A = Tr_B|\Phi\rangle\langle\Phi|, \quad \tilde{\rho}_B = Tr_A|\Phi\rangle\langle\Phi|.$$  

(b) Now consider, as an example, two spin-$1/2$ particles, labelled $A$ and $B$, in a (normalized) pure state,

$$|\Phi\rangle = \frac{1}{\sqrt{2}} |\downarrow\rangle_A \otimes |\downarrow\rangle_B + \frac{1}{\sqrt{2}} |\uparrow\rangle_A \otimes (|\uparrow\rangle_B + |\downarrow\rangle_B).$$

Obtain the Schmidt-decomposition of this state by computing and diagonalizing the two reduced density matrices.

### 5: Entanglement Entropy for 2-site Quantum Ising model in a Transverse field

Consider the Hamiltonian for two spin-$1/2$ particles, a 2-site version of the venerable Quantum-transverse field Ising model,

$$\hat{H} = -J\hat{\sigma}_1^z\hat{\sigma}_2^z - \hbar\hat{\sigma}_1^x - \hbar\hat{\sigma}_2^x.$$  

Here, as usual, the two spin-$1/2$ operators are given by $\hat{S}_j^{\mu} = \frac{\hbar}{2} \hat{\sigma}_j^{\mu}$ with $j = 1, 2$ the site-label and $\mu = x, y, z$ labeling the components of spin.

A convenient orthonormal basis of states which spans the full Hilbert space for this model consists of a direct product of eigenstates of $\hat{\sigma}^z$ denoted, for example,

$$|\phi_1\rangle = |\uparrow\rangle_1 \otimes |\downarrow\rangle_2; \quad |\phi_2\rangle = |\downarrow\rangle_1 \otimes |\downarrow\rangle_2; \quad |\phi_3\rangle = |\uparrow\rangle_1 \otimes |\uparrow\rangle_2; \quad |\phi_4\rangle = |\downarrow\rangle_1 \otimes |\uparrow\rangle_2;$$

where $\hat{\sigma}_1^z |\uparrow\rangle_1 = + |\uparrow\rangle_1$, $\hat{\sigma}_1^z |\downarrow\rangle_1 = - |\downarrow\rangle_1$, and so on.

(a) Find the matrix elements for this Hamiltonian, $\hat{h}_{\alpha\beta} = \langle \phi_\alpha | \hat{H} | \phi_\beta \rangle$, with $\alpha, \beta = 1, 2, ... 4$.

(b) Find the eigenstate and eigenvalue of the matrix $\hat{h}$ with the lowest eigenvalue. If one denotes this (normalized) eigenstate as $|\Psi\rangle$, you should be now able to express it as $|\Psi\rangle = \sum_{\alpha=1}^{4} A_\alpha |\phi_\alpha\rangle$ with known values of the coefficients $A_\alpha$.

(c) We are interested in the entanglement entropy of the state $|\Psi\rangle$ for a bipartition that divides sites 1 and 2. Consider first the full system density matrix of the system which for a pure state is simply the projection operator on to the state $|\Psi\rangle$,

$$\tilde{\rho} = |\Psi\rangle\langle\Psi|.$$  

To calculate the entanglement entropy between the 2-sites we first need to find the reduced density matrix, which we denote by $\tilde{\rho}_1$, for this bipartition. Therefore, calculate

$$\tilde{\rho}_1 = Tr_2(\tilde{\rho})$$

where $Tr_2$ denotes a trace over the Hilbert space of site 2, that is over the 2-states $|\uparrow\rangle_2, |\downarrow\rangle_2$. This gives the reduced density matrix $\tilde{\rho}_1$ for the subsystem consisting of site 1.
(d) Re-express the density-matrix operator, \( \hat{\rho}_1 \) as a \( 2 \times 2 \) matrix in the basis \(|\uparrow\rangle_1, |\downarrow\rangle_1 \), with matrix elements, for example, \( \langle\uparrow| \hat{\rho}_1 |\uparrow\rangle_1 \) and so on.

(e) Diagonalize your \( 2 \times 2 \) matrix representation of \( \hat{\rho}_1 \) to obtain its eigenvalues \( \lambda_i \).

(f) The von Neumann (bi-partite entanglement) entropy is defined as,

\[
S_{1}^{vN} = -Tr[\hat{\rho}_1 \ln(\hat{\rho}_1)] = -\sum_i \lambda_i \ln(\lambda_i). \tag{11}
\]

Calculate \( S_{1}^{vN} \) as a function of \( h/J \) and make a sketch of \( S_{1}^{vN} \) versus \( h/J \).

(g) What is the value of \( S_{1}^{vN} \) as \( h/J \to \infty \)? As \( h/J \to 0 \)? Explain the physics behind these two limits.