CAM 389C Exercise Set II.2

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Problem i

Reproduce the proof of

$$\langle p \rangle = m\frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t} = \int_{-\infty}^{\infty} \Psi^* p \Psi \,\mathrm{d}x\,.$$

We can evaluate

$$\begin{aligned}
\frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}} x(\Psi^*\Psi)\,\mathrm{d}x \\
&= \int_{\mathbb{R}} x\frac{\partial}{\partial t}(\Psi^*\Psi)\,\mathrm{d}x \\
&= \frac{i\hbar}{2m}\int_{\mathbb{R}} x\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\,\mathrm{d}x \\
&= \frac{i\hbar}{2m}x\left(\cancel{\Psi^*}\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\cancel{\Psi}\right)\Bigg|_{-\infty}^{\infty} - \frac{i\hbar}{2m}\int_{\mathbb{R}}\left(\Psi^*\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\,\mathrm{d}x \\
&= -\frac{i\hbar}{2m}\int_{\mathbb{R}}\Psi^*\frac{\partial \Psi}{\partial x}\,\mathrm{d}x + \frac{i\hbar}{2m}\underbrace{\int_{\mathbb{R}}\frac{\partial \Psi^*}{\partial x}\Psi\,\mathrm{d}x}_{\cancel{\Psi\Psi^*}\big|_{-\infty}^{\infty} - \int_{\mathbb{R}}\Psi^*\frac{\partial \Psi}{\partial x}\,\mathrm{d}x} \\
&= -\frac{i\hbar}{m}\int_{\mathbb{R}}\Psi^*\frac{\partial \Psi}{\partial x}\,\mathrm{d}x \\
&= \frac{1}{m}\int_{\mathbb{R}}\Psi^*\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi\,\mathrm{d}x \\
&= \frac{1}{m}\int_{\mathbb{R}}\Psi^* p\Psi\,\mathrm{d}x \\
&= \frac{\langle p \rangle}{m}\,.
\end{aligned}$$

Therefore

$$\langle p \rangle = m\frac{\mathrm{d}\langle x \rangle}{\mathrm{d}t} = \int_{-\infty}^{\infty} \Psi^* p \Psi \,\mathrm{d}x\,.$$

Problem ii

Reproduce the proof of

$$\frac{\mathrm{d}\langle p\rangle}{\mathrm{d}t} = \langle F\rangle.$$

Taking the time derivative of $\langle p\rangle$,

$$\begin{aligned}
\frac{\mathrm{d}\langle p\rangle}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}} (\Psi^* p \Psi)\,\mathrm{d}x \\
&= \int_{\mathbb{R}} \underbrace{\frac{\partial \Psi^*}{\partial t}}_{-\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} - \frac{i}{\hbar}V\Psi^*} p\Psi\,\mathrm{d}x + \int_{\mathbb{R}} \Psi^* p \underbrace{\frac{\partial \Psi}{\partial t}}_{\frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} + \frac{i}{\hbar}V\Psi} \mathrm{d}x \\
&= -\frac{1}{i\hbar}\int_{\mathbb{R}} \left(-\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*}{\partial x^2} - V\Psi^*\right) p\Psi + \Psi^* p \left(\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi\right)\mathrm{d}x \\
&= -\frac{1}{i\hbar}\int_{\mathbb{R}} (H-2V)\Psi^* p\Psi - \Psi^* p(H-2V)\Psi\,\mathrm{d}x \\
&= -\frac{1}{i\hbar}\int_{\mathbb{R}} \Psi^*(H-\cancel{2V})p\Psi - \Psi^* p(H-\cancel{2V})\Psi\,\mathrm{d}x && H \text{ is Hermitian} \\
&= -\frac{1}{i\hbar}\int_{\mathbb{R}} \Psi^* H p\Psi - \Psi^* pH\Psi\,\mathrm{d}x \\
&= -\frac{1}{i\hbar}\int_{\mathbb{R}} \Psi^* \underbrace{(\underbrace{Hp}_{-\frac{\hbar^2}{2m}\frac{\partial^3}{\partial x^3} + V\frac{\hbar}{i}\frac{\partial}{\partial x}} - \underbrace{pH}_{-\frac{\hbar^2}{2m}\frac{\partial^3}{\partial x^3} + \frac{\hbar}{i}\frac{\partial}{\partial x}V})}_{V\frac{\hbar}{i}\frac{\partial}{\partial x} - \frac{\hbar}{i}\frac{\partial}{\partial x}V} \Psi\,\mathrm{d}x \\
&= \int_{\mathbb{R}} \Psi^*(\cancel{V\frac{\partial\Psi}{\partial x}} - \underbrace{\frac{\partial}{\partial x}(V\Psi)}_{\cancel{V\frac{\partial\Psi}{\partial x}} + \frac{\partial V}{\partial x}\Psi})\,\mathrm{d}x \\
&= \int_{\mathbb{R}} \Psi^*\left(-\frac{\partial V}{\partial x}\right)\Psi\,\mathrm{d}x \\
&= \left\langle -\frac{\partial V}{\partial x}\right\rangle.
\end{aligned}$$

Problem 1

The proof of

$$\sigma_Q^2\sigma_M^2 \geq \left(\frac{1}{2i}\langle[Q,M]\rangle\right)^2$$

follows from several algebraic steps and the Cauchy-Schwarz inequality. Let

$$u = (\tilde{Q} - \langle Q\rangle)\Psi \quad \text{and} \quad v = (\tilde{M} - \langle M\rangle)\Psi\,.$$

a)

$$\begin{aligned}
\sigma_Q^2 &= \langle Q^2\rangle - \langle Q\rangle^2 \\
&= \underbrace{\langle \Psi, \tilde{Q}(\tilde{Q}\Psi)\rangle}_{\text{Expected value of } Q^2} - \underbrace{\langle \Psi, \langle Q\rangle^2\Psi\rangle}_{\langle Q\rangle^2 \underbrace{\int_{\mathbb{R}} \Psi^*\Psi \,\mathrm{d}x}_{1}} \\
&= \underbrace{\langle \tilde{Q}\Psi, \tilde{Q}\Psi\rangle}_{Q \text{ is Hermitian}} - \langle \langle Q\rangle\Psi, \langle Q\rangle\Psi\rangle \\
&= \int_{\mathbb{R}} (\tilde{Q}\Psi)^*\tilde{Q}\Psi - \langle Q\rangle\Psi^*\langle Q\rangle\Psi \,\mathrm{d}x \\
&= \int_{\mathbb{R}} (\tilde{Q}\Psi)^*\tilde{Q}\Psi - 2\langle Q\rangle \underbrace{\Psi^*\langle Q\rangle\Psi}_{\tilde{Q}} + \langle Q\rangle\Psi^*\langle Q\rangle\Psi \,\mathrm{d}x \\
&= \langle (\tilde{Q} - \langle Q\rangle)\Psi, (\tilde{Q} - \langle Q\rangle)\Psi\rangle \\
&= \langle u, u\rangle \\
&= \|u\|^2\,,
\end{aligned}$$

and similarly $\sigma_M^2 = \|v\|^2$. Thus, by Cauchy-Schwarz,

$$\sigma_Q^2\sigma_M^2 = \|u\|^2\|v\|^2 \geq |\langle u, v\rangle|^2\,.$$

b) Show that

$$\langle u, v\rangle = \langle QM\rangle - \langle Q\rangle\langle M\rangle\,.$$

Note that

$$\begin{aligned}
\langle u, v\rangle &= \langle (\tilde{Q} - \langle Q\rangle)\Psi, (\tilde{M} - \langle M\rangle)\Psi\rangle \\
&= \underbrace{\langle \tilde{Q}\Psi, \tilde{M}\Psi\rangle}_{\text{Hermitian}} - \langle M\rangle \underbrace{\langle \tilde{Q}\Psi, \Psi\rangle}_{\langle Q\rangle} - \langle Q\rangle \underbrace{\langle \Psi, \tilde{M}\Psi\rangle}_{\langle M\rangle} + \langle Q\rangle\langle M\rangle \underbrace{\langle \Psi, \Psi\rangle}_{1} \\
&= \langle \Psi, \tilde{Q}\tilde{M}\Psi\rangle - \langle M\rangle\langle Q\rangle - \cancel{\langle Q\rangle\langle M\rangle} + \cancel{\langle Q\rangle\langle M\rangle} \\
&= \langle QM\rangle - \langle Q\rangle\langle M\rangle\,.
\end{aligned}$$

c) The number $\langle u, v\rangle$ is complex. From the fact that any complex number z satisfies

$$|z|^2 \geq \left(\frac{1}{2i}(z - z^*)\right)^2\,,$$

where z^* is the complex conjugate of z, show that

$$\sigma_Q^2 \sigma_M^2 \geq \left(\frac{1}{2i} (\langle u, v \rangle - \langle v, u \rangle) \right)^2 .$$

From the properties of complex inner products, we know that

$$\langle u, v \rangle = \overline{\langle v, u \rangle} .$$

Therefore,

$$|\langle u, v \rangle|^2 \geq \left(\frac{1}{2i} (\langle u, v \rangle - \langle v, u \rangle) \right)^2 .$$

And from Cauchy-Schwarz we know that

$$\sigma_Q^2 \sigma_M^2 \geq |\langle u, v \rangle|^2 \geq \left(\frac{1}{2i} (\langle u, v \rangle - \langle v, u \rangle) \right)^2 .$$

Therefore,

$$\sigma_Q^2 \sigma_M^2 \geq \left(\frac{1}{2i} (\langle u, v \rangle - \langle v, u \rangle) \right)^2 .$$

d) Now we can show that

$$\begin{aligned}
\sigma_Q^2 \sigma_M^2 &\geq \left(\frac{1}{2i} (\langle u, v \rangle - \langle v, u \rangle) \right)^2 \\
&= \left(\frac{1}{2i} \left((\langle QM \rangle - \langle Q \rangle \langle M \rangle) - (\langle MQ \rangle - \langle M \rangle \langle Q \rangle) \right) \right)^2 \\
&= \left(\frac{1}{2i} (\langle QM \rangle - \cancel{\langle Q \rangle \langle M \rangle} - \langle MQ \rangle + \cancel{\langle M \rangle \langle Q \rangle}) \right)^2 \\
&= \left(\frac{1}{2i} \langle [Q, M] \rangle \right)^2 ,
\end{aligned}$$

where

$$[Q, M] = \tilde{Q}\tilde{M} - \tilde{M}\tilde{Q} .$$

This finishes the proof.

Problem 2

A classical textbook example of the time-independent Schrodinger equation for a single particle moving along the x-axis is the problem of the infinite square well for which the potential V is of the form

$$V(x) = \begin{cases} 0 , & \text{if } 0 \leq x \leq a , \\ \infty , & \text{otherwise} . \end{cases}$$

The particle is confined to this “well” so $\psi(x) = 0$ if $x < 0$ and $x > a$ while $V(x) \equiv 0$ inside the well.

a) Show that Schrodinger’s equation reduces to

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + k^2\psi = 0\,, \quad \psi(0) = \psi(a) = 0\,,$$

with $k^2 = 2mE/\hbar^2$.

The time-independent Schrodinger’s equation is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V\psi = E\psi\,.$$

With infinite potential outside the box, the particle is regulated to $0 \leq x \leq a$. So, within these bounds, with zero potential the time-independent equation becomes

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi\,.$$

Moving everything to one side and dividing by $\hbar^2/2m$,

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + \frac{2mE}{\hbar^2}\psi = 0\,.$$

Let $k^2 = 2mE/\hbar^2$, then

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + k^2\psi = 0\,.$$

b) Show that the possible values of the energy are

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}\,, \quad n = 1, 2, \ldots$$

We know that solutions to this type of ordinary differential equation take the form

$$\psi(x) = A\cos(kx) + B\sin(kx)\,.$$

Our boundary conditions dictate that $\psi = 0$ outside the box, and ψ must be continuous, therefore

$$\psi(0) = A = 0\,,$$

and

$$\psi(a) = B\sin(ka) = 0\,.$$

The solution is trivial if $B = 0$, then we have a non-trivial solution when

$$ka = \frac{\sqrt{2mE}}{\hbar}a = n\pi\,, \quad n = 1, 2, \ldots\,.$$

Therefore, we have a series of solutions for increasing n,

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}\,, \quad n = 1, 2, \ldots\,.$$

c) Show that the wave function is a superposition of solutions,

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) , \quad 0 \le x \le a \,,$$

which are orthonormal in $L^2(0,a)$.
First of all, substituting E into k, please note that

$$k = \frac{n\pi}{a} \,.$$

We wish that $\psi_n(x)$ are orthonormal, then

$$\langle \psi_n(x), \psi_m(x) \rangle = \delta_{mn} \,.$$

But,

$$\langle B \sin(\frac{n\pi}{a} x), B \sin(\frac{m\pi}{a} x) \rangle = \begin{cases} B^2 \frac{a}{2} \,, & n = m \,, \\ 0 \,, & n \neq m \,. \end{cases}$$

In order to normalize this, we need $B = \sqrt{2/a}$. Therefore,

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \,.$$

If any one $\psi_n(x)$ is a solution, then the superposition of solutions is also a solution. Thus the wave function can be written as a sum of $\psi_n(x) \,, \quad n = 1, 2, \dots$.
d) Given that the functions ψ_n form a complete orthonormal basis for $L^2(0,a)$, develop a Fourier series representation of the function $f(x) = x$ as an infinite sum of these functions.
If any one $\psi_n(x)$ satisfies the time-independent Schrodinger equation, then the infinite sum of these will also satisfy it. In general we can write

$$f(x) = \sum_{n=1}^{\infty} b_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) , \quad 0 \le x \le a \,,$$

where

$$b_n = \langle \psi_n, x \rangle = \sqrt{\frac{2}{a}} \int_0^a x \sin\left(\frac{n\pi x}{a}\right) \, \mathrm{d}x \,.$$

which is in fact a Fourier sine series representation for $f(x) = x$.
e) Let

$$Q(x,p)\Psi = \frac{\mathrm{d}^2\Psi(x)}{\mathrm{d}x^2} \,, \quad 0 \le x \le a \,.$$

Is Q observable?
We can substitute for Q in the reduced Schrodinger equation,

$$Q\psi = -\frac{n^2\pi^2}{a^2}\psi \,.$$

Therefore Q has a discrete spectrum of eigenvalues $\{-\frac{n^2\pi^2}{a^2}\}$. It is only left to prove that Q is Hermitian. Integrating by parts twice,

$$\begin{aligned}
\langle \psi, Q\psi \rangle &= \int_{\mathbb{R}} \psi^* \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}\,\mathrm{d}x \\
&= \cancel{\psi^*}\frac{\mathrm{d}\psi}{\mathrm{d}x}\bigg|_0^a - \int_{\mathbb{R}} \frac{\mathrm{d}\psi}{\mathrm{d}x}\frac{\mathrm{d}\psi^*}{\mathrm{d}x}\,\mathrm{d}x \\
&= -\frac{\mathrm{d}\psi^*}{\mathrm{d}x}\cancel{\psi}\bigg|_0^a + \int_{\mathbb{R}} \psi\frac{\mathrm{d}^2\psi^*}{\mathrm{d}x^2}\,\mathrm{d}x \\
&= \langle Q\psi, \psi \rangle\,.
\end{aligned}$$

Therefore Q is Hermitian and has a discrete spectrum of eigenvalues, so Q must be observable.

Problem 3

Consider a quantum system consisting of a single particle in a straight line with position x and momentum p. Define the following operators:

$$\begin{aligned}
A\phi &= x\psi & (A &= x)\,, \\
B\phi &= \partial\phi/\partial x & (B &= \partial/\partial x)\,.
\end{aligned}$$

Do A and B commute?
The commutator of A and B applied to ϕ is

$$\begin{aligned}
[A,B]\phi &= x\frac{\partial}{\partial x}\phi - \frac{\partial}{\partial x}x\phi \\
&= x\frac{\partial}{\partial x}\phi - x\frac{\partial}{\partial x} - \phi \\
&= -\phi \neq 0\,.
\end{aligned}$$

Therefore A and B do not commute.

Problem 4

Let

$$Q = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x^2} \quad \text{and} \quad M = -i\hbar\frac{\partial}{\partial x}\,.$$

a) Show that these operators commute.
The commutator of Q and M applied to ϕ is

$$\begin{aligned}
[Q,M]\phi &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(-i\hbar\frac{\partial}{\partial x}\right)\phi - \left(-i\hbar\frac{\partial}{\partial x}\right)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\phi \\
&= \frac{i\hbar^3}{2m}\frac{\partial^3}{\partial x^3}\phi - \frac{i\hbar^3}{2m}\frac{\partial^3}{\partial x^3}\phi = 0
\end{aligned}$$

b) Show that e^{ikx} is a simultaneous eigenfunction of these operators and, indeed, $p^2/2m = E$.
To show that e^{ikx} is a simultaneous eigenfunction of Q and M, we need

$$Q\mathrm{e}^{ikx} = \lambda_Q \mathrm{e}^{ikx}\,,$$

and

$$M\mathrm{e}^{ikx} = \lambda_M \mathrm{e}^{ikx}\,.$$

Then,

$$Q\mathrm{e}^{ikx} = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x^2}\mathrm{e}^{ikx} = \underbrace{\frac{\hbar^2 k}{2m}}_{\lambda_Q}\mathrm{e}^{ikx}\,.$$

Similarly for M,

$$M\mathrm{e}^{ikx} = -i\hbar\frac{\partial}{\partial x}\mathrm{e}^{ikx} = \underbrace{\frac{\hbar^2 k}{2m}}_{\lambda_M}\mathrm{e}^{ikx}\,.$$

Therefore e^{ikx} is a simultaneous eigenfunction for Q and M.
If we assume the absence of a potential, the Hamiltonian becomes $H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}$, and the Schrodinger equation reads

$$H\Psi = E\Psi\,.$$

Then

$$\frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} = H = E\,.$$