PHY V2500: QUANTUM MECHANICS I

Problem Set 1

Due September 11, 2025

Problem 1

In class I calculated the elements $X_{nn'}$. In a similar way, we define

$$P_{nn'} = \int_0^L dx\, v_n(x) \left(-i\hbar \frac{\partial}{\partial x}\right) v_{n'}(x)$$

where

$$v_n(x) = \sqrt{\frac{2}{L}} \sin\bigl(n\pi x/L\bigr), \qquad x \in [0, L]$$

Carry out the integration to obtain $P_{nn'}$. Also show that $P^*_{nn'} = P_{n'n}$.

Solution

Carrying out the indicated differentiation,

$$\begin{aligned} P_{nn'} &= (-i\hbar)\frac{2}{L}\frac{n'\pi}{L}\int_0^L dx\, \sin\bigl(n\pi x/L\bigr)\cos\bigl(n'\pi x/L\bigr) \\ &= (-i\hbar)\frac{n'\pi}{L^2}\int_0^L \Bigl[\sin\bigl((n+n')\pi x/L\bigr) + \sin\bigl((n-n')\pi x/L\bigr)\Bigr] \\ &= (-i\hbar)\frac{n'\pi}{L^2}\frac{L}{\pi}\left[-\frac{\cos\bigl((n+n')\pi x/L\bigr)}{n+n'} - \frac{\cos\bigl((n-n')\pi x/L\bigr)}{n-n'}\right]_0^L \\ &= -i\frac{2\hbar}{L}\frac{nn'}{n^2-n'^2}\Bigl[1-(-1)^{n+n'}\Bigr] \end{aligned}$$

This result applies for $n \neq n'$. For $n = n'$, we have

$$P_{nn} = (-i\hbar)\frac{n'\pi}{L^2}\int_0^L \sin\bigl(2\pi nx/L\bigr) = (-i\hbar)\frac{n'\pi}{L^2}\frac{L}{2\pi n}\Bigl[-\cos(2\pi nx/L)\Bigr]_0^L = 0$$

Taking the complex conjugate of $P_{nn'}$, we see

$$P^*_{nn'} = i\frac{2\hbar}{L}\frac{nn'}{n^2-n'^2}\Bigl[1-(-1)^{n+n'}\Bigr] = -i\frac{2\hbar}{L}\frac{nn'}{n'^2-n^2}\Bigl[1-(-1)^{n+n'}\Bigr] = P_{n'n}$$

Problem 2

Consider the function

$$\psi(x) = \mathcal{C}\, x\, \sin(\pi x/L)$$

which is defined on the interval $[0, L]$.

a) Identify the value of $\mathcal{C}$ such that ψ is normalized, i.e., such that

$$\int_0^L dx\, \psi^*\psi = 1$$

b) The function ψ is square-integrable over the interval $[0, L]$ and vanishes at $x = 0, L$. So it can be expanded in terms of the basis $\{v_n(x)\}$ given in Problem 1 as

$$\psi(x) = \sum_n c_n \, v_n(x)$$

Calculate the coefficients c_n.

<u>**Solution**</u>

a) $\mathcal{C}$ is determined by

$$1 = |\mathcal{C}|^2 \int_0^L dx \, x^2 \, \sin^2(\pi x/L) = \frac{|\mathcal{C}|^2}{2} \int_0^L dx \, x^2 \, \left(1 - \cos(2\pi x/L)\right)$$

We note that

$$\frac{\partial}{\partial x}\left[\frac{x^3}{3} - \left(\frac{x^2 \sin \alpha x}{\alpha} + \frac{2x \cos \alpha x}{\alpha^2} - \frac{2 \sin \alpha x}{\alpha^3}\right)\right] = x^2 - x^2 \cos \alpha x$$

Taking $\alpha = 2\pi/L$, we find

$$\begin{aligned} 1 &= \frac{|\mathcal{C}|^2}{2}\left[\frac{x^3}{3} - \left(\frac{x^2 \sin \alpha x}{\alpha} + \frac{2x \cos \alpha x}{\alpha^2} - \frac{2 \sin \alpha x}{\alpha^3}\right)\right]_0^L \\ &= \frac{|\mathcal{C}|^2}{2} L^3 \left(\frac{1}{3} - \frac{1}{2\pi^2}\right) \end{aligned}$$

This identifies $\mathcal{C}$ as

$$\mathcal{C} = \frac{1}{L^{\frac{3}{2}}}\left(\frac{1}{6} - \frac{1}{4\pi^2}\right)^{-\frac{1}{2}}$$

b) From the orthonormality of v_n, we have

$$c_n = \int_0^L dx \, v_n(x)\psi(x) = \sqrt{\frac{2}{L}}\mathcal{C} \int_0^L dx \, x \, \sin(n\pi x/L) \sin(\pi x/L)$$

We can now write

$$\sin(n\pi x/L) \sin(\pi x/L) = \frac{1}{2}\left[\cos\big((n-1)\pi x/L\big) - \cos\big((n+1)\pi x/L\big)\right]$$

We then note that

$$\frac{\partial}{\partial x}\left[\frac{x \sin \alpha x}{\alpha} + \frac{\cos \alpha x}{\alpha^2}\right] = x \cos \alpha x$$

Using these two results, we find

$$\begin{aligned} c_n &= \frac{\mathcal{C}}{\sqrt{2L}}\Big[\frac{L}{\pi}\frac{x \sin((n-1)\pi x/L)}{n-1} + \frac{L^2}{\pi^2}\frac{\cos((n-1)\pi x/L)}{(n-1)^2} \\ &\quad - \frac{L}{\pi}\frac{x \sin((n+1)\pi x/L)}{n+1} + \frac{L^2}{\pi^2}\frac{\cos((n+1)\pi x/L)}{(n+1)^2}\Big]_0^L \\ &= \frac{\mathcal{C}L^2}{\sqrt{2L}}\left(1 - (-1)^{n+1}\right)\left[\frac{1}{(n+1)^2} - \frac{1}{(n-1)^2}\right] \end{aligned}$$

This applies for $n \neq 1$. For $n = 1$, we have, with $\alpha = 2\pi/L$,

$$\begin{aligned} c_1 &= \sqrt{\frac{2}{L}}\frac{\mathcal{C}}{2}\int dx\, x\,(1-\cos(2\pi x/L)) = \sqrt{\frac{2}{L}}\frac{\mathcal{C}}{2}\left[\frac{x^2}{2} - \left(\frac{x\sin\alpha x}{\alpha} + \frac{\cos\alpha x}{\alpha^2}\right)\right]_0^L \\ &= \mathcal{C}\sqrt{\frac{1}{8L}} \end{aligned}$$

Problem 3

Consider a Hilbert space and a basis of vectors $\{|e_i\rangle\}$, $i = 1, 2, 3, \cdots$. Unlike what we did in class, we will not assume that these are orthonormal. Thus

$$\langle e_i|e_j\rangle = g_{ij}$$

where g_{ij} is not δ_{ij}, but can be taken to be invertible.

a) Show that the matrix $\mathbf{g}$ (with matrix elements g_{ij}) is hermitian.

b) Expand an arbitrary vector in terms of this basis as

$$|a\rangle = \sum_i a_i\,|e_i\rangle$$

Calculate the coefficients a_i in terms of the inner product $\langle e_i|a\rangle$.

c) Using the solution for part b), obtain the completeness relation for the basis $\{|e_i\rangle\}$.

Solution

a) From the properties of the Hilbert space discussed in class,

$$\langle a|b\rangle = \langle b|a\rangle^*$$

Thus

$$g_{ij} = \langle e_i|e_j\rangle = \langle e_j|e_i\rangle^* = g^*_{ji} = (g^T*)_{ij} = (g^\dagger)_{ij}$$

Thus we have $\mathbf{g}^\dagger = \mathbf{g}$, showing that $\mathbf{g}$ is hermitian.

b) Taking the inner product of $|a\rangle$ with $\langle e_j|$, we get

$$\langle e_j|a\rangle = \sum_i a_i\,\langle e_j|e_i\rangle = \sum_i g_{ji}a_i$$

Multiplying by $(g^{-1})_{kj}$ and summing over j, we find

$$\sum_j (g^{-1})_{kj}\,\langle e_j|a\rangle = \sum_{j,i}(g^{-1})_{kj}g_{ji}a_i = \sum_i \delta_{ki}a_i = a_k$$

Thus $a_k = \sum_j (g^{-1})_{kj}\,\langle e_j|a\rangle$, or $a_i = \sum_j (g^{-1})_{ij}\,\langle e_j|a\rangle$. Using this in the expansion for $|a\rangle$,

$$|a\rangle = \sum_i |e_i\rangle \sum_j (g^{-1})_{ij}\,\langle e_j|a\rangle = \left(\sum_{i,j} |e_i\rangle\,(g^{-1})_{ij}\,\langle e_j|\right)|a\rangle$$

Since this applies for any $|a\rangle$, we get the relation

$$\sum_{i,j} |e_i\rangle\, (g^{-1})_{ij}\, \langle e_j| = \mathbb{1}$$

This is the completeness relation when we do not have orthonormality.

Problem 4

We have considered the basis $\{v_n\}$ as in Problem 1. Now consider a different set of functions defined on the interval $[0, L]$ as

$$u_n(x) = \sqrt{\frac{2}{L}} \cos\bigl(n\pi x/L\bigr), \qquad n = 1, 2, \cdots .$$

These functions do not vanish at the boundaries. Rather they obey $u_n'(x) = 0$ at $x = 0, L$. (These are what are called Neumann boundary conditions.) Carry out the needed integration to identify the integral

$$\int_0^L dx\, u_n(x)\, u_{n'}(x)$$

Solution

We write the integral as

$$\begin{aligned}
\int_0^L dx\, u_n(x)\, u_{n'}(x) &= \frac{2}{L}\int_0^L dx\ \cos(n\pi x/L)\ \cos(n'\pi x/L) \\
&= \frac{1}{L}\int_0^L dx\, \Bigl[\cos[(n+n')\pi x/L] + \cos[(n-n')\pi x/L]\Bigr] \\
&= \frac{1}{L}\frac{L}{\pi}\left[\frac{\sin[(n+n')\pi x/L]}{n+n'} + \frac{\sin[(n-n')\pi x/L]}{n-n'}\right]_0^L = 0
\end{aligned}$$

This applies for $n \neq n'$. For $n = n'$, we get

$$\int_0^L dx\, u_n(x)\, u_{n'}(x) = \frac{1}{L}\int_0^L dx\, \Bigl[\cos[2\pi n x/L] + 1\Bigr] = 1$$

Combining these two results we have

$$\int_0^L dx\, u_n(x)\, u_{n'}(x) = \delta_{nn'}$$