**PHY V2500: QUANTUM MECHANICS I**

**Problem Set 2**

**Due September 25, 2025**

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**Problem 1**

Consider a wave function in one dimension of the form

$$\psi = A\, e^{-i\omega t}\, x^2\, e^{-ax}$$

where $A$, $a$ are constants and $x$ is in the range $[0, \infty]$.

a) From the normalization condition $\int dx \psi^* \psi = 1$, determine the constant $A$ in terms of $a$.

b) Calculate the expectation values $\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$, $\langle p^2 \rangle$.

**Solution**

a) The normalization condition is

$$\begin{aligned} \int dx\, \psi^* \psi &= |A|^2 \int dx\, x^4 e^{-2ax} = |A|^2 \frac{1}{(2a)^5} \int du\, u^4 e^{-u} \qquad \Big[u = 2ax \\ &= |A|^2 \frac{4!}{(2a)^5} = |A|^2 \frac{3}{4a^5} \end{aligned}$$

Setting this to $1$, $|A| = \sqrt{\frac{4a^5}{3}}$.

b) For the expectation value of $x$, we get

$$\langle x \rangle = \int dx\, \psi^*\, x\, \psi = |A|^2 dx\, x^5 e^{-2ax} = |A|^2 \frac{1}{(2a)^6} 5! = \frac{5}{2a}$$

For the expectation value of $p$, we get

$$\begin{aligned} \langle p \rangle &= -i\hbar \int dx\, \left(x^2 e^{-ax}\right) \left[\frac{\partial}{\partial x}\left(x^2 e^{-ax}\right)\right] = -i\frac{\hbar}{2} \int dx\, \frac{\partial}{\partial x}\left[\left(x^2 e^{-ax}\right)^2\right] \\ &= -i\frac{\hbar}{2}\left[\left(x^2 e^{-ax}\right)^2\right]_0^\infty = 0 \end{aligned}$$

$$\langle x^2 \rangle = |A|^2 \int dx\, x^6 e^{-2ax} = |A|^2 \frac{6!}{(2a)^7} = \frac{15}{2a^2}$$

For $\langle p^2 \rangle$, we first note that

$$\frac{\partial}{\partial x}(x^2 e^{-ax}) = (2x - ax^2) e^{-ax}, \qquad \frac{\partial^2}{\partial x^2}(x^2 e^{-ax}) = (2 - 4ax + a^2 x^2) e^{-ax}$$

Thus

$$\langle p^2 \rangle = -\hbar^2 |A|^2 \int dx\, x^2 e^{-ax} \frac{\partial^2}{\partial x^2}(x^2 e^{-ax})$$

$$\begin{aligned} &= -\hbar^2|A|^2 \int dx\,(2x^2 - 4ax^3 + a^2x^4)e^{-2ax} \\ &= -\hbar^2|A|^2 \left[\frac{2\times 2!}{(2a)^3} - \frac{4a\times 3!}{(2a)^4} + \frac{a^2 4!}{(2a)^5}\right] \\ &= \frac{\hbar^2 a^2}{3} \end{aligned}$$

**Problem 2**

Consider the problem of the particle in a one-dimensional box of length $L$ which was worked out in class. Consider a wave function

$$\psi = A\,\sin^2(n\pi x/L)$$

a) Find $A$ from the normalization condition.

b) Expand the given $\psi$ as a linear combination of the eigenstates of the Hamiltonian.

**Solution**

a) For the normalization condition, we need

$$\begin{aligned} \int_0^L dx\,|\psi|^2 &= |A|^2 \int dx\,\sin^4(n\pi x/L) = |A|^2 \int dx\,\frac{1}{4}\,(1-\cos(2\pi n x/L))^2 \\ &= |A|^2 \int dx\,\frac{1}{4}\left[1 - 2\cos(2\pi n x/L) + \frac{1}{2}\,(1+\cos(4\pi n x/l))\right] \\ &= |A|^2 \frac{1}{4}\left[L + \frac{L}{2}\right] = |A|^2 \frac{3L}{8} \end{aligned}$$

This identifies $A = \sqrt{8/3L}$.

b) The eigenstates of the Hamiltonian were obtained in class as

$$u_n = \sqrt{\frac{2}{L}}\,\sin(n\pi x/L)$$

The expansion of $\psi$ in terms of these takes the form

$$\sqrt{\frac{3}{8L}}\,\sin^2(n\pi x/L) = \sum_k c_k\,u_k$$

The coefficients $c_k$ can be obtained as

$$\begin{aligned} c_k &= \int_0^L dx\,u_k\,\psi = \sqrt{\frac{3}{8L}}\sqrt{\frac{2}{L}}\int_0^L dx\,\sin^2(n\pi x/L)\sin(k\pi x/L) \\ &= \sqrt{\frac{3}{4L^2}}\frac{1}{2}\int dx\,\left[1-\cos(2\pi n x/L)\right]\sin(k\pi x/L) \\ &= \sqrt{\frac{3}{4L^2}}\frac{1}{2}\left\{\frac{L}{k\pi}\Big[-\cos(k\pi x/L)\Big]_0^L - \frac{1}{2}\int dx\,\sin((k+2n)\pi x/L) - \frac{1}{2}\int dx\,\sin((k-2n)\pi x/L)\right\} \end{aligned}$$

$$= \frac{\sqrt{3}}{4L}\left\{\frac{L}{k\pi}(1-(-1)^k) - \frac{1}{2}\frac{L}{(k+2n)\pi}(1-(-1)^{k+2n}) - \frac{1}{2}\frac{L}{(k-2n)\pi}(1-(-1)^{k-2n})\right\}$$
$$= -\frac{\sqrt{3}}{4\pi}\left[1-(-1)^k\right]\frac{2n^2}{k(k^2-4n^2)}$$

Notice that this vanishes for even values of $k$. This result applies for $k \neq 2n$. For $k = 2n$ the second term of the integral is $\int dx \cos(2\pi n x/L)\sin(2\pi n x/L) = 0$, giving zero again. Thus

$$\psi = -\frac{1}{4\pi}\sqrt{\frac{6}{L}}\sum_k \left[1-(-1)^k\right]\frac{2n^2}{k(k^2-4n^2)}\ \sin(k\pi x/L)$$

**Problem 3**

a) Determine the eigenvalues and eigenvectors of the matrix

$$M = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & e^{i\varphi} \end{bmatrix}$$

where $\theta$, $\varphi$ are some angular variables.

b) Is this matrix hermitian, unitary or neither?

**Solution**

a) The eigenvalues are given by $\det(M - \lambda \mathbb{1}) = 0$. This becomes

$$(\lambda - e^{i\varphi})\left[(\cos\theta - l)^2 + \sin^2\theta\right] = 0$$

with the solutions

$$\lambda = e^{i\varphi}, \cos\theta \pm i\sin\theta = e^{\pm i\theta}$$

The eigenvalue equation for $\lambda = e^{i\theta}$ is

$$\begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & e^{i\varphi} \end{pmatrix}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = e^{i\theta}\begin{pmatrix} u \\ v \\ w \end{pmatrix}$$

This can be written out as

$$\cos\theta\, u - \sin\theta\, v = \cos\theta\, u + i\sin\theta\, u, \qquad e^{i\varphi}w = e^{i\theta}w$$

which gives $w = 0$ and $v = -iu$. Normalizing, the eigenvector is

$$U^{(1)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}$$

The other eigenvector (for $\lambda = e^{-i\theta}$) can be obtained in a similar manner, and it is given by

$$U^{(2)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}$$

The third eigenvector, corresponding to $\lambda = e^{i\varphi}$, is given by

$$U^{(3)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

b) From the definition of the matrix

$$M^{\dagger} = (M^*)^T = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & e^{-i\varphi} \end{pmatrix}$$

So by explicit calculation

$$M^{\dagger}M = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & e^{i\varphi} \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & e^{-i\varphi} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathbb{1}$$

This shows that $M$ is unitary.

**Problem 4**

a) Starting with the Heisenberg algebra, calculate the commutators $[\hat{x}, \hat{p}^n]$, $[\hat{p}, \hat{x}^n]$.

b) Recall the familiar identity

$$e^a\, e^b = e^{a+b}$$

Let $\hat{A}$ and $\hat{B}$ be two operators which do not necessarily commute. *Then a similar identity as given above does not hold*. A more general identity is of the form

$$e^{\hat{A}}\, e^{\hat{B}} = e^{\hat{A}+\hat{B}+F_2+F_3+\cdots}$$

where $F_2$ is quadratic in $\hat{A}$, $\hat{B}$, $F_3$ is cubic and so on. Expanding both sides to quadratic order and comparing, calculate $F_2$.

**Solution**

Define

$$A(n) = [\hat{x}, \hat{p}^n]$$

Writing $\hat{p}^n = \hat{p}\,\hat{p}^{n-1}$ and using $[A, BC] = [A, B]C + B[A, C]$,

$$A(n) = [\hat{x}, \hat{p}]\hat{p}^{n-1} + \hat{p}A(n-1) = i\hbar\,\hat{p}^{n-1} + \hat{p}A(n-1) \tag{1}$$

The same equation, with $n$ replaced by $n-1$ gives

$$A(n-1) = i\hbar\,\hat{p}^{n-2} + \hat{p}A(n-2)$$

Thus we can write (1) as

$$A(n) = 2i\hbar\,\hat{p}^{n-1} + \hat{p}^2 A(n-2)$$

Iterating

$$A(n) = ki\hbar\,\hat{p}^{n-1} + \hat{p}^k A(n-k)$$

Taking $k = n$ and using $A(0) = 0$, we find

$$A(n) = [\hat{x}, \hat{p}^n] = i\hbar\,n\,\hat{p}^{n-1}$$

The same kind of argument leads to

$$[\hat{p}, \hat{x}^n] = -i\hbar\,n\,\hat{x}^{n-1}$$

b) We expand the left hand side to quadratic order to get

$$\begin{aligned} e^{\hat{A}}\,e^{\hat{B}} &\approx \left(1 + \hat{A} + \frac{1}{2!}\hat{A}^2 + \cdots\right)\left(1 + \hat{B} + \frac{1}{2!}\hat{B}^2 + \cdots\right) \\ &\approx 1 + \hat{A} + \hat{B} + \hat{A}\hat{B} + \frac{1}{2!}\hat{A}^2 + \frac{1}{2!}\hat{B}^2 + \cdots \end{aligned} \tag{2}$$

Expanding the right hand side to the same order

$$\begin{aligned} e^{\hat{A}+\hat{B}+F_2+F_3+\cdots} &\approx 1 + \hat{A} + \hat{B} + F_2 + \frac{1}{2!}(\hat{A} + \hat{B})^2 + \cdots \\ &\approx 1 + \hat{A} + \hat{B} + F_2 + \frac{1}{2!}\hat{A}^2 + \frac{1}{2!}\hat{B}^2 + \frac{1}{2}(\hat{A}\hat{B} + \hat{B}\hat{A}) + \cdots \end{aligned} \tag{3}$$

Comparing (2) and (3), we get

$$F_2 = \frac{1}{2}[\hat{A}, \hat{B}]$$

Thus

$$e^{\hat{A}}\,e^{\hat{B}} = e^{\hat{A}+\hat{B}+\frac{1}{2}[\hat{A},\hat{B}]+\cdots}$$