Sample: Quantum Mechanics - Quantum Mechanics Problems

2. Particle in a Box.

One knows the solution for a one-dimensional box: $\psi_{n_1}(x)=\sqrt{\frac{2}{a}}\sin(\pi n_1 \frac{x}{a})$. In the same way, plugging in the solution into Schrodinger equation in 3D in form $\psi(x,y,z)=\psi(x)\psi(y)\psi(z)$, it is easy to obtain $\psi_{n_1 n_2 n_3}(x,y,z)=\sqrt{\frac{8}{3a^3}}\sin(\frac{\pi n_1 x}{a})\sin(\frac{\pi n_2 y}{3a})\sin(\frac{\pi n_3 z}{a})$ - these are the normalized solutions.

Let us find $<x>_{n_1 n_2 n_3}=$

$$\frac{8}{3a^3}\int_0^a x\sin^2(\pi\frac{n_1}{a}x)\int_0^{3a}\sin^2(\pi\frac{n_2}{3a}y)dy\int_0^a\sin^2(\pi\frac{n_3}{a}z)dz=\frac{8}{3a^3}\cdot\frac{a}{2}\cdot\frac{3a}{2}\cdot(\frac{-a^2}{8\pi^2 n_1^2}(-1-2n_1^2\pi^2+\cos 2\pi n_1))=$$

$$\frac{2a^2 n_1^2\pi^2}{8\pi^2 n_1^2}\cdot\frac{8}{3a^3}\cdot\frac{3a}{4}\cdot\frac{a}{2}=\frac{a}{4}\quad .$$

In the same way, $<y>_{n_1 n_2 n_3}=$

$$\frac{8}{3a^3}\int_0^a\sin^2(\pi\frac{n_1}{a}x)\int_0^{3a}y\sin^2(\pi\frac{n_2}{3a}y)dy\int_0^a\sin^2(\pi\frac{n_3}{a}z)dz=\frac{8}{3a^3}\cdot\frac{a}{2}\cdot\frac{a}{2}\cdot(-9\frac{a^2}{8\pi^2 n_2^2}(-1-2n_2^2\pi^2+\cos 2\pi n_2))=\frac{3}{2}a$$

and $<z>_{n_1 n_2 n_3}=$

$$\frac{8}{3a^3}\int_0^a\sin^2(\pi\frac{n_1}{a}x)\int_0^{3a}\sin^2(\pi\frac{n_2}{3a}y)dy\int_0^a z\sin^2(\pi\frac{n_3}{a}z)dz=\frac{8}{3a^3}\cdot\frac{a}{2}\cdot\frac{3a}{2}\cdot(\frac{2a^2 n_3^2\pi^2}{8\pi^2 n_3^2})=\frac{a}{2}\quad .$$

3. Velocity equals velocity

First, let us write Schrodinger equation $i\hbar\frac{\partial\psi}{\partial t}=\frac{-\hbar^2}{2m}\nabla^2\psi+V\psi$.

$\frac{d}{dt}<x>=\int\bar{\psi}x\frac{\partial\psi}{\partial t}d\tau+\int\psi x\frac{\partial\bar{\psi}}{\partial t}d\tau$. Now let us plug in derivatives from Schrodinger equation.

Obtain: $\frac{d}{dt}<x>=\frac{i\hbar}{2m}\int[\bar{\psi}x(\nabla^2\psi)-(\nabla^2\bar{\psi})x\psi]d\tau$ (the parts with potential V vanished).

Let us rewrite the last term in $\frac{d}{dt}<x>$. First, let us use equality

$\nabla(x\psi\nabla\bar{\psi})=(\nabla^2\bar{\psi})x\psi+(\nabla\bar{\psi})\nabla(x\psi)$.

Then, $\int(\nabla^2\bar{\psi})x\psi d\tau=-\int(\nabla\bar{\psi})\nabla(x\psi)d\tau+\int\nabla(x\psi\bar{\psi})d\tau$. The last integral according to divergence theorem is equal to $\int_S(x\psi\nabla\bar{\psi})d\vec{S}$. It vanishes on infinity.

Now, use the given equality one more time for term which left:

$\int(\nabla^2\bar{\psi})x\psi d\tau=-\int(\nabla\bar{\psi})\nabla(x\psi)d\tau=\int\bar{\psi}\nabla^2(x\psi)d\tau$ (one more time, the term with divergence converted into integral over surface and vanished).

Hence, $\frac{d}{dt}<x>=\frac{i\hbar}{2m}\int\bar{\psi}[x\nabla^2\psi-\nabla^2(x\psi)]d\tau$.

The last term is $\nabla^2(x\psi)=2\nabla x\nabla\psi+x\nabla^2\psi=2\frac{\partial\psi}{\partial x}+x\nabla^2\psi$. Plugging this into previous equation, obtain $\frac{d}{dt}<x>=\frac{-i\hbar}{m}\int\bar{\psi}\frac{\partial\psi}{\partial x}d\tau=\frac{1}{m}<p_x>$, because $p_x=-i\hbar\frac{\partial}{\partial x}$.

The average value $<p_x>$ is simply $p_x=mv_x=mv$, so $\frac{d}{dt}<x>=v$.

4. Acceleration

One might use equation $\frac{d\hat{f}}{dt}=\frac{1}{i\hbar}[\hat{p},\hat{H}]$. But according to canonical quantization relations, $[\hat{p},\hat{H}]\rightarrow -i\hbar\{f,H\}$, where $\{f,g\}=\sum_k\frac{\partial f}{\partial q_k}\frac{\partial g}{\partial p_k}-\frac{\partial g}{\partial q_k}\frac{\partial f}{\partial p_k}$.

a) Poisson bracket $\{p_x,H\}=0$, hence acceleration is zero.

b) Poisson bracket is $\{p_x,H\}=-c$, so $\frac{d}{dt}\hat{p}=c$ and $a=\frac{c}{m}$.

c) Poisson bracket is $\{p_x,H\}=-mw^2x$, so $\frac{d}{dt}\hat{p}=mw^2x$ and $a=w^2x$.