Solutions to Mid-Term Test

1. (a) Write down the Hamiltonian of a particle of the mass *M* moving in the *xy* plane subject to the potential energy $V = k(x^2 + y^2)/2$.

$$\widehat{H} = -\frac{\hbar^2}{2M} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + \frac{k}{2} (x^2 + y^2)$$

(b) Given a wave function $\psi = Ne^{-|x|}$. Evaluate the normalization coefficient N.

$$\int_{-\infty}^{\infty} |\psi|^2 dx = N^2 \int_{-\infty}^{\infty} e^{-2|x|} dx$$
$$= N^2 \left(\int_{-\infty}^{0} e^{2x} dx + \int_{0}^{\infty} e^{-2x} dx \right)$$
$$= 2N^2 \int_{0}^{\infty} e^{-2x} dx$$
$$= N^2$$

Thus N = 1.

2. (a) What is the Hermitian operator? Discuss the properties of a Hermitian operator.

For any two functions, if the following equation holds, then $\hat{\Omega}$ is called Hermitian operator.

$$\int \mathrm{d}\tau \psi_j^* \widehat{\Omega} \psi_i = \left(\int \mathrm{d}\tau \psi_i^* \widehat{\Omega} \psi_j \right)^*$$

Any eigenvalue of Hermitian operator is a real number. Eigenfunctions of Hermitian operator with different eigenvalues are orthogonal.

(b) Prove that $\frac{d^2}{dx^2}$ is a Hermitian operator.

Given any two functions ψ_i and ψ_j ,

$$\int_{-\infty}^{+\infty} \mathrm{d}x\psi_j^* \frac{\mathrm{d}^2\psi_i}{\mathrm{d}x^2} = \psi_j^* \frac{\mathrm{d}\psi_i}{\mathrm{d}x}\Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \mathrm{d}x \frac{\mathrm{d}\psi_j^*}{\mathrm{d}x} \frac{\mathrm{d}\psi_i}{\mathrm{d}x}$$
$$= -\frac{\mathrm{d}\psi_j^*}{\mathrm{d}x}\psi_i\Big|_{-\infty}^{+\infty} + \int_{-\infty}^{+\infty} \mathrm{d}x \frac{\mathrm{d}^2\psi_j^*}{\mathrm{d}x^2}\psi_i$$
$$= \left(\int_{-\infty}^{+\infty} \mathrm{d}x\psi_i^* \frac{\mathrm{d}^2\psi_j}{\mathrm{d}x^2}\right)^*$$

Thus $\frac{d^2}{dx^2}$ is a Hermitian operator.

Q.E.D.

3. What is the Heisenberg's uncertainty principle for position and momentum? Why is it related to the commutator of the two operators?

(a) For position and momentum along its direction, their uncertainties satisfy the following Heisenberg's uncertainty principle

$$\Delta x \cdot \Delta p_x \ge \frac{\hbar}{2}$$

For position and momentum along other directions, we have

$$\Delta x \cdot \Delta p_y \ge 0$$

(b) For two observables A and B, the product of their uncertainty is related to the expectation value of the commutator of the corresponding operators \hat{A} and \hat{B} .

$$\Delta A \cdot \Delta B \geq \frac{1}{2} \left| \left\langle \left[\hat{A}, \hat{B} \right] \right\rangle \right|$$

Specify $\hat{A} = \hat{x}$, $\hat{B} = \hat{p}_x = -i\hbar \frac{\partial}{\partial x}$, we have $[\hat{x}, \hat{p}_x] = i\hbar$, thus $\Delta x \cdot \Delta p_x \ge \frac{\hbar}{2}$

For
$$\hat{A} = \hat{x}$$
, $\hat{B} = \hat{p}_y = -i\hbar \frac{\partial}{\partial y}$, we have $[\hat{x}, \hat{p}_y] = 0$, thus
 $\Delta x \cdot \Delta p_y \ge 0$

4. An electron resides within a potential well of infinite depth and a width *L*.(a) Write down its Schrödinger equation;

Denote the mass of electron as *m*. Suppose it is confined in [0, L], then $\widehat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$ where the potential is $V(x) = \begin{cases} 0, \ 0 < x < L \\ +\infty, \ x \le 0 \text{ or } x \ge L \end{cases}$

The Schrödinger equation is

$$\widehat{H}\psi(x) = E\psi(x)$$

(b) Confirm $\psi = N \sin \frac{n\pi x}{L}$ where *n* is an integer is the solution of the above Schrödinger equation;

This wavefunction is the solution of above Schrödinger equation in [0, L].

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 N\sin\frac{n\pi x}{L} = \frac{n^2\pi^2\hbar^2}{2mL^2}\psi(x)$$
$$E = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

It also satisfies boundary conditions $\psi(0) = \psi(L) = 0$, thus $\psi(x)$ is indeed the solution of above Schrödinger equation.

(c) Calculate the normalization coefficient *N*.

$$\int_{-\infty}^{\infty} |\psi|^2 dx = N^2 \int_0^L \sin^2 \frac{n\pi x}{L} dx$$

= $N^2 \int_0^L \frac{1 - \cos \frac{2n\pi x}{L}}{2} dx$
= $\frac{N^2 L}{2} - \frac{1}{2} \left(\frac{L}{2n\pi} \sin \frac{2n\pi x}{L}\right) \Big|_0^L$
= $\frac{N^2 L}{2}$

Thus

$$N = \sqrt{\frac{2}{L}}$$