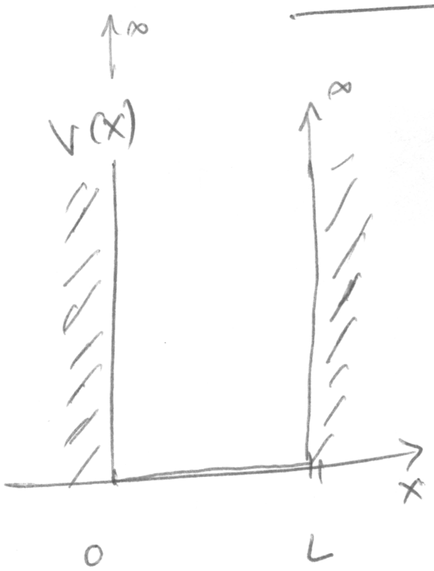
QMA.

Solution to Problem Set 2

Problem 1



1

Schrödinger equation in space $0 \leq x \leq L$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad (1)$$

The general solution to (1) is:

$$\psi_k(x) = A\sin(kx) + B\cos(kx) \qquad (2)$$

where $$E = \frac{\hbar^2 k^2}{2m} \qquad (3)$$

Boundary conditions: $\psi(0) = \psi(L) = 0$

$$\psi(0) = 0 \xrightarrow{(2)} B = 0 \Rightarrow \psi_k(x) = A\sin(kx) \qquad (4)$$

$$\psi(L) = 0 \xrightarrow{(4)} k\cancel{x}L = n\pi \Rightarrow k = n\frac{\pi}{L} \qquad n = 1, 2, \dots$$

Normalization of $\psi_k(x)$:

$$\int_0^L |\psi_k(x)|\, dx = 1 \Rightarrow |A|^2 \int_0^L \sin^2\left(n\pi\frac{x}{L}\right) dx = 1 \Rightarrow$$

$$\Rightarrow |A|^2 \frac{L}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{L}}$$

Thus, energy eigenstates $\psi_k(x) = \sqrt{\frac{2}{L}}\sin(kx)$ $\quad k = n\frac{\pi}{L}$

" " eigenvalue $E = \hbar^2 k^2/2m$.

2. Let's test to see if the eigenstates of energy are eigenstates of the momentum operator $\hat{P}_x = -i\hbar\partial_x$

$$\hat{P}_x \psi_k(x) = -i\hbar\, \partial_x\left[\sqrt{\frac{2}{L}}\sin(kx)\right] = -i\hbar k\sqrt{\frac{2}{L}}\cos(kx)$$

therefore, $\psi_k(x)$ is not an eigenstate of $\hat{P}_x$.

3.

$$\langle\psi_k|\hat{P}_x|\psi_k\rangle = \int_0^L \psi_k^*(x)\,(-i\hbar\,\partial_x\psi_k(x))\,dx$$

$$= \frac{2}{L}(-i\hbar)k\int_0^L \sin(kx)\cos(kx)\,dx = 0$$

Problem 2

1. $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$, $\psi_k(x) = \sqrt{\frac{1}{L}}\, e^{ikx}$

$$\hat{H}\psi_k(x) = \frac{\hbar^2 k^2}{2m}\psi_k(x)$$

it is an eigenstate of $\hat{H}$ with energy eigenvalue given by

$$E(k) = \frac{\hbar^2 k^2}{2m}$$

2. $$\hat{p}\,\psi_k(x) = -i\hbar\frac{\partial}{\partial x}\left(\sqrt{\frac{1}{L}}\, e^{ikx}\right) = \hbar k \underbrace{\sqrt{\frac{1}{L}}\, e^{ikx}}_{\psi_k(x)}$$

Therefore, $\psi_k(x)$ is a momentum eigenstate with momentum eigenvalue $\hbar k$.

3. Periodic boundary conditions:

$$\psi_k(x+L) = \psi_k(x), \quad \forall x$$

$$\frac{1}{\sqrt{L}} e^{ik(x+L)} = \frac{1}{\sqrt{L}} e^{ikx}, \quad \forall x \Rightarrow e^{ikL} = 1 \Rightarrow kL = n2\pi$$

Thus, $k = \frac{2\pi}{L} n$.

Problem 4

1. $$\psi_{\vec{k}}(x,y,z) = \left(\frac{2}{L}\right)^{3/2} \sin(k_x x)\,\sin(k_y y)\,\sin(k_z z)$$

and
$$k_x L = n_x \pi \Rightarrow k_x = n_x \frac{\pi}{L} \quad n_x = 1,2,\dots$$
$$k_y L = n_y \pi \Rightarrow k_y = n_y \frac{\pi}{L} \quad n_y = 1,2,\dots$$
$$k_z = n_z \frac{\pi}{L} \quad n_z = 1,2,\dots$$

$$E(k_x,k_y,k_z) = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

2. They are not eigenstates of the momentum operator.

3. $$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$$

$$\text{P.B.C} \Longrightarrow \begin{array}{l} k_x L = 2\pi n_x \Rightarrow k_x = \frac{2\pi}{L} n_x \quad n_x = 0,\pm1,\pm2,\dots \\ k_y L = 2\pi n_y \Rightarrow k_y = \frac{2\pi}{L} n_y \quad n_y = 0,\pm1,\pm2,\dots \\ k_z L = 2\pi n_z \Rightarrow k_z = \frac{2\pi}{L} n_z \quad n_z = 0,\pm1,\pm2,\dots \end{array}$$

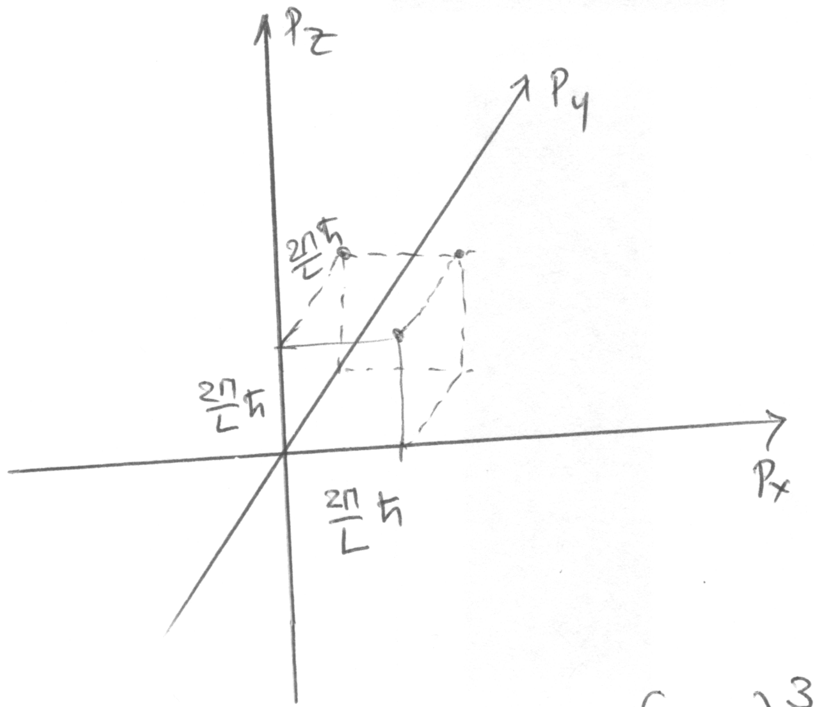
$$E(k_x,k_y,k_z) = \frac{\hbar^2 k^2}{2m}, \quad k^2 = k_x^2 + k_y^2 + k_z^2$$

4. $\psi_k(\vec{r})$ is simultaneous eigenstate of $\hat{\vec{P}} = -i\hbar\vec{\nabla}$ with eigenvalue $\hbar\vec{k}$.

5. Momentum $\vec{P} = \hbar \vec{k} = \frac{\hbar 2\pi}{L}(n_x, n_y, n_z)$

$$n_{x,y,z} = 0, \pm 1, \pm 2, \ldots$$

i.e in momentum space



Every cube of size $\left(\frac{2\pi}{L}\hbar\right)^3$ corresponds to 1 momentum state. Therefore, the density of states is

$$\frac{1 \text{ state}}{\left(\frac{2\pi\hbar}{L}\right)^3} = \frac{L^3}{(2\pi\hbar)^3} = \frac{V}{(2\pi\hbar)^3}$$

6.

$$\sum_{p_x} \sum_{p_y} \sum_{p_z} f(p_x, p_y, p_z) =$$

$$\left(\frac{L}{2\pi\hbar}\right)^3 \quad \left(\frac{2\pi\hbar}{L}\right) \sum_{p_x} \left(\frac{2\pi\hbar}{L}\right) \sum_{p_y} \left(\frac{2\pi\hbar}{L}\right) \sum_{p_z} f(\vec{p})$$

Namely, I multiplied and divide by $\left(\frac{2\pi\hbar}{L}\right)^3$.

Notice that

$$\underbrace{\frac{2\pi\hbar}{L}}_{\Delta p_x} \sum_{p_x} \xrightarrow[\lim L\to\infty]{} \int dp_x$$

Because we sum over values of $p_x = \frac{2\pi\hbar}{L} n_x$

i.e in increments of $\Delta p_x = \frac{2\pi\hbar}{L}$.

Therefore

$$\sum_{\vec{p}} f(\vec{p}) \rightarrow V \int \frac{d^3p}{(2\pi\hbar)^3} f(\vec{p})$$

Problem 4

1. Fourier transform:

$$f(\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \tilde{f}(\vec{p})$$

where

$$\tilde{f}(\vec{p}) = \int d^3r \; e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}} f(\vec{r})$$

Then for the δ-function

$$\tilde{f}(\vec{p}) = \int d^3r \; e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \delta(\vec{r}-\vec{r}\,') = e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}\,'}$$

2. $$\langle\vec{p}|\vec{p}\,'\rangle = \int d^3r \; \langle\vec{p}|\vec{r}\rangle\langle\vec{r}|\vec{p}\,'\rangle =$$

$$= \int d^3r \; e^{\frac{i}{\hbar}\vec{r}\cdot(\vec{p}\,'-\vec{p})} = (2\pi\hbar)^3 \delta(\vec{p}-\vec{p}\,')$$

3. $$\tilde{\psi}(p) = \langle\vec{p}|\psi\rangle = c \; e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2\sigma^2}}$$

and c is determined by the normalization

$$\int \frac{d^3p}{(2\pi\hbar)^3} \left|\tilde{\psi}(\vec{p})\right|^2 = 1 \Rightarrow \frac{|c|^2}{(2\pi\hbar)^3} \int d^3p \; e^{-\frac{(\vec{p}-\vec{p}_0)^2}{\sigma^2}} = 1$$

$$\Rightarrow \quad \frac{|c|^2}{(2\pi\hbar)^3} \left(\sqrt{\pi}\,\sigma\right)^3 = 1 \Rightarrow |c|^2 = \left(\frac{2\sqrt{\pi}\,\hbar}{\sigma}\right)^3$$

$$\Rightarrow \quad c = \left(\frac{2\sqrt{\pi}\,\hbar}{\sigma}\right)^{3/2}$$

Thus

$$\tilde{\psi}(\vec{p}) = \left(\frac{2\sqrt{\pi}\,\hbar}{\sigma}\right)^{3/2} e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2\sigma^2}}$$

Therefore

$$\psi(\vec{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} \; e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \; \tilde{\psi}(\vec{p})$$

$$= \frac{1}{(\sqrt{\pi}\,\sigma)^{3/2}} \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p \; e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} \; e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2\sigma^2}}$$

$$= \frac{1}{(\sqrt{\pi}\,\sigma)^3} \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p \; e^{-\frac{1}{2\sigma^2}\left[(\vec{p}-\vec{p}_0)^2 - \frac{2i\sigma^2}{\hbar}\vec{p}\cdot\vec{r}\right]}$$

The exponent should be written in a way to complete the square:

$$(\vec{p}-\vec{p}_0)^2 - \frac{2i\sigma^2}{\hbar}\vec{p}\cdot\vec{r} = (\vec{p}-\vec{p}_0)^2 - \frac{2i\sigma^2}{\hbar}(\vec{p}-\vec{p}_0)\cdot\vec{r} + \frac{2i\sigma^2\vec{p}_0\cdot\vec{r}}{\hbar}$$

$$= \left(\vec{p}-\vec{p}_0-\frac{i\sigma^2}{\hbar}\vec{r}\right)^2 - \left(\frac{i\sigma^2}{\hbar}\vec{r}\right)^2 + \frac{2i\sigma^2\vec{p}_0\cdot\vec{r}}{\hbar}$$

Therefore

$$\psi(\vec{r}) = \frac{1}{(\sqrt{\pi}\,\sigma)^{3/2}}\frac{1}{(2\pi\hbar)^{3/2}} e^{-\frac{1}{2\sigma^2}\left[\frac{\sigma^4}{\hbar^2}r^2 + \frac{2i\sigma^2}{\hbar}\vec{p}_0\cdot\vec{r}\right]}$$

$$\int d^3p \; e^{-\frac{1}{2\sigma^2}(\vec{p}-\vec{p}\,')^2}$$

where $\vec{p}\,' = \vec{p}_0 + \frac{i\sigma^2}{\hbar}\vec{r}$ which is a constant vector, i.e. independent of $\vec{p}$.

Thus, $\int d^3p \; e^{-\frac{1}{2\sigma^2}(\vec{p}-\vec{p}\,')^2} = \int d^3p'' e^{-\frac{1}{2\sigma^2}p''^2} = (\sqrt{2\pi}\,\sigma)^3$

and

$$\psi(\vec{r}) = \left(\frac{\sqrt{\pi}\,\sigma}{\hbar}\right)^3 e^{-\frac{i}{\hbar}\vec{p}_0\cdot\vec{r}} \; e^{-\frac{\sigma^2}{2\hbar^2}r^2}$$

Problem 5

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \frac{1}{2} G \hat{\vec{r}}^{\,2} \qquad (1)$$

$$\hat{\mathcal{H}} |\psi\rangle_t = i\hbar \partial_t |\psi\rangle_t \qquad (2)$$

we consider the momentum space basis:

$$\langle \vec{p} | \mathcal{H} | \psi_t \rangle = i\hbar \partial_t \langle \vec{p} | \psi_t \rangle \overset{(1)}{\Longrightarrow}$$

$$\langle \vec{p} | \frac{\hat{\vec{p}}^{\,2}}{2m} + \frac{1}{2} G \hat{\vec{r}}^{\,2} | \psi_t \rangle = i\hbar \partial_t \langle \vec{p} | \psi_t \rangle$$

but

$$\langle \vec{p} | \frac{\hat{\vec{p}}^{\,2}}{2m} = \frac{\vec{p}^{\,2}}{2m} \langle \vec{p} |$$

and

$$\langle \vec{p} | \frac{1}{2} G \hat{\vec{r}}^{\,2} | \psi_t \rangle = \frac{1}{2} G \langle \vec{p} | \hat{\vec{r}}^{\,2} | \psi_t \rangle$$

Now

$$\langle \vec{p} | \hat{\vec{r}}^2 | \psi_t \rangle = \int d^3r' \, \langle \vec{p} | \hat{\vec{r}}^2 | \vec{r}' \rangle \langle \vec{r}' | \psi_t \rangle =$$

$$= \int d^3r' \, \vec{r}'^2 \, \langle \vec{p} | \vec{r}' \rangle \langle \vec{r}' | \psi_t \rangle =$$

$$= \int d^3r' \, \vec{r}'^2 \, e^{-\frac{i}{\hbar} \vec{p} \cdot \vec{r}'} \langle \vec{r}' | \psi_t \rangle$$

because $\langle \vec{p} | \vec{r}' \rangle = e^{-\frac{i}{\hbar} \vec{p} \cdot \vec{r}'}$, thus:

$$\langle \vec{p} | \hat{\vec{r}}^2 | \psi_t \rangle = \int d^3r' (i\hbar \nabla_p)^2 \, e^{-\frac{i}{\hbar} \vec{p} \cdot \vec{r}'} \langle \vec{r}' | \psi_t \rangle$$

$$= (i\hbar \nabla_p)^2 \int d^3r' \, \langle \vec{p} | \vec{r}' \rangle \langle \vec{r}' | \psi_t \rangle$$

$$= (i\hbar \nabla_p)^2 \langle \vec{p} | \psi_t \rangle$$

Therefore we have

$$\left[\frac{p^2}{2m} + \frac{1}{2} G (i\hbar \nabla_p)^2 \right] \langle \vec{p} | \psi_t \rangle = i\hbar \partial_t \langle \vec{p} | \psi_t \rangle$$