Solutions Final exam 633

S.J. van Enk

(Dated: June 9, 2008)

(1) [25 points] You have a source that produces pairs of spin-1/2 particles. With probability p they are in the singlet state,

$$(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)/\sqrt{2}$$

and with probability 1 - p they are in the state (note the i!)

$$(\sqrt{3}|\uparrow\rangle|\downarrow\rangle + i|\downarrow\rangle|\uparrow\rangle)/2.$$

Unfortunately, that is all you know, and so you have to ascribe a mixed state ρ to your pairs of spin-1/2 particles.

- (a) [10] Write down ρ as a matrix in the basis $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$, and make sure it is a hermitian matrix.
- (b) [15] How much entanglement does ρ possess? Calculate the negativity (or the logarithmic negativity if you want), and check your answer for p = 1.

Answers: (a)

$$\rho = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 3/4 - p/4 & -p/2 - i\sqrt{3}(1-p)/4 & 0 \\ 0 & -p/2 + i\sqrt{3}(1-p)/4 & 1/4 + p/4 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

This matrix has the property that $\rho_{ij}^* = \rho_{ji}$, so ρ is hermitian.

(b) Taking the partial transpose of ρ can be done in two ways. One way gives

$$\rho^{\Gamma} = \begin{pmatrix} 0 & 0 & 0 & -p/2 - i\sqrt{3}(1-p)/4 \\ 0 & 3/4 - p/4 & 0 & 0 \\ 0 & 0 & 1/4 + p/4 & 0 \\ -p/2 + i\sqrt{3}(1-p)/4 & 0 & 0 & 0 \end{pmatrix},$$

and the other way gives the complex conjugate of this expression. In any case, the eigenvalues are the same: the two entries on the diagonal give $\lambda_1 = 3/4 - p/4$ and

 $\lambda_2 = 1/4 + p/4$, which are both positive. The off-diagonal elements give rise to two eigenvalues

$$\lambda_{\pm} = \pm \frac{1}{2} \sqrt{p^2 + 3(1-p)^2/4}.$$

For the negativity we need only the negative eigenvalue λ_{-} , and

$$N(\rho) = 2|\lambda_{-}| = \sqrt{p^2 + 3(1-p)^2/4}$$

Similarly, the logarithmic negativity is $E_N(\rho) = \log_2(1 + \sqrt{p^2 + 3(1-p)^2/4})$. For p = 1 both quantities equal 1, as they should for the singlet state.

(2) [40 points] Suppose we have a cubic box with sides L. The potential is zero inside the box, and infinite outside the box. We put 10 identical and noninteracting spin-1/2 fermions of mass m in the box. Everyone remembers, of course, the eigenenergies for a single particle in a 1-D box:

$$E_n = n^2 \frac{\hbar^2 \pi^2}{2mL^2} := n^2 E_1$$
 for integer $n > 0$

- (a) [15] What is the ground-state energy (expressed in E_1) of the system of 10 fermions in the box? Also, verify there is a 15-fold degeneracy in the ground state.
- (b) [15] What are the possible values for the $total \, spin \, S$ in the ground state manifold? (**Do not** list 15 orthogonal ground states and determine the total spin in each; just argue which values of S could occur in the 15-D space spanned by those states)
- (c) [10] Suppose there is actually a very short-range pair-wise interaction between the fermions that we describe by a delta-function potential:

$$V(\vec{x}_1, \vec{x}_2) = \lambda \delta(\vec{x}_1 - \vec{x}_2),$$

with λ a small constant and \vec{x}_1 and \vec{x}_2 position coordinates of a pair of fermions. We consider V as a perturbation. Explain how perturbation theory can be valid at all for this perturbation, even though the potential contains a singularity.

(d) [extra credit*] [5*] Suppose $\lambda > 0$ and sufficiently small to allow perturbation theory to be applicable. What is the total spin of the perturbed ground state?

Answers: (a) There are three quantum numbers: n_x, n_y, n_z . The lowest-energy single-particle state has $(n_x, n_y, n_z) = (1, 1, 1)$ with energy $3E_1$. Next, there are three different (spatial) states which we can indicate by the quantum numbers (1,1,2),

(1,2,1), and (2,1,1) with energy $6E_1$; and then there are three different spatial states (2,2,1), (2,1,2), and (1,2,2) with energy $9E_1$. We can put 2 fermions in each different spatial state, because there are 2 different spin states for each fermion. So, we can put 2 fermions in a state with $3E_1$, 6 can be put in states with $6E_1$ and the remaining 2 can be put in states with $9E_1$. Adding up all energies gives

$$E = (2 \times 3 + 6 \times 6 + 2 \times 9)E_1 = 60E_1$$

The last two fermions can be put in any pair of 6 different states (3 spatial states multiplied by 2 possibilities for the spin), but the order doesn't matter: so the number of different ground states is 6 choose 2 = 6!/(2!4!) = 15

- (b) The first 8 fermions are all in pairwise symmetric spatial states, so their spin states must be pairwise antisymmetric, hence singlet, hence spin-0. The last two fermions can be in either a triplet state or a singlet state, and so the total spin can be 0 or 1
- (c) What counts is [matrix elements] of the perturbation. A matrix element involves integrating over spatial coordinates, which gets rid of the delta function. As long as the matrix elements of V are small compared to energy differences between unperturbed energy eigenstates, perturbation theory applies.
- (d) There is still no choice for the 8 fermions in the single-particle lowest-energy states [so their total spin is zero, see part (b)], but the last two do have a choice: if they are in a symmetric spatial state the perturbation will increase the energy, but in an antisymmetric spatial state the perturbation, to first order at least, does not change the energy (particles cannot be in the same location in an antisymmetric spatial state). So, the ground state will have an antisymmetric spatial part and hence a symmetric spin part: the total spin is S = 1
- (3) [25 points] Suppose the electron possesses not just a magnetic moment but also a small electric dipole moment proportional to its spin \vec{S} . Consider the nonrelativistic hydrogen atom with the standard Hamiltonian $H_0 = \vec{p}^2/2\mu + V_{Coulomb}(\vec{r})$ (where \vec{p} and \vec{r} are, of course, the momentum and position vectors of the electron, relative to the nucleus). We add a perturbation of the form

$$V \propto \vec{S} \cdot \vec{E}$$
,

where \vec{E} is the electric field. Here we assume there is no external field, so \vec{E} is just

the Coulomb field of the proton. That makes the perturbation of this form:

$$V = \lambda \vec{S} \cdot \vec{r}/r^3,$$

with λ a small constant. Consider the unperturbed eigenstates $|n, l, m_l, m_s\rangle$ of H_0, L^2 , L_z, S_z .

- (a) [10] Using degenerate perturbation theory, show that the first-order energy shift due to V of the degenerate unperturbed ground states $|1, 0, 0, \pm 1/2\rangle$ is zero.
- (b) [15] Consider the second-order energy shifts of the ground states. One of the terms that determines this shift is

$$\Delta_{++}^{(2)} = -\sum_{n'l'm'_lm'_s} \frac{|\langle n', l', m'_l, m'_s | V | 1, 0, 0, +1/2 \rangle|^2}{E_{n'l'm'} - E_{100}}.$$

Which terms in this sum are nonzero? Hint: it may be a good idea to write V in terms of $S_x \pm iS_y$, S_z , and $x \pm iy$, z.

Answers: (a) You need all 4 matrix elements between the two states $|1,0,0,m_s\rangle$ for $m_s = \pm 1/2$. But for all m_s, m_s'

$$\langle 1, 0, 0, m'_s | V | 1, 0, 0, m_s \rangle = 0$$

because all of the following matrix elements (involving just the spatial part, not the spin part) are zero by parity

$$\langle 1, 0, 0 | \vec{r} / r^3 | 1, 0, 0 \rangle = 0.$$

(The $1/r^3$ part is not really relevant, neither here nor in part (b): it's just a scalar). All eigenvalues of the zero matrix are zero, of course.

(b) Write $\vec{S} \cdot \vec{r}$ as

$$\vec{S} \cdot \vec{r} = \frac{1}{2} (S_x + iS_y)(x - iy) + \frac{1}{2} (S_x - iS_y)(x + iy) + S_z z.$$

The first term raises m_s by 1 unit, and lowers m_l by 1 unit; the second term lowers m_s by 1 unit and raises m_l by 1 unit; the last term leaves both the same. (In other words, total angular momentum is conserved, consistent with $\vec{S} \cdot \vec{r}$ being a scalar.) All of the $x \pm iy$, z terms are rank-1 tensors, so they change l by 1. So, starting at l = 0 we must have l' = 1. Moreover, m'_s can be equal to m_s , but then m'_l must be equal to

 m_l : so, $m'_s = 1/2, m'_l = 0$ is possible; or m'_s can decrease but then m_l must increase: so $m'_s = -1/2, m'_l = 1$ is possible, too. The quantum number n' can be any integer $n' \geq 2$ (since l' = 1, n' cannot be equal to 1).

- (4) [30+10* points] You have a measurement device that you tested many times by sending in single spin-1/2 particles in states that you prepared. The device contains 3 light bulbs of different colors, red (R), blue (B), and green (G). The device always responds to your spin-1/2 particle by lighting one and only one light bulb. So, the different measurement outcomes correspond to R, B, and G. You notice that the following states give the following measurement results:
 - 1. $|\downarrow\rangle$ sometimes lights the green bulb, sometimes the blue one, but never the red one.
 - 2. $(|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$ sometimes lights the blue bulb, sometimes the red one, but never the green one.
 - 3. $(2|\uparrow\rangle |\downarrow\rangle)/\sqrt{5}$ sometimes lights the green bulb, sometimes the red one, but never the blue one.
 - (a) [5] Give the simple argument that shows the measurement performed by the device cannot be a von Neumann measurement on the spin-1/2 system, but must be a POVM.
 - (b) [10] The POVM consists of three operators of the form $E_k = w_k \Pi_k$, in terms of projectors Π_k —which we label k = G, B, R for the three measurement outcomes—and in terms of three weights w_k . Write down the Π_k (this includes, of course, identifying with which color each projector corresponds).
 - (c) [15] Determine the weights w_k . You can either choose the weights such that $\sum_k w_k \Pi_k = 1$ or (perhaps this is easier) try to make the projectors orthogonal by extending them to a 3-D Hilbert space, and extracting the weights from those.
 - (d) [extra credit*] [10*] When you open the device it turns out there is another spin-1/2 particle (the "ancilla") inside. You suspect what happens is the following. The particle you send in interacts with the ancilla in the following way:

$$(\alpha|\uparrow\rangle+\beta|\downarrow\rangle)|\uparrow\rangle\mapsto\alpha|\uparrow\rangle|\uparrow\rangle+\beta|\downarrow\rangle|\downarrow\rangle,$$

followed by the device performing a von Neumann measurement on the two spins together. (i) Construct such a measurement consistent with the three "experimental

results" described above. (ii) Why would repeating this POVM on a given spin-1/2 particle *not* necessarily lead to the same measurement outcome, even though we just managed to model it as a von Neumann measurement?

Answers: (a) The measurement has *three* different outcomes: a von Neumann measurement on a spin-1/2 system can have only two outcomes. $\boxed{3>2}$:-)

(b) Since there is always one outcome not occurring at all for the three particular input states, the three projectors in the 2-D space of the test spin-1/2 particle of the POVM must be projections onto the states orthogonal to those. For instance,

$$\Pi_R = |\uparrow\rangle\langle\uparrow|$$

because the state $|\downarrow\rangle$ never lights the red bulb. Similarly, $\Pi_G = |-\rangle\langle -|$ with $|-\rangle = (|\uparrow\rangle - |\downarrow\rangle)/\sqrt{2}$, and $\Pi_B = |B\rangle\langle B|$ with $|B\rangle = (|\uparrow\rangle + 2|\downarrow\rangle)/\sqrt{5}$.

(c) Extending the vectors $|\uparrow\rangle$, $|-\rangle$ and $|B\rangle$ to a third dimension and making them orthogonal doesn't leave much choice (actually, the only choice left is an arbitrary phase factor in front of the extra basis vector, which I call $|2\rangle$ here). We get

$$|R\rangle := |\uparrow\rangle \mapsto (|\uparrow + |2\rangle)/\sqrt{2},$$

$$|G\rangle := |-\rangle \mapsto (|\uparrow\rangle - |\downarrow\rangle - |2\rangle)/\sqrt{3},$$

and

$$|B\rangle \mapsto (|\uparrow +2|\downarrow\rangle - |2\rangle)/\sqrt{6}.$$

The weights for the 2-D projectors can then be seen to be

$$w_R = 1/2 \text{ and } w_G = 2/3 \text{ and } w_B = 5/6$$

(d) (i) Just identify $|\uparrow\rangle|\uparrow\rangle$ with $|\uparrow\rangle$, $|\downarrow\rangle|\downarrow\rangle$ with $|\downarrow\rangle$, and then for instance $|\uparrow\rangle|\downarrow\rangle$ with $|2\rangle$. Three von Neumann projectors are onto the states corresponding to those found in part (c) [with a zero component onto the fourth basis vector $|\downarrow\rangle|\uparrow\rangle$], and the fourth projector projects onto the fourth basis state $|\downarrow\rangle|\uparrow\rangle$. Thus,

$$|R\rangle := |\uparrow\rangle \mapsto (|\uparrow + |2\rangle)/\sqrt{2} \mapsto (|\uparrow\rangle|\uparrow\rangle + |\uparrow\rangle|\downarrow\rangle)/\sqrt{2}$$

etcetera.

(ii) The ancilla will have to be reset to $|\uparrow\rangle$, and that prevents the same outcome from having to occur again (it still could occur, but it doesn't have to).