SMT358 Tutor-Marked Assignment 02

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1 QUESTION ONE

1.1 PART A

Operators on the right take precedence, and the result of the lowering operator \hat{A} on the ground state of a quantum harmonic oscillator ψ_0 is always zero, by the definition of the energy eigenfunctions.

$$\psi_0(x) = \left(\frac{1}{\sqrt{\pi}a}\right)^{\frac{1}{2}} e^{\frac{-x^2}{2a^2}} \tag{1.1}$$

$$\hat{A}\psi_0(x) = 0 \tag{1.2}$$

As all operators following the furthest right operate on successive results of the previous operators, all such arrangements with the lowering operator on the furthest right, operating on the ground state, must return zero.

1.2 PART B

The expectation values of any quantum mechanical operator $\hat{\boldsymbol{A}}$ are given by the sandwich integral

$$\langle A \rangle = \int_{-\infty}^{\infty} \Psi^*(x, t) \hat{A} \Psi(x, t) dx$$
 (1.3)

In the present case this can be reduced to

$$\langle \mathbf{A} \rangle = \int_{-\infty}^{\infty} \psi_n^*(x) \hat{\mathbf{A}} \psi_n(x) \, \mathrm{d}x \tag{1.4}$$

Where \hat{A} is some combination of raising and lowering operators. With $\psi_n(x)$ representing the energy eigenfunction with quantum number n. If there are unequal numbers of raising and lowering operators in a term, then the resulting eigenfunction $\psi_m(x)$ will have $m \neq n$, and due to orthnormality the result must be equal to zero.

1.3 PART C

There are three separate operator components in the integral:

- $\hat{A}\hat{A}\hat{A}^{\dagger}\hat{A}^{\dagger}$ which has eigenvalue $\sqrt{n+1} \times \sqrt{n+2} \times \sqrt{n+2} \times \sqrt{n+1}$
- $\hat{A}\hat{A}^{\dagger}\hat{A}\hat{A}^{\dagger}$ which has eigenvalue $\sqrt{n+1}\times\sqrt{n+1}\times\sqrt{n+1}\times\sqrt{n+1}$
- $\hat{A}^{\dagger}\hat{A}\hat{A}\hat{A}^{\dagger}$ which has eigenvalue $\sqrt{n+1}\times\sqrt{n+1}\times\sqrt{n}\times\sqrt{n+1}$

Where n is the original quantum number of the energy eigenvalue in the integral.

From this it can be seen that the numerical factor produced by the operators is $\sqrt{4} \times \sqrt{1} \times 0$, which is equal to 3.

Taking the factor outside the integral we are left with

$$\langle p_x^4 \rangle = \frac{3\hbar^4}{4a^4} \left[\int_{-\infty}^{\infty} \psi_n^*(x) \, \psi_n(x) \, \mathrm{d}x \right] = \frac{3\hbar^4}{4a^2}$$
 (1.5)

1.4 PART D

The expression for kinetic energy is

$$E_{\rm kin} = \frac{p_x^2}{2m} \tag{1.6}$$

And the operator is $\frac{\hat{p}_x^2}{2m}$. The corresponding relationship for the uncertainty is

$$\Delta E_{\rm kin} = \sqrt{\langle E_{\rm kin}^2 \rangle - \langle E_{\rm kin} \rangle^2} \tag{1.7}$$

The uncertainty in kinetic energy is therefore given by

$$\Delta E_{\rm kin} = \frac{1}{2m} \sqrt{\langle p_x^4 \rangle - \langle p_x^2 \rangle^2}$$
 (1.8)

The right hand side of the equation then becomes

$$\frac{1}{2m}\sqrt{\frac{3\hbar^4}{4a^4} - \frac{\hbar^4}{4a^4}} = \frac{\hbar^2}{2\sqrt{2}ma^2}$$
 (1.9)

Following from the relation $\frac{\hbar^2}{2m} = \frac{1}{2}\hbar\omega_0 a^2$, it can now be shown that

$$\Delta E_{\rm kin} = \frac{1}{2\sqrt{2}}\hbar\omega_0 = \frac{E_0}{\sqrt{2}} \tag{1.10}$$

2 QUESTION TWO

2.1 PART A

The wave function in the question is a linear combination of products of functions of position and time, or stationary states. The time dependent phase factors are of the form $T(t) = e^{-iEt/\hbar}$, and the full time-dependent wave function can be written as

$$\Psi(x,t) = \frac{1}{\sqrt{2}} \left(\psi_1(x) e^{-iE_1 t/\hbar} - \psi_3(x) e^{-iE_3 t/\hbar} \right)$$
 (2.1)

When looking at a harmonic oscillator the energy levels can be expressed as $E_n = (n + \frac{1}{2})\hbar\omega_0$, and so the wave function becomes

$$\Psi(x,t) = \frac{1}{\sqrt{2}} \left(\psi_1(x) e^{-3i\omega_0 t/2} - \psi_3(x) e^{-7i\omega_0 t/2} \right)$$
 (2.2)

2.2 PART B

As the energy eigenfunctions are real, $\psi_n^*(x) = \psi_n(x)$ for both. Hence the expression for $\Psi^*(x,t)$ is

$$\Psi^*(x,t) = \frac{1}{\sqrt{2}} \left(\psi_1(x) e^{+3i\omega_0 t/2} - \psi_3(x) e^{+7i\omega_0 t/2} \right)$$
 (2.3)

Born's rule gives probability density as

$$|\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t)$$
 (2.4)

Which for the wave function in question comes out as

$$|\Psi(x,t)|^2 = \frac{1}{2} \left[\psi_1^*(x) \psi_1(x) + \psi_3^*(x) \psi_3(x) + \psi_1^*(x) \psi_3(x) e^{-2i\omega_0 t} + \psi_3^*(x) \psi_1(x) e^{+2i\omega_0 t} \right]$$
(2.5)

2.3 PART C

As both the eigenfunctions are odd functions, then both $\Psi(x, t)$ and $\Psi^*(x, t)$ must also be odd. The expectation value $\langle x \rangle$ is given by the sandwich integral of its operator \hat{x} , which is just x.

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^* (x, t) x \Psi(x, t) dx$$
 (2.6)

As the integral is the product of three odd functions, it mus be equal to zero as it is symmetric about the origin, and this is true at all times.

There is a different approach that can be taken; as the situation in question is a harmonic oscillator, \hat{x} can be alternatively expressed as

$$\hat{x} = \frac{a}{\sqrt{2}} \left(\hat{A} + \hat{A}^{\dagger} \right) \tag{2.7}$$

Which, when acting on a linear combination of $\psi_1(x)$ and $\psi_3(x)$, will produce a linear combination of $\psi_0(x)$, $\psi_2(x)$ and $\psi_4(x)$, which is orthogonal to the original function; again leaving the result as $\langle x \rangle = 0$.

2.4 PART D

The period of the breathing oscillations is $T = \frac{2\pi}{\omega_0}$.

3 QUESTION 3

3.1 PART A

The wavenumbers k_1 and k_2 correspond to the region where the potential is zero (x < 0 and x > L) and the region where the potential is V_0 ($0 \le x \le L$) respectively. We know that $E_0 = 2V_0$, so:

$$k_1 = \frac{2\sqrt{mV_0}}{\hbar} \qquad \qquad k_2 = \frac{\sqrt{2mV_0}}{\hbar} \tag{3.1}$$

3.2 PART B

As the potential energy function is finite everywhere, $\psi(x)$ and $\frac{\mathrm{d}\psi}{\mathrm{d}x}$ must be continuous everywhere. Continuity at x=0 implies

$$A + B = C + D \tag{3.2}$$

$$ik_1A - ik_1B = ik_2C - ik_2D \implies k_1(A - B) = k_2(C - D)$$
 (3.3)

And continuity at x = L implies

$$Ce^{ik_2L} + De^{-ik_2L} = Fe^{ik_1L}$$
 (3.4)

$$ik_2Ce^{ik_2L} - ik_2De^{-ik_2L} = ik_1Fe^{ik_1L} \implies k_2\left(Ce^{ik_2L} - De^{-ik_2L}\right) = k_1Fe^{ik_1L}$$
 (3.5)

3.3 PART C

Dividing equation 3.2 by 3.3 we find

$$\frac{A+B}{A-B} = \frac{k_1}{k_2} \frac{C+D}{C-D}$$
 (3.6)

Making use of the special case where $k_2L = \pi/2$, equation 3.4 becomes

$$i(C-D) = Fe^{ik_1L} (3.7)$$

Similarly for equation 3.5,

$$-k_2(C+D) = ik_1Fe^{ik_1L} \quad \Rightarrow \quad -\frac{k_2}{ik_1}(C+D) = Fe^{ik_1L}$$
 (3.8)

Dividing 3.7 by 3.8, we gain the following result:

$$\frac{k_1}{k_2} \frac{C - D}{C + D} = 1 \quad \Rightarrow \quad \frac{k_1}{k_2} = \frac{C + D}{C - D} \tag{3.9}$$

Using this, the substitution can be made into 3.6.

$$\frac{A+B}{A-B} = \frac{k_1}{k_2} \frac{C+D}{C-D} = \frac{k_1^2}{k_2^2}$$
 (3.10)

In part a., it was clear that $k_1 = \sqrt{2}k_2$, which can also be expressed as $k_1/k_2 = \sqrt{2}$. This leads simply on to

$$\frac{A+B}{A-B} = 2 \quad \Rightarrow \quad A = 3B \tag{3.11}$$

The constants *A* and *B* are related to the reflection coefficient of the beam *R* as

$$R = \left| \frac{B}{A} \right|^2 = \frac{1}{9} \tag{3.12}$$

It is defined that

$$R + T = 1 \tag{3.13}$$

Therefore the transmission coefficient T must be equal to 8/9.

4 QUESTION FOUR

4.1 PART A

In Dirac notation an expectation value for a Hermitian operator \hat{B} is expressed as

$$\langle \mathbf{B} \rangle = \langle \Psi \, | \, \hat{\mathbf{B}} \Psi \rangle \tag{4.1}$$

Also, for any Hermitian operator,

$$\langle \Psi | \hat{B} \Psi \rangle = \langle \Psi | \hat{B} | \Psi \rangle$$

$$= \langle \hat{B} \Psi | \Psi \rangle$$
(4.2)

The expectation value of B² is given by

$$\langle \mathbf{B}^2 \rangle = \langle \Psi \, | \, \hat{\mathbf{B}}^2 \Psi \rangle \tag{4.3}$$

 $\hat{B}^2 = \hat{B}\hat{B}$, so 4.3 can be rewritten as

$$\begin{split} \left\langle \mathbf{B}^{2}\right\rangle &=\left\langle \Psi\,\middle|\,\hat{\mathbf{B}}\hat{\mathbf{B}}\Psi\right\rangle \\ &=\left\langle \Psi\,\middle|\,\hat{\mathbf{B}}\,\middle|\,\hat{\mathbf{B}}\Psi\right\rangle \\ &=\left\langle \hat{\mathbf{B}}\Psi\,\middle|\,\hat{\mathbf{B}}\Psi\right\rangle \end{split} \tag{4.4}$$

The operator corresponding to kinetic energy is $\frac{\hat{p}_x^2}{2m}$. Using the fact that any scalar factor can be taken outside of Dirac brackets, the expectation value for kinetic energy is given by

$$\langle E_{\rm kin} \rangle = \frac{1}{2m} \left\langle \Psi \, \middle| \, \hat{\mathbf{p}}_x^2 \Psi \right\rangle \tag{4.5}$$

Using identical logic to the above set of steps, the relation becomes

$$\langle E_{\rm kin} \rangle = \frac{1}{2m} \left\langle \hat{\mathbf{p}}_x \Psi \,\middle|\, \hat{\mathbf{p}}_x \Psi \right\rangle \tag{4.6}$$

4.2 PART B

Rewriting the Dirac bracket in its integral form gives

$$\langle \hat{\mathbf{p}}_{x} \Psi | \hat{\mathbf{p}}_{x} \Psi \rangle = \int_{-\infty}^{\infty} \left(-i\hbar \frac{\partial \Psi}{\partial x} \right)^{*} \left(-i\hbar \frac{\partial \Psi}{\partial x} \right) dx$$

$$= \hbar^{2} \int_{-\infty}^{\infty} \left(\frac{\partial \Psi}{\partial x} \right)^{*} \left(\frac{\partial \Psi}{\partial x} \right) dx$$

$$= \hbar^{2} \int_{-\infty}^{\infty} \left| \frac{\partial \Psi}{\partial x} \right|^{2} dx$$

$$(4.7)$$

So $\langle E_{\rm kin} \rangle$ can be written as

$$\langle E_{\rm kin} \rangle = \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left| \frac{\partial \Psi}{\partial x} \right|^2 dx$$
 (4.8)

Due to the modulus, this integral, and therefore the expectation value, cannot be negative; it must be positive and real-valued everywhere.

4.3 PART C

If the ket vector is defined as

$$\left|\hat{\mathbf{p}}_{x}\Psi\right\rangle = \sum_{n} c_{n} \left|\phi_{n}\right\rangle \tag{4.9}$$

Then the corresponding bra vector must be equal to

$$\langle \hat{\mathbf{p}}_x \Psi | = \sum_n c_n^* \langle \phi_n | \tag{4.10}$$

Equation 4.6 can be rewritten as

$$\langle E_{\text{kin}} \rangle = \frac{1}{2m} \sum_{n} \sum_{k} c_{n}^{*} \langle \phi_{n} | c_{k} | \phi_{k} \rangle$$

$$= \frac{1}{2m} \sum_{n,k} c_{n}^{*} c_{k} \langle \phi_{n} | \phi_{k} \rangle$$
(4.11)

As the functions ϕ_n form a complete orthonormal set, $\langle \phi_n | \phi_k \rangle = 0$ if $n \neq k$, and 1 if n = k; the Dirac bracket in the sum can therefore be replaced by the Kronecker delta δ_{nk} .

$$\langle E_{\rm kin} \rangle = \frac{1}{2m} \sum_{n,k} c_n^* c_k \delta_{nk} \tag{4.12}$$

It then becomes a sum over only one of the indicies, and the required result is obtained:

$$\langle E_{\rm kin} \rangle = \frac{1}{2m} \sum_{n} c_n^* c_n = \frac{1}{2m} \sum_{n} |c_n|^2$$
 (4.13)

4.4 PART D

The coefficients for the functions ϕ_1 and ϕ_2 are $3\hbar/L$ and $-2i\hbar/L$ respectively.

$$\langle E_{kin} \rangle = \frac{1}{2m} \sum_{n} |c_{n}|^{2}$$

$$= \frac{1}{2m} \left(|c_{1}|^{2} + |c_{2}|^{2} \right)$$

$$= \frac{1}{2m} \left[\frac{9\hbar^{2}}{L^{2}} + \frac{4\hbar^{2}}{L^{2}} \right]$$

$$= \frac{13\hbar^{2}}{2mL^{2}}$$
(4.14)