

## PHYSICS 301 QUANTUM PHYSICS I (2006)

### Assignment 3 Solutions

1. In so-called isospin theory, the neutron and the proton are assumed to be two different states,  $|n\rangle$  and  $|p\rangle$  respectively, of the one particle called the nucleon. Suppose as a result of a collision between a nucleon and another particle, the state of the nucleon undergoes a change represented by the operator  $\hat{E}$  defined by

$$\begin{aligned}\hat{E}|n\rangle &= (|n\rangle + i|p\rangle)/\sqrt{2} \\ \hat{E}|p\rangle &= (i|n\rangle + |p\rangle)/\sqrt{2}\end{aligned}$$

which ‘mixes’ the two states  $|n\rangle$  and  $|p\rangle$ .

- (a) Suppose a neutron suffers such a collision. What is the probability that the nucleon could still be observed to be a neutron after the collision?
- (b) Construct the matrix representation of  $\hat{E}$  in the  $\{|n\rangle, |p\rangle\}$  basis.
- (c) (i) Write the state  $|\psi\rangle = (|n\rangle - 2i|p\rangle)/\sqrt{5}$  as a column vector, and determine the new state of the system after the collision has occurred.  
(ii) Write the bra vector  $\langle\psi|$  as a row vector, and hence show that the probability the nucleon could be observed in the state  $|\psi\rangle$  after the collision is non-zero. Evaluate this probability.
- (d) Show that  $\hat{E}\hat{E}^\dagger = \hat{1}$  where  $\hat{1}$  is the unit operator.
- (e) If the nucleon is in an arbitrary state  $|\psi\rangle = a|n\rangle + b|p\rangle$  before a collision, what is its state after the collision? If  $|\psi\rangle$  is normalized to unity, show that the state of the system after the collision is still normalized to unity.
- (f) Do there exist states of the nucleon for which the collision does not change the state? If so, determine what the state or states are that have this property.

### SOLUTION

- (a) If the particle is initially a neutron, i.e. initially in the state  $|n\rangle$ , then after the collision, it will be in the state

$$\hat{E}|n\rangle = (|n\rangle + i|p\rangle)/\sqrt{2}.$$

The probability that it will be observed to be a neutron after the collision will then be

$$|\langle n|\hat{E}|n\rangle|^2 = \frac{1}{2}\langle n|\{|n\rangle + i|p\rangle\} = \frac{1}{2}.$$

- (b) Using the ordering defined by

$$\hat{E} \doteq \begin{pmatrix} \langle n|\hat{E}|n\rangle & \langle n|\hat{E}|p\rangle \\ \langle p|\hat{E}|n\rangle & \langle p|\hat{E}|p\rangle \end{pmatrix}$$

we get

$$\hat{E} \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}.$$

- (c) (i) As a column vector, the state  $|\psi\rangle = (|n\rangle - 2i|p\rangle)/\sqrt{5}$  is, (with the states ordered as in part (b))

$$|\psi\rangle \doteq \begin{pmatrix} \langle n|\psi\rangle \\ \langle p|\psi\rangle \end{pmatrix} = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ -2i \end{pmatrix}.$$

The state of the particle after the collision has occurred will then be

$$\hat{E}|\psi\rangle \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ -2i \end{pmatrix} = \frac{1}{\sqrt{10}} \begin{pmatrix} 3 \\ -i \end{pmatrix}$$

which can also be written as

$$\hat{E}|\psi\rangle = \frac{1}{\sqrt{10}}(3|n\rangle - i|p\rangle).$$

- (ii) The probability of the particle being observed in the state  $|\psi\rangle$  after the collision will be  $|\langle\psi|\hat{E}|\psi\rangle|^2$ . Thus we need to calculate

$$\langle\psi|\hat{E}|\psi\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 2i \end{pmatrix} \frac{1}{\sqrt{10}} \begin{pmatrix} 3 \\ -i \end{pmatrix} = \frac{5}{\sqrt{50}} = \frac{1}{\sqrt{2}}.$$

Consequently the required probability is

$$|\langle\psi|\hat{E}|\psi\rangle|^2 = 0.5.$$

- (d) Since, from part (b), we have

$$\hat{E} \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$$

we immediately have

$$\hat{E}^\dagger \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}$$

and hence

$$\hat{E}\hat{E}^\dagger \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

- (e) The state before the collision is  $|\psi\rangle = a|n\rangle + b|p\rangle$  which can be represented as a column matrix

$$|\psi\rangle \doteq \begin{pmatrix} a \\ b \end{pmatrix}.$$

The effect of the collision is to change the state to

$$\hat{E}|\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} a + ib \\ ia + b \end{pmatrix}.$$

If we call this state after the collision  $|\phi\rangle$ , then what we now what to check is  $\langle\phi|\phi\rangle$ . Thus

$$\langle\phi|\phi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} a^* - ib^* & -ia^* + b^* \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} a + ib \\ ia + b \end{pmatrix} = \frac{1}{2}((a^* - ib^*)(a + ib) + (-ia^* + b^*)(ia + b)) = |a|^2 + |b|^2.$$

But we are given that the initial state  $|\psi\rangle$  was normalized to unity, i.e.

$$\langle\psi|\psi\rangle = |a|^2 + |b|^2 = 1$$

so we have shown that

$$\langle\phi|\phi\rangle = 1.$$

(f) States for which the collision has no effect will be states  $|\lambda\rangle$  such that

$$\hat{E}|\lambda\rangle = \lambda|\lambda\rangle$$

where  $\lambda$  is a complex number. In this case, the effect of  $\hat{E}$  is to simply multiply  $|\lambda\rangle$  by a constant factor. Recall that the state vector  $c|\psi\rangle$  represents the *same physical state* of the system for any value of the factor  $c$ . Thus the task is to find the eigenvectors of  $\hat{E}$ . We can do this in the usual way, that is assume the eigenstate is of the form  $|\lambda\rangle = a|n\rangle + b|p\rangle$ , so we have, in matrix form

$$\hat{E}|\lambda\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$$

or

$$\begin{pmatrix} 1/\sqrt{2} - \lambda & i/\sqrt{2} \\ i/\sqrt{2} & 1/\sqrt{2} - \lambda \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0. \quad (1)$$

This is a pair of homogeneous equations for  $a$  and  $b$ , and there will be a non-trivial solution provided

$$\begin{vmatrix} 1/\sqrt{2} - \lambda & i/\sqrt{2} \\ i/\sqrt{2} & 1/\sqrt{2} - \lambda \end{vmatrix} = 0$$

which has the solutions

$$\lambda_{\pm} = \frac{1 \pm i}{\sqrt{2}} = e^{\pm i\pi/4}.$$

We can find the associated eigenvectors by substituting the two possible values for  $\lambda$  into Eq. (1) and solving for  $a$  and  $b$ . Thus, with  $\lambda = \lambda_+ = (1 + i)/\sqrt{2}$  we get

$$-ia/\sqrt{2} + ib/\sqrt{2} = 0$$

which tells us that  $a = b$ . We need the state to be normalized to unity, which can be shown to require  $a = b = 1/\sqrt{2}$ , so we end up with one eigenstate being

$$|\lambda_+\rangle \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

In the same way, the other eigenstate can be shown to be

$$|\lambda_-\rangle \doteq \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

These states  $|\lambda_{\pm}\rangle$  are then the states for which a collision has no effect.

2. (a) With respect to a pair of orthonormal vectors  $|1\rangle$  and  $|2\rangle$  that span the state space  $\mathcal{H}$  of a certain system, the operator  $\hat{Q}$  is defined by its action on these base states as follows:

$$\hat{Q}|1\rangle = 2|1\rangle + 2i|2\rangle \quad \hat{Q}|2\rangle = \alpha|1\rangle - |2\rangle.$$

where  $\alpha$  is a quantity to be determined.

- (i) What is the matrix representation of  $\hat{Q}$  in the  $\{|1\rangle, |2\rangle\}$  basis?
- (ii)  $\hat{Q}$  is known to be an observable of the system. What is the value of  $\alpha$ , and why does it have this value?
- (iii) Show that the states

$$|q_1\rangle = \frac{1}{\sqrt{5}}(|1\rangle - 2i|2\rangle) \quad |q_2\rangle = \frac{1}{\sqrt{5}}(2|1\rangle + i|2\rangle).$$

are eigenstates of  $\hat{Q}$  and that the associated eigenvalues are  $q_1 = -2$  and  $q_2 = 3$  respectively.

- (b) The system is prepared in the state

$$|\psi\rangle = \frac{1}{\sqrt{3}}|1\rangle + \frac{1+i}{\sqrt{3}}|2\rangle.$$

- (i) What are the possible results of a measurement of the observable  $Q$ ?
- (ii) What are the probabilities of obtaining each of the possible results?
- (iii) What is the state of the system *after* the measurement is performed for each of the possible measurement outcomes?

#### SOLUTION

- (a) (i) The matrix representation is given by

$$\hat{Q} \doteq \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix}$$

where  $Q_{ij} = \langle i|\hat{Q}|j\rangle$ .

By direct calculation from the above defining properties of  $\hat{Q}$ , it follows that

$$\hat{Q} \doteq \begin{pmatrix} 2 & \alpha \\ 2i & -1 \end{pmatrix}$$

- (ii) As  $\hat{Q}$  is an observable of the system, the operator  $\hat{Q}$  must be Hermitean, so that  $\alpha = -2i$ .
- (iii) The calculation can proceed by either using the matrix representation of the operator, or by carrying out the calculation in bra-ket notation. The first will be done in the bra-ket notation. Thus, what is required is

$$\begin{aligned} \hat{Q}|q_1\rangle &= \hat{Q} \frac{1}{\sqrt{5}}(|1\rangle - 2i|2\rangle) \\ &= \frac{1}{\sqrt{5}}(\hat{Q}|1\rangle - 2i\hat{Q}|2\rangle) \\ &= \frac{1}{\sqrt{5}}[2|1\rangle + 2i|2\rangle - 2i(-2i|1\rangle - |2\rangle)] \\ &= \frac{1}{\sqrt{5}}[-2|1\rangle + 4i|2\rangle] \\ &= -2 \frac{1}{\sqrt{5}}[|1\rangle - 2i|2\rangle] \\ &= -2|q_1\rangle. \end{aligned}$$

Thus,  $|q_1\rangle$  is an eigenstate of  $\hat{Q}$  with eigenvalue  $-2$ .

The second case will be dealt with using the column vector representation of  $|q_2\rangle$ , i.e.

$$|q_2\rangle \doteq \begin{pmatrix} \langle 1|q_2\rangle \\ \langle 2|q_2\rangle \end{pmatrix} = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ i \end{pmatrix}.$$

Thus

$$\hat{Q}|q_2\rangle = \begin{pmatrix} 2 & -2i \\ 2i & -1 \end{pmatrix} \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ i \end{pmatrix} = \frac{1}{\sqrt{5}} \begin{pmatrix} 6 \\ 3i \end{pmatrix} = 3 \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ i \end{pmatrix} \doteq 3|q_2\rangle$$

i.e.  $|q_2\rangle$  is an eigenstate of  $\hat{Q}$  with eigenvalue 3.

- (b) (i) The possible results are the eigenvalues of  $\hat{Q}$ , that is  $-2$  or  $3$ .  
(ii) The probability of getting the result  $q_1 = -2$  is given by  $|\langle q_1|\psi\rangle|^2$ . So first we need the probability amplitude

$$\langle q_1|\psi\rangle = \langle q_1|\left\{\frac{1}{\sqrt{3}}|1\rangle + \frac{1+i}{\sqrt{3}}|2\rangle\right\} = \frac{1}{\sqrt{3}}(\langle q_1|1\rangle + (1+i)\langle q_1|2\rangle).$$

To calculate the inner products appearing in this expression, it is necessary to make use of the expressions for the eigenstates in terms of the basis states  $\{|1\rangle, |2\rangle\}$ .

Thus

$$\langle q_1|1\rangle = \frac{1}{\sqrt{5}}(\langle 1| + 2i\langle 2|)|1\rangle = \frac{1}{\sqrt{5}}$$

and

$$\langle q_1|2\rangle = \frac{1}{\sqrt{5}}(\langle 1| + 2i\langle 2|)|2\rangle = \frac{2i}{\sqrt{5}}$$

and hence

$$\langle q_1|\psi\rangle = \frac{1}{\sqrt{15}}(1 + 2i(1+i)) = \frac{1}{\sqrt{15}}(-1 + 2i).$$

Thus

$$|\langle q_1|\psi\rangle|^2 = \frac{1}{3}.$$

The probability of getting the result  $q_2 = 3$  is calculated in a similar fashion. We require  $|\langle q_2|\psi\rangle|^2$  which means we first need

$$\langle q_2|\psi\rangle = \langle q_2|\left\{\frac{1}{\sqrt{3}}|1\rangle + \frac{1+i}{\sqrt{3}}|2\rangle\right\} = \frac{1}{\sqrt{3}}(\langle q_2|1\rangle + (1+i)\langle q_2|2\rangle).$$

The expression for  $|q_2\rangle$  gives us the corresponding expression for the bra vector  $\langle q_2|$ , so we have

$$\langle q_2|1\rangle = \frac{1}{\sqrt{5}}(2\langle 1| - i\langle 2|)|1\rangle = \frac{2}{\sqrt{5}}$$

and

$$\langle q_2|2\rangle = \frac{1}{\sqrt{5}}(2\langle 1| - i\langle 2|)|2\rangle = -\frac{i}{\sqrt{5}}$$

and hence

$$\langle q_2|\psi\rangle = \frac{1}{\sqrt{15}}(2 - i(1+i)) = \frac{1}{\sqrt{15}}(3 - i).$$

Thus

$$|\langle q_2|\psi\rangle|^2 = \frac{2}{3}.$$

- (iii) If the result  $q_1 = -2$  is obtained, then the system ends up in the state  $|q_1\rangle$  immediately after the measurement, and if the result  $q_2 = 3$  is obtained, the system ends up in the state  $|q_2\rangle$  immediately after the measurement.

3. (a) The negative oxygen molecular ion  $O_2^-$  consists of a pair of oxygen atoms separated by a distance  $2a$ . As an approximation, the electron can be assumed to be found only on one or the other of the oxygen atoms, at  $x = \pm a$ .

- (i) Within this approximation, write down the eigenvalue equation for the position operator  $\hat{x}$  for the electron.
- (ii) The momentum  $\hat{p}$  for the electron can be represented by a  $2 \times 2$  matrix.
- A. Why would the matrix be  $2 \times 2$  in size?
- B. Given that the matrix representing the momentum is, in the position representation

$$\hat{p} \doteq p_0 \begin{pmatrix} 0 & -ie^{-i\phi} \\ ie^{i\phi} & 0 \end{pmatrix}$$

show that the eigenvalues are  $\pm p_0$  and prove that the associated eigenvectors  $|\pm p_0\rangle$  of  $\hat{p}$  are given by

$$|p_0\rangle \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ ie^{i\phi} \end{pmatrix} \quad \text{and} \quad |-p_0\rangle \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -ie^{i\phi} \end{pmatrix}.$$

C. Show that the states  $|\pm p_0\rangle$  are orthonormal.

- (b) The quantum system is prepared in the state  $|\psi\rangle = \frac{1}{\sqrt{3}} [ | + a\rangle + i\sqrt{2}| - a\rangle ]$ . A measurement is made of the momentum and the result  $p_0$  is obtained.
- (i) What is the state of the system *after* this measurement was performed?
- (ii) If, after the above result for the momentum was obtained, the position of the electron was measured, what is the probability of obtaining the result  $+a$ ?
- (iii) What would be the probability of getting the result  $-a$  if the position of the electron was measured when the system was in the original state  $|\psi\rangle$ ?
- (iv) Could the system ever be found in a state in which the position of the electron was  $x = +a$  and the momentum was  $p_0$ ? Explain your answer.

### SOLUTION

- (a) (i) The eigenvalues will be  $\pm p_0$ .
- (ii) A. As the state space has dimension 2, all operators will be represented by a  $2 \times 2$  matrix.
- B. To determine the eigenvalues and eigenvectors of  $\hat{p}$ , the solution must be found of the eigenvalue equation

$$\hat{p}|p\rangle = p|p\rangle.$$

In matrix form, this equation is

$$\hat{p} \doteq p_0 \begin{pmatrix} 0 & -ie^{-i\phi} \\ ie^{i\phi} & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = p \begin{pmatrix} a \\ b \end{pmatrix}$$

or

$$\begin{pmatrix} -p & -ip_0e^{-i\phi} \\ ip_0e^{i\phi} & -p \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0.$$

The associated equation for the eigenvalues will be

$$\begin{vmatrix} -p & -ip_0e^{-i\phi} \\ ip_0e^{i\phi} & -p \end{vmatrix} = 0$$

or

$$p^2 - p_0^2 = 0$$

which gives

$$p = \pm p_0.$$

For  $p = p_0$ , the equation for the coefficients  $a$  and  $b$  of the momentum eigenvector will be

$$-p_0 a - i p_0 e^{-i\phi} b = 0$$

which has the solution

$$a = -i e^{-i\phi} b.$$

To fix the values of  $a$  and  $b$ , the eigenstate must be normalized to unity, i.e.

$$|a|^2 + |b|^2 = 1$$

which yields

$$2|a|^2 = 1$$

and hence

$$a = \frac{1}{\sqrt{2}} e^{i\theta} \quad \text{and} \quad b = \frac{1}{\sqrt{2}} i e^{i\phi} e^{-i\theta}$$

where  $\theta$  is a phase whose value we are free to choose. If we put  $\theta = 0$  we get

$$a = \frac{1}{\sqrt{2}} \quad \text{and} \quad b = \frac{1}{\sqrt{2}} i e^{i\phi}$$

so that the eigenvector associated with the eigenvalue  $p = p_0$  will be

$$|p_0\rangle \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i e^{i\phi} \end{pmatrix}.$$

The procedure is much the same for  $p = -p_0$ . The equation for the coefficients  $a$  and  $b$  of the momentum eigenvector will be

$$p_0 a - i p_0 e^{-i\phi} b = 0$$

which has the solution

$$a = i e^{-i\phi} b.$$

Using the normalization condition

$$|a|^2 + |b|^2 = 1$$

we get in a similar way to the previous case

$$a = \frac{1}{\sqrt{2}} e^{i\theta} \quad \text{and} \quad b = -\frac{1}{\sqrt{2}} i e^{i\phi} e^{-i\theta}$$

where  $\theta$  is a phase whose value we are free to choose. If we put  $\theta = 0$  we get

$$a = \frac{1}{\sqrt{2}} \quad \text{and} \quad b = -\frac{1}{\sqrt{2}} i e^{i\phi}$$

so that the eigenvector associated with the eigenvalue  $p = -p_0$  will be

$$|-p_0\rangle \doteq \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i e^{i\phi} \end{pmatrix}.$$

C. To check orthonormality we have to calculate

$$\langle p_0 | p_0 \rangle = \frac{1}{2} \begin{pmatrix} 1 & -ie^{-i\phi} \end{pmatrix} \begin{pmatrix} 1 \\ ie^{i\phi} \end{pmatrix} = 1.$$

Similarly,  $\langle -p_0 | -p_0 \rangle = 1$ . Finally we need to check  $\langle p_0 | -p_0 \rangle$ :

$$\langle p_0 | -p_0 \rangle = \frac{1}{2} \begin{pmatrix} 1 & -ie^{-i\phi} \end{pmatrix} \begin{pmatrix} 1 \\ -ie^{i\phi} \end{pmatrix} = 0$$

as required.

- (b) (i) The state will be  $|p_0\rangle$ .  
(ii) This probability will be  $|\langle +a | p_0 \rangle|^2$ . Given the expression for  $|p_0\rangle$  in part (b), this is

$$|\langle +a | p_0 \rangle|^2 = \left| \frac{1}{\sqrt{2}} \right|^2 = \frac{1}{2}.$$

- (iii) This probability is given by

$$|\langle -a | \psi \rangle|^2 = \left| \frac{i\sqrt{2}}{\sqrt{3}} \right|^2 = \frac{2}{3}$$

- (iv) If the system is in the state  $|\psi\rangle$  and the momentum is measured, and the result  $p_0$  obtained, then the system ends up in the state  $|p_0\rangle$ . If then the position of the electron is measured, then the probability of getting either result  $\pm a$  is  $\frac{1}{2}$ . Suppose we get the result  $+a$ , which means that the system is now in the state  $|+a\rangle$ , and then remeasure the momentum. The probability of regaining the result  $p_0$  is now  $|\langle p_0 | +a \rangle|^2$ , which is  $\frac{1}{2}$ , i.e. there is no guarantee that the result  $p_0$  will be observed again – there is a probability  $\frac{1}{2}$  of obtaining the result  $p = -p_0$ . Thus, the system cannot be found in a state in which the position of the electron will be observed to have the same value whenever measured and its momentum of the system can be observed to have the same value whenever measured.

4. For the  $O_2^-$  of the previous question, the Hamiltonian  $\hat{H}$  is such that:

$$\begin{aligned} \hat{H}|+a\rangle &= \frac{1}{2}E(|+a\rangle + e^{i\phi}|-a\rangle) \\ \hat{H}|-a\rangle &= \frac{1}{2}E(e^{-i\phi}|+a\rangle + |-a\rangle) \end{aligned}$$

- (a) Write down the matrix representing  $\hat{H}$  in the position representation.  
(b) Assuming that the state of the system at time  $t$  can be expressed as

$$|\psi(t)\rangle = C_+(t)|+a\rangle + C_-(t)|-a\rangle,$$

write down the Schrödinger equation for this system in matrix form.

- (c) Confirm, by direct substitution into the equations for  $C_1(t)$  and  $C_2(t)$  that the solutions for these coefficients are

$$\begin{aligned} C_+(t) &= \frac{1}{2} \left( ae^{-i\omega t} + b \right) \\ C_-(t) &= \frac{1}{2} e^{i\phi} \left( ae^{-i\omega t} - b \right) \end{aligned}$$

where  $a$  and  $b$  are unknown constants and  $\omega = E/\hbar$ .



- (d) The system is initially, at  $t = 0$  in the state  $| - a \rangle$ . Solve for the probability of observing the system in state  $| + a \rangle$  at a later time  $t$ .
- (e) At what time  $t = T$  would the probability of the electron being observed on the oxygen atom at  $+a$  first be a maximum?
- (f) Assuming it is valid to do so, analyse this result classically to estimate the momentum that the electron would have to have in order to cross from the left hand to the right hand atom in time  $T$ . [It turns out that the momentum of the electron can have the magnitude  $p_0 = mEa/\hbar$ . Your result here will be slightly different.]

### SOLUTION

- (a) The matrix representing  $\hat{H}$  will be

$$\frac{1}{2}E \begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix}$$

- (b) The Schrödinger equation will be

$$\frac{1}{2}E \begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix} \begin{pmatrix} C_1(t) \\ C_2(t) \end{pmatrix} = i\hbar \frac{d}{dt} \begin{pmatrix} C_1(t) \\ C_2(t) \end{pmatrix}$$

- (c) From the expressions given for  $C_{\pm}(t)$  it follows that

$$i\hbar \frac{d}{dt} \begin{pmatrix} C_+(t) \\ C_-(t) \end{pmatrix} = \frac{1}{2}\hbar\omega a e^{-i\omega t} \begin{pmatrix} 1 \\ e^{i\phi} \end{pmatrix}$$

while

$$\begin{aligned} \frac{1}{2}E \begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix} \begin{pmatrix} C_+(t) \\ C_-(t) \end{pmatrix} &= \frac{1}{4}\hbar\omega \begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix} \begin{pmatrix} ae^{-i\omega t} + b \\ e^{i\phi}(ae^{-i\omega t} - b) \end{pmatrix} \\ &= \frac{1}{4}\hbar\omega \begin{pmatrix} 2a e^{-i\omega t} \\ 2a e^{i\phi} e^{-i\omega t} \end{pmatrix} \\ &= \frac{1}{2}\hbar\omega a e^{-i\omega t} \begin{pmatrix} 1 \\ e^{i\phi} \end{pmatrix} \\ &= i\hbar \frac{d}{dt} \begin{pmatrix} C_+(t) \\ C_-(t) \end{pmatrix} \end{aligned}$$

as required.

- (d) If the system is initially in the state  $| - a \rangle$ , then we have  $C_-(0) = 1$  and  $C_+(0) = 0$ . If we substitute this into the expressions for  $C_{\pm}(t)$  evaluated at  $t = 0$  we get

$$C_+(0) = \frac{1}{2}(a + b) = 0 \quad \text{and} \quad C_-(0) = \frac{1}{2}e^{i\phi}(a - b) = 1.$$

Solving these equations for  $a$  and  $b$  gives

$$a = e^{-i\phi} \quad \text{and} \quad b = -e^{-i\phi}$$

and hence

$$C_-(t) = \frac{1}{2}e^{-i\phi}(e^{-i\omega t} + 1) \quad \text{and} \quad C_+(t) = \frac{1}{2}e^{-i\phi}(e^{-i\omega t} - 1)$$

The probability of the system being in the state  $| + \rangle$  at a time  $t$  is then

$$| \langle + | \psi(t) \rangle |^2 = |C_+(t)|^2 = \frac{1}{4}|e^{-i\omega t} - 1|^2.$$

When calculating this last quantity it, recall that  $|u + v|^2 = (u + v)(u^* + v^*)$  where  $u$  and  $v$  are both complex numbers. In this case this gives

$$|\langle + | \psi(t) \rangle|^2 = \frac{1}{4}(e^{-i\omega t} - 1)(e^{i\omega t} - 1) = \frac{1}{2} \left( 1 - \frac{e^{i\omega t} + e^{-i\omega t}}{2} \right) = \frac{1}{2}(1 - \cos \omega t).$$

This can also be written

$$|\langle + | \psi(t) \rangle|^2 = \sin^2 \frac{1}{2} \omega t.$$

- (e) The probability of observing the electron at  $x = +a$  will then be a maximum at a time  $T$  such that  $\sin^2 \frac{1}{2} \omega T = 1$ , i.e.

$$T = \pi/\omega.$$

- (f) Assuming a classical interpretation, this results suggests that the electron started out at  $x = -a$  at a time  $t = 0$  and arrived at  $x = +a$  at a time  $t = \pi/\omega$ . This implies an average speed of  $v = 2a\omega/\pi$  and hence a momentum of

$$p = \frac{2a\omega m}{\pi} = \frac{2}{\pi} \frac{mEa}{\hbar}$$

as compared to  $p_0 = mEa/\hbar$  that can be shown to be the case in the previous question.

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