1. (a) Consider a system consisting of two spin half atoms (or qubits), usually referred to as a ‘bipartite system’. Each of these atoms can be put into a spin state for which \( S_z = \pm \frac{1}{2} \hbar \). Using the notation 0 \( \leftrightarrow S_z = -\frac{1}{2} \hbar \) and 1 \( \leftrightarrow S_z = +\frac{1}{2} \hbar \) the four possible states for this system are \(|00\rangle, |01\rangle\) and two others.

(i) What are the other possible states?

The state of this bipartite system can be manipulated by the use of magnetic fields. Suppose this bipartite system is initially prepared in the state \(|\psi\rangle\).

(ii) What is the symbol in bra-ket notation for the probability amplitude of finding the system in state \(|m,n\rangle, m, n = 0 \text{ or } 1\) given that it was initially prepared in the state \(|\psi\rangle\)?

(iii) What is the symbol in bra-ket notation for the probability amplitude of finding the system in the final state \(|\phi\rangle\) given that it was in one of the intermediate states \(|mn\rangle\)?

(iv) What is the symbol in bra-ket notation for the probability amplitude of finding the system in the final state \(|\phi\rangle\) given that it ‘passed through’ the intermediate state \(|mn\rangle\)? (Recall that the system was initially prepared in the state \(|\psi\rangle\).)

(v) Expressed as a sum over appropriate terms, write down an expression for the total probability amplitude of finding the atom in the final state \(|\phi\rangle\) if the intermediate state through which it passed is not observed.

(b) Suppose the initial and final states are such that the probability amplitudes of part (a)(iv) above have the values \(\frac{1}{2^m+n}, i = \sqrt{-1}, \) if the system has passed through the intermediate state \(|mn\rangle, m, n = 0 \text{ or } 1\).

(i) What is the total probability of finding the system in the final state \(|\phi\rangle\) if the intermediate state through which it passed is not observed?

(ii) Decoherence (as produced by external ‘noise’ affecting the atoms) is a physical process which is equivalent to an observer determining which state each atom is in by some suitable measuring process. What is the total probability of finding the system in the final state \(|\phi\rangle\) if the intermediate state through which it passed is ‘observed’ through decoherence?

SOLUTION

(a) (i) \(|mn|\psi\rangle\)

(ii) \(|\phi|mn\rangle\)

(iii) \(|\phi|mn\rangle\langle mn|\psi\rangle\)

(iv) Since the intermediate state is not observed, the total probability amplitude of observing the atom in the \(|\phi\rangle\) is the sum of the probability amplitudes of arriving in this final state via each of the possible intermediate states. Since the initial state is \(|\psi\rangle\), the required probability amplitude is \(|\phi|\psi\rangle\), and this is

\[
|\phi|\psi\rangle = \sum_{mn} \langle \phi|mn\rangle \langle mn|\psi\rangle
\]

where the sum is over the four possible values of \(mn\).
(b) Given that the probability amplitudes $\langle \phi | mn \rangle \langle mn | \psi \rangle = (i)^{m+n}/2$, then

(i) The total probability amplitude of finding the atom in the final state $\langle \phi |$ if the intermediate state through which it passed is not observed is given in answer 1(a)iv i.e.

$$\langle \phi | \psi \rangle = \sum_{mn} \langle \phi | i \rangle \langle i | \psi \rangle$$

$$= \frac{i}{2} (i^0 + i^1 + i^1 + i^2)$$

$$= \frac{i}{2} (1 + i + i - 1)$$

$$= i.$$

Thus the probability of finding the atom in the final state $\langle \phi |$ is

$$|\langle \phi | \psi \rangle|^2 = 1.$$

(ii) If the intermediate state through which it passed is observed then the total probability of finding the atom in the final state $\langle \phi |$ is just the sum of the probabilities of the the system passing through the various possible intermediate states. Thus, in this case

$$|\langle \phi | \psi \rangle|^2 = \sum_{mn} |\langle \phi | n \rangle \langle n | \psi \rangle|^2 = 4 \times \frac{1}{4} = 1$$

i.e. if the intermediate states are observed, there is no interference, and the total probability of finding the atom in the state $\langle \phi |$ is unity. That this is the same as the case where interference would have been present implies that these interference terms are, in fact, zero, so that the ‘observed’ and ‘unobserved’ results are the same.

2. A beam of spin half particles (e.g. silver atoms) heading in the $y$ direction passes through a Stern-Gerlach apparatus and the separate beams corresponding to $S_z = \pm \frac{1}{2} \hbar$ then pass through two separate slits. The atoms then strike an observation screen. Using the notation $\pm$ to represent the atom having spin of $S_z = \pm \frac{1}{2} \hbar$, and 1 or 2 to represent the atom positioned at either slit 1 or slit 2, the state in which an atom is positioned at slit 1 and has spin up ($S_z = \frac{1}{2} \hbar$) can be written $| +, 1 \rangle$, and similarly for the state in which the atom is positioned at slit 2 with spin down.

(a) Write down in Dirac notation the state vector corresponding to the atom positioned at slit 2 with spin down.

Magnetic fields can be set up at the positions of each slit so as to flip the spin from + to – or vice versa.

(b) Write down, in Dirac notation, the two further states that the atoms be prepared in by use of these fields.

(c) Assign values for the probability amplitudes $\langle +, 1 | +, 1 \rangle$, $\langle -, 1 | -, 1 \rangle$, $\langle -, 1 | -, 2 \rangle$, $\langle +, 1 | +, 2 \rangle$ and any four other possible combinations (there are sixteen all together) and justify the values assigned in each case.
The Stern-Gerlach apparatus will prepare an atom in a state $|\psi\rangle$ in which there is equal probability of the atom having spin up and passing through slit 1, or having spin down and passing through slit 2. Which of the four possible states listed below could be used to describe this situation (Assume, for the present, that there are no magnetic fields at the positions of the slits.):

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

(ii) $|\psi\rangle = \frac{1}{2} |\uparrow, 1\rangle - \frac{\sqrt{3}}{2} |\downarrow, 2\rangle$.

(iii) $|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow, 1\rangle - |\downarrow, 2\rangle)$.

(iv) $|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow, 1\rangle + i|\downarrow, 2\rangle)$.

In each case, explain why the state could or could not be used to describe the situation.

If we let $|\pm, x\rangle$ represent the state in which the atom is observed to have spin $S_z = \pm \frac{1}{2} \hbar$ and to be at the position $x$ on the observation screen, what do $|\langle +, x | \psi \rangle|^2$ and $|\langle -, x | \psi \rangle|^2$ represent?

The probability of observing the atom to be at position $x$ on the observation screen irrespective of the spin of the atom is the sum of the probability to be observed at position $x$ with spin up plus the probability of it being observed at $x$ but with spin down. Using an appropriate choice of the state $|\psi\rangle$ from part (d), show that this is given by

$$|\langle +, x | \psi \rangle|^2 + |\langle -, x | \psi \rangle|^2 = \frac{1}{2} |\langle +, x | +, 1 \rangle|^2 + \frac{1}{2} |\langle -, x | -, 2 \rangle|^2.$$ 

Suppose that a magnetic field at slit 1 flips the spin to spin down. Calculate, once again, $|\langle +, x | \psi \rangle|^2 + |\langle -, x | \psi \rangle|^2$ for the state used in part (f), the detection probability of observing the atom to be at position $x$ on the observation screen irrespective of the spin of the atom. In what way does this result differ from that found in part (f)?

**SOLUTION**

(a) $|\downarrow, 2\rangle$.

(b) $|\downarrow, 1\rangle$ and $|\uparrow, 2\rangle$.

(c) Set up a table:

|           | $|\downarrow, 1\rangle$ | $|\downarrow, 2\rangle$ | $|\uparrow, 1\rangle$ | $|\uparrow, 2\rangle$ |
|-----------|--------------------------|--------------------------|--------------------------|--------------------------|
| $\langle -, 2 \rangle$ | 0                         | 1                         | 0                         | 0                         |
| $\langle +, 1 \rangle$ | 0                         | 1                         | 0                         | 0                         |
| $\langle +, 2 \rangle$ | 0                         | 0                         | 1                         | 0                         |

The diagonal elements of this table are all unity, for instance, $\langle +, 1 | +, 1 \rangle = 1$, as the initial and final states are identical while the off-diagonal elements are all zero, for instance $\langle +, 1 | -, 1 \rangle = 0$, as the initial and final states represent mutually exclusive alternatives.

(d) (i) For the state $|\psi\rangle = (|\downarrow, 1 \rangle + |\uparrow, 2\rangle)/\sqrt{2}$ we see that this corresponds to an atom with spin down passing through slit 1 or an atom with spin up passing through slit 2, which is not possible given the experimental setup.
(ii) For the state $|\psi\rangle = (|+, 1\rangle - \sqrt{3}|-, 2\rangle)/2$ we see that the probability of the atom passing through slit 1 will be

$$|\langle +, 1|\psi\rangle|^2 = \frac{1}{4},$$

while the probability of it passing through slit 2 will be

$$|\langle -, 2|\psi\rangle|^2 = \frac{3}{4}.$$  

These probabilities are not equal, so the state cannot be accepted.

(iii) For the state $|\psi\rangle = \frac{1}{\sqrt{2}}(|+, 1\rangle - |-, 2\rangle)$ we see that

$$|\langle +, 1|\psi\rangle|^2 = |\langle -, 2|\psi\rangle|^2 = \frac{1}{2}$$

i.e. the probabilities are equal, so this is a possible state for the atom.

(iv) Finally, for the state $|\psi\rangle = (|+, 1\rangle + i|-, 2\rangle)\sqrt{2}$ we find that

$$|\langle +, 1|\psi\rangle|^2 = |\langle -, 2|\psi\rangle|^2 = \frac{1}{2}$$

i.e. the probabilities are equal once again, so this is also a possible state for the atom.

(e) $|\langle +, x|\psi\rangle|^2$ is the probability of observing the atom at position $x$ on the observation screen and for this atom to have spin up;

$|\langle -, x|\psi\rangle|^2$ is the probability of observing the atom at position $x$ on the observation screen and for this atom to have spin down.

(f) In the following, we shall use the state $|\psi\rangle = (|+, 1\rangle + i|-, 2\rangle)\sqrt{2}$ from part (d). The probability of finding a particle at $x$ irrespective of its spin will then be

$$|\langle +, x|\psi\rangle|^2 + |\langle -, x|\psi\rangle|^2 = \frac{1}{2}|\langle +, x|(|+, 1\rangle + i|-, 2\rangle)|^2 + \frac{1}{2}|\langle -, x|(|+, 1\rangle + i|-, 2\rangle)|^2$$

$$= \frac{1}{2}|\langle +, x|+\rangle|^2 + \frac{1}{2}|\langle -, x|\rangle|^2.$$  

All the terms involving a different spin state in the inner products will vanish by virtue of the orthogonality relations in part (c). There is no interference term in this result – it is simply the probability of the particle passing through slit 1 and arriving at $x$ plus the probability of the particle passing through slit 2 and arriving at $x$.

(g) If there is a magnetic field at slit 1 that flips the spin to spin down, then the new state is

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|-, 1\rangle + i|-, 2\rangle).$$

The detection probability will then be

$$|\langle +, x|\psi_1\rangle|^2 + |\langle -, x|\psi_1\rangle|^2$$

$$= 0 + \frac{1}{2}|\langle -, x|\rangle|^2$$

$$= \frac{1}{2}|\langle -, x|\rangle|^2 + \frac{1}{2}|\langle -, x|\rangle|^2 = \text{Re}[i\langle -, x|\rangle\langle -, 2|\rangle - \text{Re}[i\langle -, x|\rangle\langle -, 2|\rangle]$$

$$= \frac{1}{2}|\langle -, x|\rangle|^2 + \frac{1}{2}|\langle -, x|\rangle|^2 + \text{Im}[\langle -, x|\rangle\langle -, 2|\rangle - \text{Im}[\langle -, x|\rangle\langle -, 2|\rangle]$$

i.e. there is now an interference term (the last term). Here we have used the algebraic result $|a + b|^2 = |a|^2 + |b|^2 + a^*b + ab^*$.  

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4
3. (a) The state of a system is given by

\[ |\psi\rangle = \frac{1}{3} \left[ (1 - i)|1\rangle + \sqrt{2} e^{-i\pi/4}|2\rangle - (2 + i)|3\rangle \right]. \]

What is the probability amplitude of finding the system, in each of the states |1⟩ and |2⟩? What are the probabilities of finding the system in each of these states?

(b) What is the associated bra vector ⟨ψ|?

(c) Another state of the system is given by

\[ |\phi\rangle = \frac{1}{\sqrt{6}} \left[ (1 - i)|1\rangle - 2i|2\rangle \right]. \]

Calculate the inner product ⟨ψ|φ⟩ and determine the probability of observing the system in the state |ψ⟩ given that it was in the state |φ⟩.

**SOLUTION**

(a) The probability amplitude of finding the system in the state |1⟩ is the coefficient of |1⟩, i.e.

\[ \langle 1|\psi \rangle = (1 - i)/3. \]

The probability amplitude of finding the system in the state |2⟩ is

\[ \langle 2|\psi \rangle = \sqrt{2} e^{-i\pi/4}/3. \]

Finally, the probability amplitude of finding the system in the state |3⟩ will be

\[ \langle 3|\psi \rangle = -(2 + i)/3. \]

The corresponding probabilities will then be

\[ |\langle 1|\psi \rangle|^2 = \left| \frac{1 - i}{3} \right|^2 = \frac{2}{9} \]

and

\[ |\langle 2|\psi \rangle|^2 = \left| \frac{\sqrt{2} e^{-i\pi/4}}{3} \right|^2 = \frac{2}{9} \]

and

\[ |\langle 3|\psi \rangle|^2 = \left| \frac{2 + i}{3} \right|^2 = \frac{5}{9} \]

Note that these probability amplitudes add to give unity, i.e. the initial state was correctly normalized.

(b) The bra vector corresponding to the ket

\[ |\psi\rangle = \frac{1}{3} \left[ (1 - i)|1\rangle + \sqrt{2} e^{-i\pi/4}|2\rangle - (2 + i)|3\rangle \right] \]

is obtained by taking the complex conjugate of the coefficients, and replacing the ket vectors |1⟩, |2⟩ and |3⟩ by the corresponding bras i.e.

\[ \langle \psi| = \frac{1}{3} \left[ (1 + i)|1\rangle + \sqrt{2} e^{i\pi/4}\langle 2| - (2 - i)\langle 3| \right]. \]
(c) The inner product $\langle \psi | \phi \rangle$ is then

$$
\langle \psi | \phi \rangle = \frac{1}{3} \left( (1 + i)(1 + \sqrt{2} e^{i\pi/4}) (2) - (2 - i)(3i) \right) \cdot \frac{1}{\sqrt{6}} \left( (1 - i)(1) - 2i(2) \right)
$$

$$
= \frac{1}{3\sqrt{6}} \left[ (1 + i)(1 - i) - 2i\sqrt{2} e^{i\pi/4} \right]
$$

$$
= \frac{1}{3\sqrt{6}} (4 - 2i).
$$

where we have used

$$
e^{i\pi/4} = \cos(\pi/4) + i \sin(\pi/4) = \frac{1 + i}{\sqrt{2}}.
$$

The probability of observing the system in the state $|\psi\rangle$ given that it was in the state $|\phi\rangle$ will is

$$
|\langle \psi | \phi \rangle|^2 = \left| \frac{1}{3\sqrt{6}} (4 - 2i) \right|^2 = \frac{10}{27}.
$$

For this to be a true probability, the final state $|\phi\rangle$ must be normalized to unity. To check this, the inner product $\langle \phi | \phi \rangle$ must be evaluated. This is just

$$
\langle \phi | \phi \rangle = \frac{1}{6} \left( |1 - i|^2 + |2i|^2 \right) = 1.
$$

Hence the probability $|\langle \phi | \psi \rangle|^2$ is the true probability.

4. An ozone molecule consists of three oxygen atoms arranged to form a triangle. If an electron is attached to the molecule, it can attach itself to any of the oxygen atoms. Let the possible states of the electron be $\{|i\rangle; i = 1, 2, 3\}$ where $|i\rangle$ is the state in which the electron is on the $i^{th}$ atom.

(a) What is the dimension of the state space for the system?

(b) The states $\{|i\rangle; i = 1, 2, 3\}$ form a complete, orthonormal basis for the system.

(i) State mathematically what orthonormality means here.

(ii) What does it mean that the basis states are complete?

(c) The system is prepared in the state $|\phi\rangle = a(1) + (1 - i)|2\rangle - |3\rangle$.

(i) What value will $a$ have to have in order for this state to be normalized to unity?

(ii) On which atom is it most likely to find the electron? What is the probability of finding it there?

(iii) On which atom is it least likely to find the electron?

SOLUTION

(a) As there are three basis states, the dimension of the state space is 3.

(b) (i) $\langle i | j \rangle = \delta_{ij}, \ i, j = 1, 2, 3$. 
(ii) The basis states are complete in the sense that any state of the system can be written as a linear combination of the three basis states \( \{|i\rangle; i = 1, 2, 3\} \). If the states were incomplete, then this would mean that the electron could be found elsewhere other than on one of the three oxygen atoms, which, within the context of the model being considered here, is not possible.

(c) (i) Checking that the state \( |\phi\rangle \) is normalized to unity requires calculating \( \langle \phi|\phi\rangle \):

\[
\langle \phi|\phi\rangle = |a|^2 (-i|1\rangle + (1 + i)|2\rangle - |3\rangle)(i|1\rangle + (1 - i)|2\rangle - |3\rangle) \\
= |a|^2(1 + (1 + i)(1 - i) + 1) \\
= 4|a|^2 = 1.
\]

So the state \( |\phi\rangle \) is normalized to unity provided \( 4|a|^2 = 1 \), which requires

\[
a = \frac{e^{i\theta}}{2}
\]

where \( \theta \) is an unknown phase which we can freely set to zero. Thus we have \( a = \frac{1}{2} \).

(ii) The required probabilities are

\[
|\langle 1|\phi\rangle|^2 = \frac{1}{4} \\
|\langle 2|\phi\rangle|^2 = \frac{|1 - i|^2}{4} = \frac{1}{2} \\
|\langle 3|\phi\rangle|^2 = \frac{1}{4}.
\]

Thus the electron is most likely to be found on atom 2.

(iii) The electron is equally likely to be found on either atom 1 or atom 3.

5. An ‘atom’ with two energy levels has two states, the excited and ground states, represented by the kets \( |e\rangle \) and \( |g\rangle \) respectively.

(a) The states \( |e\rangle \) and \( |g\rangle \) form a complete orthonormal basis for the system. What does this statement mean?

(b) The atom is prepared in the state

\[
|\psi\rangle = (2 - i)|e\rangle + (4 + 2i)|g\rangle.
\]

(i) Show that this state is not normalized to unity.

(ii) Show that the state \( \frac{1}{5}|\psi\rangle \) is normalized to unity.

(iii) Using the normalized state, what are the probability amplitudes of observing the atom in the excited state and in the ground state?

(iv) What are the probabilities of finding the atom in the excited and ground states?

(v) The state of the atom for which its electric dipole moment has the value \( \mu \) is given by

\[
|\mu\rangle = \frac{1}{\sqrt{2}}(|e\rangle + |g\rangle).
\]

Given that the atom is in the state \( |\psi\rangle \), what is the (correctly normalized) probability of finding the atom to be in a state for which the dipole moment has the value \( \mu \)?
SOLUTION

(a) Orthonormality means that

\[ \langle e | e \rangle = \langle g | g \rangle = 1 \]
\[ \langle e | g \rangle = \langle g | e \rangle = 0. \]

Completeness means that any state of the system can be described as a linear combination of these two states, i.e. there does not exist any states of the system that cannot be expressed in terms of these basis states. If there were, then it would mean, for instance, that the atom has more than two energy levels.

(b) (i) \[ \langle \psi | \psi \rangle = \left[ (1 - 2i) \langle e | + (2 + 4i) \langle g | \left] \left[ (1 + 2i) | e \rangle + (2 - 4i) | g \rangle \right] \right] \]
\[ = (1 - 2i)(1 + 2i) + (2 + 4i)(2 - 4i) \]
\[ = 25. \]

Thus the state is not normalized to unity.

(ii) Since \( \langle \psi | \psi \rangle \) has just been shown to be equal to 25, then \( \langle \overline{\psi} | \overline{\psi} \rangle = \frac{1}{25} \langle \psi | \psi \rangle = 1. \) Thus the state \( | \overline{\psi} \rangle = \frac{1}{5} | \psi \rangle \) is normalized to unity.

(iii) In order to calculate probabilities, it is necessary to use normalized states. Thus, using the normalized state \( | \overline{\psi} \rangle \), the probability amplitudes of observing the atom in the excited state and in the ground state will be

\[ \langle e | \overline{\psi} \rangle = \frac{1 + 2i}{5} \quad \text{and} \quad \langle g | \overline{\psi} \rangle = \frac{2 - 4i}{5}. \]

(iv) The probabilities of finding the atom in the excited and ground states will then be

\[ |\langle e | \overline{\psi} \rangle|^2 = \left| \frac{1 + 2i}{5} \right|^2 = \frac{1}{5} \quad \text{and} \quad |\langle g | \overline{\psi} \rangle|^2 = \left| \frac{2 - 4i}{5} \right|^2 = \frac{4}{5}. \]

(v) The probability of finding the atom in the state \( | \mu \rangle \) will be \( |\langle \mu | \psi \rangle|^2 \). However, in calculating this, it is necessary to use the correctly normalized state \( | \overline{\psi} \rangle \). Thus we need

\[ \langle \mu | \overline{\psi} \rangle = \frac{1}{5\sqrt{2}} \left[ \langle e | + \langle g | \left] \left[ (2 - i) | e \rangle + (4 + 2i) | g \rangle \right] \right] = \frac{6 + i}{5\sqrt{2}}. \]

The required probability is then

\[ |\langle \mu | \psi \rangle|^2 = \left| \frac{6 + i}{5\sqrt{2}} \right|^2 = \frac{37}{50} = 0.74. \]