Quantum Mechanics Assignment 2

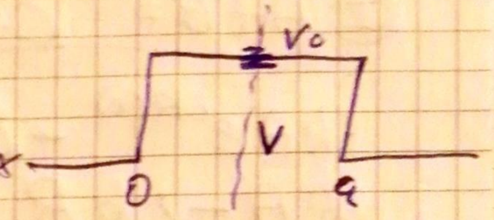
Q1 (a) $KE = \frac{1}{2m}p^2 = \frac{1}{2}V_0$

$$V(x) = \begin{cases} 0, & x \leq 0 \\ V_0, & 0 \leq x \leq a \\ 0, & x > a \end{cases}$$

$\boxed{E < V_0}$

$\cancel{E = \frac{1}{2m}p^2}$ $\quad E = \frac{1}{2}V_0$

① $x \leq 0$



$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi = E\psi$$

$V(x) = 0, \quad x \leq 0$

$$-\frac{\hbar^2}{2m}\psi'' = E\psi$$

$$\psi'' = -k^2\psi$$

$$\boxed{k = \frac{\sqrt{2mE}}{\hbar} = \frac{\sqrt{mV_0}}{\hbar}}$$

$$\psi = A\cos(kx) + B\sin(kx)$$
$$= Ae^{ikx} + Be^{-ikx}$$

② $0 < x \leq a$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi = E\psi$$

$V(x) = V_0, \quad 0 \leq x \leq a$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi = (E - V(x))\psi$$

$$\frac{\hbar^2}{2m}\psi'' = (V(x) - E)\psi$$

$$\psi'' = K^2\psi$$

$$K = \frac{\sqrt{(V(x) - E)2m}}{\hbar} = \frac{\sqrt{2m(V_0 - E)}}{\hbar} = \sqrt{\frac{mV_0}{\hbar}}$$

$$\psi = Ce^{Kx} + De^{-Kx}$$

③ $x > a$ → since wave is only coming from $+x$ direction

$$\psi(x) = Fe^{ikx}$$

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & , x \le 0 \\ Ce^{Kx} + De^{-Kx} & , 0 \le x < a \\ Fe^{ikx} & , x > a \end{cases}$$

$$k = \frac{\sqrt{mV_0}}{\hbar}$$

$$K = \frac{\sqrt{mV_0}}{\hbar}$$

$K = k$

denote k by K

ψ, ψ' continuous at $x = 0$

$$Ae^{ik(0)} + Be^{-ik(0)} = Ce^{K(0)} + De^{-K(0)}$$

$$\text{I} \quad \boxed{A + B = C + D}$$

$$ikAe^{ik(0)} - ikBe^{-ik(0)} = KCe^{K(0)} - KDe^{-K(0)}$$

$$ikA - ikB = KC - KD$$

$$\text{II} \quad ik(A - B) = K(C - D) \rightarrow \boxed{i(A - B) = C - D}$$

ψ, ψ' continuous at $x = a$

$$\text{III} \quad Ce^{Ka} + De^{-Ka} = Fe^{ika}$$

$$\text{IV} \quad CKe^{Ka} - DKe^{-Ka} = ikFe^{ika}$$

$$\boxed{Ce^{Ka} - De^{-Ka} = iFe^{ika}}$$

Using II: $ik(A-B) = K(C-D)$.

$$ikA - ikB = K(C - D)$$

$$ikB = ikA + K(D - C)$$

$$B = A + \frac{K}{ik}(D - C)$$

$k = K$ $\quad B = A - \frac{iK}{k}(D - C) \rightarrow B = A + i(C - D)$

$$A = B + i(D - C)$$

$$C = 1/K(KD + ik(A - B)) \rightarrow C = D + i(A - B)$$

$$D = C + i(B - A)$$

$$F = (Ce^{Ka} + De^{-Ka}) \cdot e^{-ika}$$

(F is transmitted wave)

$$i(A-B) = C-D$$

$$\boxed{B-A = i(C-D)}$$

$$B = i(C-D) + A$$

$$A+B = C+D \quad + \quad B-A = i(C-D)$$

$$2B = i(C-D) + C+D$$

$$C = Fe^{ika-ka} - De^{-2ka}$$

$$D = Fe^{ika+ka} - Ce^{2ka}$$

$$2B = i\left(Fe^{ika-ka} - Fe^{ika+ka} - De^{-2ka} + Ce^{2ka}\right)$$
$$+ Fe^{ika-ka} + Fe^{ika+ka} - De^{-2ka} - Ce^{2ka}$$

(B is reflected wave)

$$B = \frac{i}{2}\left(Fe^{ika-ka} - Fe^{ika+ka} - De^{-2ka} + Ce^{2ka}\right)$$
$$+ \frac{1}{2}\left[Fe^{ika-ka} + Fe^{ika+ka} - De^{-2ka} - Ce^{2ka}\right]$$

(b) $T = \left|\frac{F}{A}\right|^2$

$$F = (Ce^{ka} - De^{-ka})e^{-ika}$$
$$F = i(De^{-ka} - Ce^{ka})e^{-ika}$$

$$A = B + i(D - C)$$

$$D - C = Fe^{ika+ka} - Fe^{ika-ka} - Ce^{2ka} + De^{-2ka}$$

$$A = \frac{i}{2}\left[Fe^{ika-ka} - Fe^{ika+ka} - De^{-2ka} + Ce^{2ka}\right]$$
$$+ \frac{1}{2}\left[Fe^{ika-ka} + Fe^{ika+ka} - De^{-2ka} - Ce^{2ka}\right]$$

$$A = \frac{i}{2}\left[-Fe^{ika-ka} + Fe^{ika+ka} + De^{-2ka} - Ce^{2ka}\right]$$
$$+ \frac{1}{2}\left[Fe^{ika-ka} + Fe^{ika+ka} - De^{-2ka} - Ce^{2ka}\right]$$

$$A = \frac{1}{2}\left[-iFe^{ika-ka} + iFe^{ika+ka} + Fe^{ika-ka}\right.$$
$$\left. + Fe^{ika+ka} + iDe^{-2ka} - De^{-2ka} - iCe^{2ka} - Ce^{2ka}\right]$$

$$A = \frac{1}{2}\left[-iFe^{ika-ka} + iFe^{ika+ka} + Fe^{ika-ka} + Fe^{ika+ka}\right.$$
$$\left. + (-1-i)Ce^{2ak} - (1-i)De^{-2ak}\right]$$

Want to show $\left|\frac{F}{A}\right|^2$ is equal to $\cosh^{-2}(ka)$

Quantum Mechanics

Q2. Use Gram-Schmidt Process to find a basis of real polynomials $e_n(x)$ of degree n $(n=0,1,2,3)$ which are mutually orthonormal with respect to inner product:

$$\langle f,g\rangle = \int_{-1}^{1} f(x)\,g(x)\,dx$$

$$\underline{e}_0 = 1,\quad \underline{e}_1 = x,\quad \underline{e}_2 = x^2,\quad \underline{e}_3 = x^3$$

$$\|e_0\|^2 = \langle e_1, e_1\rangle = \int_{-1}^{1} 1^2\,dx = [x]_{-1}^{1} = 2$$

$$e_0' = \frac{1}{\|e_0\|} = \frac{1}{\sqrt{2}}$$

$$e_1' = \underline{e}_1 - \langle \underline{e}_0', \underline{e}_1\rangle \underline{e}_0' \cdot \frac{1}{\|e_1\|} \neq 0$$

$$\langle \underline{e}_0', \underline{e}_1\rangle = \int_{-1}^{1} \tfrac{1}{\sqrt{2}} x = \tfrac{1}{\sqrt{2}} \tfrac{x^2}{2}\Big|_{-1}^{1} = 0$$

$$\|e_1\|^2 = \langle e_1, e_1\rangle = \int_{-1}^{1} x^2 = \frac{x^3}{3}\Big|_{-1}^{1} = \frac{2}{3}$$

$$\underline{e}_1' = \frac{x}{\sqrt{2/3}} = \sqrt{3/2}\,x$$

then we have $\underline{e}_2 - \langle \underline{e}_0', \underline{e}_2\rangle \underline{e}_0' - \langle \underline{e}_1', \underline{e}_2\rangle e_1' \neq 0$

$$x^2 - \langle 1/\sqrt{2}, x^2\rangle 1/\sqrt{2} - \langle \sqrt{3/2}\,x, x^2\rangle \sqrt{3/2}\,x^2$$

$$\langle 1/\sqrt{2}, x^2\rangle = \int_{-1}^{1} \tfrac{1}{\sqrt{2}} x^2\,dx = \tfrac{1}{\sqrt{2}} \tfrac{x^3}{3}\Big|_{-1}^{1} = \frac{2}{\sqrt{2}\,3}$$

$$\langle \sqrt{3/2}\,x, x^2\rangle = \int_{-1}^{1} \sqrt{3/2}\,x^3\,dx = \sqrt{3/2}\,\frac{x^4}{4}\Big|_{-1}^{1} = 0$$

$$x^2 - \left(\tfrac{2}{3}\cdot \tfrac{1}{\sqrt{2}} \cdot \tfrac{1}{\sqrt{2}}\right) = x^2 - 1/3 - 0$$
$$= 1/3\,(3x^2 - 1)$$

normalise → can remove multiplicative constant $1/3$

$$\|3x^2-1\|^2 = \int_{-1}^{1} (3x^2-1)^2 dx = \int_{-1}^{1} 9x^4 - 6x^2 + 1\, dx$$

$$= \frac{9x^5}{5} - 2x^3 + x \Big|_{-1}^{1} = \left[\frac{2\cdot 9}{5} - 4 + 2\right]$$

$$= 8/5 \rightarrow \|3x^2-1\| = \sqrt{8/5}$$

$$\underline{e}_2' = \sqrt{5/8}\,(3x^2-1) = \sqrt{5/2}\cdot \tfrac{1}{2}(3x^2-1)$$

$$= \sqrt{5/2}\left(\tfrac{3}{2}x^2 - \tfrac{1}{2}\right)$$

$$\underline{e}_3' \rightarrow \underline{e}_3 - \langle \underline{e}_0', \underline{e}_3\rangle \underline{e}_0' - \langle \underline{e}_1', \underline{e}_3\rangle \underline{e}_1' - \langle \underline{e}_2', \underline{e}_3\rangle \underline{e}_2'$$

$$x^3 - \langle 1/\sqrt{2}, x^3\rangle \frac{1}{\sqrt{2}} - \langle \sqrt{3/2}\,x, x^3\rangle \sqrt{3/2}\,x - \langle \sqrt{5/8}(3x^2-1), x^3\rangle \cdot \sqrt{5/8}(3x^2-1)$$

$$\langle 1/\sqrt{2}, x^3\rangle = \int_{-1}^{1} 1/\sqrt{2}\, x^3 dx = \frac{1}{\sqrt{2}} \frac{x^4}{4}\Big|_{-1}^{1} = 0$$

$$\langle \sqrt{3/2}\,x, x^3\rangle = \int_{-1}^{1} \sqrt{3/2}\, x^4 dx = \sqrt{3/2}\, \frac{x^5}{5}\Big|_{-1}^{1} = \sqrt{3/2}\cdot 2/5$$

$$\langle \sqrt{5/8}(3x^2-1), x^3\rangle = \int_{-1}^{1} \sqrt{5/8}(3x^2-1)x^3 dx = \int_{-1}^{1} \sqrt{5/8}(3x^5 - x^3)dx$$

$$= \left[\sqrt{5/8}\left(1/2\, x^6 - \frac{x^4}{4}\right)\right]_{-1}^{1} = 0$$

$$x^3 - \sqrt{3/2}\,x \cdot \sqrt{3/2}\cdot 2/5 = x^3 - 3/5\, x$$

$$\|x^3 - 3/5\, x\|^2 = \int_{-1}^{1} (x^3 - 3/5\, x)^2 dx = \int_{-1}^{1} x^6 - 6/5\, x^4 + \frac{9}{25}x^2 dx$$

$$= \left[\frac{x^7}{7} - \frac{6}{5}\cdot\frac{x^5}{5} + 9/25\,\frac{x^3}{3}\right]_{-1}^{1} = \frac{4}{175} - \left[-\frac{4}{175}\right] = \frac{8}{175}$$

$$\|x^3 - 3/5\, x\| = \sqrt{\frac{8}{175}} = \frac{2\sqrt{14}}{35}$$

$$\underline{e}_3' = \sqrt{\frac{175}{8}}\,(x^3 - 3/5\, x) = \frac{5\sqrt{14}}{4}(x^3 - 3/5\, x)$$

$$\underline{e}_3' = \sqrt{14}\left(5/4\, x^3 - 3/4\, x\right)$$

Q3 (a) Show $[AB, C] = A[B, C] + [A, C]B$ for general operators A, B and C

RHS $\rightarrow$ $[AB, C] = ABC - CAB$

LHS $\rightarrow$ $A[B, C] = A(BC - CB)$

$[A, C]B = (AC - CA)B$

$A[B, C] + [A, C]B = ABC - ACB + ACB - CAB$

$= ABC - CAB$

LHS $A[B, C] + [A, C]B = ABC - CAB$

RHS $[AB, C] = ABC - CAB$

So therefore $[AB, C] = A[B, C] + [A, C]B$

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

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

$[x^{n-1}, \hat{p}]f = x^{n-1} \cdot -i\hbar \partial/\partial x f + i\hbar \partial/\partial x \, x^{n-1} f$

$= -x^{n-1} \cdot i\hbar \partial f/\partial x + i\hbar(x^{n-1} \partial f/\partial x + f(n-1)x^{n-2})$

$[x^{n-1}, \hat{p}]f = i\hbar(n-1)x^{n-2} f$ ~~$[x^{n-1}, \hat{p}] = i\hbar$~~

$\rightarrow [x^{n-1}, \hat{p}] = i\hbar(n-1)x^{n-2}$

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

$[x, \hat{p}]f = x\hat{p}f - \hat{p}xf = -xi\hbar \partial f/\partial x + i\hbar \partial/\partial x(xf)$

$= -xi\hbar \partial f/\partial x + xi\hbar \partial f/\partial x + fi\hbar$

$[x, \hat{p}]f = fi\hbar \rightarrow [x, \hat{p}] = i\hbar$

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

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

$= i\hbar n x^{n-1} + i\hbar x^{n-1} - i\hbar x^{n-1}$

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

Q3(c) $[x, p^n] = x p^n - p^n x$

$$[x, p^n] f = x p^n f - p^n x f$$

$$= x(-i\hbar)^n \frac{\partial^n}{\partial x^n} f - (-i\hbar)^n \frac{\partial^n}{\partial x^n}(x f)$$

$$= x(-i\hbar)^n \frac{\partial^n f}{\partial x^n} - (-i\hbar)^n \left(\left(\frac{\partial^n}{\partial x^n} x\right) \cdot f + x \cdot \frac{\partial^n f}{\partial x^n} \right)$$

$$= \cancel{x(-i\hbar)^n \frac{\partial^n f}{\partial x^n} - x(-i\hbar)^n \frac{\partial^n f}{\partial x^n}} - f(-i\hbar)^n \frac{\partial^n x}{\partial x^n}$$

$$= -f(-i\hbar)^n \frac{\partial^n x}{\partial x^n} = [x, \hat{p}^n] f$$

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

$$= -i\hbar(-i\hbar)^{n-1} \frac{\partial^{n-1}}{\partial x^{n-1}}$$

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

QM

Q4 (a) Show for Hermitian Operators $\hat{A}$ and $\hat{B}$ that $\langle[\hat{A},\hat{B}]\rangle$ is purely imaginary

We know $\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right)^2$

$$\langle[\hat{A},\hat{B}]\rangle = \int_{-\infty}^{\infty}\Psi^*[\hat{A},\hat{B}]\Psi\,dx$$

$$= \int_{-\infty}^{\infty}\Psi^*(\hat{A}\hat{B}-\hat{B}\hat{A})\Psi\,dx$$

We know $\hat{A}$ and $\hat{B}$ are Hermitian (Self-adjoint)

$\hat{A}^* = \hat{A}$ $\quad\hat{B}^* = \hat{B}$

$\hat{A}^\dagger = \hat{A}$ $\quad\hat{B}^\dagger = \hat{B}$

$$[A,B]^\dagger = (AB-BA)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger$$

Since A & B Hermitian $\Rightarrow$ $[A,B]^\dagger = BA - AB = -[A,B]$

$$\int\Psi^*(\hat{Q}\Psi)dx = \int(\hat{Q}^\dagger\Psi)^*\Psi\,dx$$

for an operator $\hat{Q}$

So we have

$$\int_{-\infty}^{\infty}\Psi^*[\hat{A},\hat{B}]\Psi\,dx = \int_{-\infty}^{\infty}(-[A,B]\Psi)^*\Psi\,dx$$

$$= \int_{-\infty}^{\infty}-[A,B]^*\Psi^*\Psi\,dx$$

So $\langle[\hat{A},\hat{B}]\rangle = \langle-[\hat{A},\hat{B}]^*\rangle$ $\boxed{\text{if \& only if } \hat{A} \text{ and } \hat{B} \text{ are imaginary}}$ is this possible

$\langle[\hat{A},\hat{B}]\rangle = \langle[\hat{B},\hat{A}]^*\rangle = \langle[\hat{A},\hat{B}]\rangle$

(Minus sign cancels with complex conjugation $\Leftrightarrow$ A & B purely imaginary) $\boxed{\text{Since } [\hat{A},\hat{B}] \text{ is anti-hermitian, the expectation value of } [A,B] \text{ must be imaginary}}$

Q4 (b) Show for Hamiltonian $\hat{H} = \frac{1}{2m}\hat{p}^2 + V(x)$

that $\sigma_x \sigma_{\hat{H}} \geq \frac{\hbar}{2m} |\langle \hat{p} \rangle|$

Using $\sigma_A^2 \sigma_B^2 \geq \left[\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right]^2$

where $A = x$ and $B = \hat{H}$

find $[x, \hat{H}]$

$$[\hat{x}, \hat{H}] = \hat{x}\hat{H} - \hat{H}\hat{x}$$

$$[x, \hat{H}]\psi = x\hat{H}\psi - \hat{H}x\psi$$

$$= x\left(\tfrac{1}{2m}\hat{p}^2 + V(x)\right)\psi - \left(\tfrac{1}{2m}\hat{p}^2 + V(x)\right)x\psi$$

$\hat{p} = -i\hbar \partial/\partial x$

$$= \left(-\frac{x}{2m} i^2\hbar^2 \frac{\partial^2}{\partial x^2} + xV(x)\right)\psi - \left(-\tfrac{1}{2m} i^2\hbar^2 \frac{\partial^2}{\partial x^2} + V(x)\right)x\psi$$

$$= -\tfrac{x}{2m} i^2\hbar^2 \frac{\partial^2\psi}{\partial x^2} + xV(x)\psi - xV(x)\psi + \tfrac{1}{2m} i^2\hbar^2 \frac{\partial^2}{\partial x^2}(x\psi)$$

$$= -x \cdot \tfrac{1}{2m} i^2\hbar^2 \frac{\partial^2\psi}{\partial x^2} + \tfrac{1}{2m} i^2\hbar^2 \frac{\partial^2}{\partial x^2}(x\psi)$$

$$\frac{\partial^2}{\partial x^2}(x\psi) = \frac{\partial}{\partial x}\left(\frac{\partial x}{\partial x}\psi + \frac{\partial\psi}{\partial x}x\right) = \frac{\partial}{\partial x}\left(\psi + \frac{\partial\psi}{\partial x}x\right)$$

$$= \frac{\partial^2\psi}{\partial x^2}x + 2\frac{\partial\psi}{\partial x}$$

$$[x, \hat{H}]\psi = -x \cdot \tfrac{1}{2m} i^2\hbar^2 \frac{\partial^2\psi}{\partial x^2} + \tfrac{1}{2m} i^2\hbar^2 \left(\frac{\partial^2\psi}{\partial x^2}x + 2\frac{\partial\psi}{\partial x}\right)$$

$$[x, \hat{H}]\psi = \tfrac{1}{2m} i^2\hbar^2 \left(2\frac{\partial\psi}{\partial x}\right) = \frac{1}{m} i^2\hbar^2 \frac{\partial}{\partial x}\psi$$

$$[x, \hat{H}] = \frac{1}{m} i^2\hbar^2 \frac{\partial}{\partial x} = \frac{1}{m} i\hbar\hat{p}$$

so $\sigma_x^2 \sigma_{\hat{H}}^2 \geq \left[\frac{1}{2i} \langle \tfrac{1}{m} i\hbar\hat{p} \rangle \right]^2$

$\sigma_x \sigma_{\hat{H}} \geq \frac{\hbar}{2m} |\langle \hat{p} \rangle|$ as required.

~~For a stationary state~~ $\cancel{\hat{H} = E = \text{const}}$. ~~This implies that neither the position of a particle or the total energy of the system can have a definite solution at the same time.~~

For a stationary state $\hat{p} = 0$.

So for a stationary state:

$$\sigma_x \sigma_{\hat{H}} \geqq 0$$

This means that the product of uncertainty in x and uncertainty in $\hat{H}$ can take any positive, real value greater than or equal to zero.

$\hat{H} = E$.

This implies that with a known uncertainty ~~in either~~ σ_x or $\sigma_{\hat{H}}$, that it is not possible to approximate the other uncertainty.