PHYS 606 – Spring 2015 – Homework V – Solution

Problem [1]

(a) Simultaneous momentum eigenstates: separation $\psi(\vec{r}) = X(x)\,Y(y)\,Z(z)$

$$-i\hbar\frac{\partial}{\partial x}\psi(x,y,z) = \underset{\uparrow\text{ eigenvalue}}{p_x}\,\psi(x,y,z) \quad\Rightarrow\quad X(x) = \text{const} * e^{\frac{i}{\hbar}p_x x}, \quad p_x \in \mathbb{R}$$

(p_x hermitian op.)

Same for y, z-directions

$$\Rightarrow \psi(x,y,z) = \text{const.} * e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}$$ eigenfct. for P_x, P_y, P_z simultaneously

with $(p_x, p_y, p_z) \in \mathbb{R}^3$

Instead of the separation ansatz you can also use our results for free particles

Impose boundary conditions: for periodic boundary cond. on box of size L the fct. $\psi(\vec{r})$ needs to be periodic w/ period L:

$$\psi(x,y,z) = \psi(x+n_1L,\, y+n_2L,\, z+n_3L) \qquad \text{with } (n_1,n_2,n_3)\in\mathbb{Z}^3$$

$$\Rightarrow \frac{i}{\hbar}p_i L = 2\pi i n_i \quad\Rightarrow\quad p_i = \frac{2\pi\hbar}{L}n_i = \frac{h}{L}n_i$$

$\Rightarrow$ eigenvalues that obey B.c. are $\vec{p}_N = \frac{h}{L}\underbrace{(n_1, n_2, n_3)}_{=:N\in\mathbb{Z}^3}$

with eigenfcts. $\psi_N(\vec{r}) = \underset{\uparrow}{L^{-3/2}}\, e^{\frac{i}{\hbar}\vec{p}_N\cdot\vec{r}}$

normalization from $\int_{\text{Box}} |\psi_N|^2 d^3r = 1$

$$H\psi_N(\vec{r}) = \frac{p_N^2}{2m}\psi_N(\vec{r}) \quad\Rightarrow\quad \psi_N \text{ are eigenstate of } H \text{ with eigenvalues}$$

$$E_N = \frac{h^2}{2mL^2}\left(n_1^2+n_2^2+n_3^2\right) \geq 0$$

For $L\to\infty$ the lattice of the $\vec{p}_N = \frac{h}{L}N$ has lattice spacing $\frac{h}{L}\to 0$

i.e. it will cover all of $\mathbb{R}^3$ with eigenfcts. $\sim e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}$ (as in I.II.4, case (B))

(b) Number of states in a $\Delta n_x \Delta n_y \Delta n_z$ cube of the lattice is $\Delta n_x \Delta n_y \Delta n_z = \Delta N$.

Its momentum space volume is $\Delta p_x \Delta p_y \Delta p_z = \frac{h^3}{L^3} \Delta n_x \Delta n_y \Delta n_z$

$$\Rightarrow \rho = \frac{\Delta N}{L^3 \Delta p_x \Delta p_y \Delta p_z} = \frac{1}{h^3}$$

, i.e. we have one eigenstate per elementary phase space volume h^3

(c) An energy interval ΔE cuts out a spherical shell in the $\mathbb{Z}^3$ lattice of momentum eigenvalues.

The number of eigenvalues in that shell grows quadratically with its radius.

For large E (large radius) we should be able to approximate the sum over points in the shell by an integral over the shell

Number of eigenstates $\Delta N \approx \underset{\substack{\text{phase space} \\ \text{density}}}{\rho} L^3 \underbrace{4\pi p^2 \Delta p}_{\substack{\text{shell volume} \\ \text{in } \vec{p}\text{-space}}}$ for large p but $\Delta p \ll p$

$p^2 = 2mE \Rightarrow \Delta p = \frac{m \Delta E}{p}$

$$\Rightarrow \sigma = \frac{\Delta N}{\Delta E} = \frac{L^3}{h^3} 4\pi \sqrt{2mE}\, m = \frac{m^{3/2} L^3}{\sqrt{2}\, \pi^2 \hbar^3} \sqrt{E}$$

Problem [2]

(a) Eigenvalues and eigenfcts. for mom. operator p are usually $K \in \mathbb{R}$ and $\sim e^{\frac{i}{\hbar}Kx}$. Since p and U_a commute try the same eigenfcts:

$$U_a\, e^{\frac{i}{\hbar}Kx} = \sum_{j=0}^{\infty} \left(\frac{i}{\hbar} p\, a\right)^j e^{\frac{i}{\hbar}Kx} = e^{-\frac{i}{\hbar}Ka}\; e^{\frac{i}{\hbar}Kx}$$

$\Rightarrow$ eigenvalues are $e^{\frac{i}{\hbar}Ka}$ with eigenfct. $\sim e^{\frac{i}{\hbar}Kx}$

But eigenvalues $e^{-\frac{i}{\hbar}Ka}, e^{-\frac{i}{\hbar}K'a}$ with $K-K' = \frac{2\pi\hbar}{a}$ are actually the same

$\Rightarrow$ The set $e^{-\frac{i}{\hbar}Ka}$ with $-\frac{h}{2a} < K < \frac{h}{2a}$ is a unique set of eigenvalues, each with an infinite but countable degeneracy. As a set it covers the unit circle in $\mathbb{C}$.

The fcts. $e^{\frac{i}{\hbar}(K+\frac{2\pi\hbar n}{a})x}$ for $n \in \mathbb{Z}$ have all the same eigenvalue $e^{-\frac{i}{\hbar}Ka}$, and they are mutually orthogonal.

(b) Fourier's Theorem: the fcts. $e^{i2\pi n\frac{x}{a}}$ $n\in\mathbb{Z}$ are periodic with period a. They are a complete basis spanning the space of square-integrable periodic fcts with period a.

Thus: arbitrary fct. in eigenspace of eigenvalue $e^{-\frac{i}{\hbar}Ka}$ is a linear combination

$$\sum_{n\in\mathbb{Z}} c_n\, e^{\frac{i}{\hbar}(K+\frac{2\pi\hbar n}{a})x} = e^{\frac{i}{\hbar}Kx} \underbrace{\sum_{n\in\mathbb{Z}} c_n e^{i2\pi n\frac{x}{a}}}_{\text{Fourier series}} = e^{\frac{i}{\hbar}Kx} \underbrace{u(x)}_{a\text{-periodic fct.}}$$

Problem [3]

$$(a)\quad D_{w_i} = e^{\frac{i}{\hbar}(mr_i - p_i t)w_i} = e^{\frac{i}{\hbar}(mr_i - p_i t)w_i + \overbrace{[\frac{i}{\hbar}mr_i w_i, -\frac{i}{\hbar}p_i w_i t]/2}^{\frac{i}{2\hbar}mw_i^2 t}}\, e^{-\frac{i}{2\hbar}mw_i^2 t}$$

exponent just a number, so can be pulled out

just numbers

$$\underset{BCH}{=} e^{\frac{i}{\hbar}mr_i w_i}\, e^{-\frac{i}{\hbar}p_i w_i t}\, e^{-\frac{i}{\hbar}\frac{mw_i^2}{2}t}$$

commutes here

$$\Rightarrow D_{w_i}\psi(\vec{r},t) = e^{\frac{i}{\hbar}(mw_i r_i - \frac{mw_i^2}{2}t)}\, \underbrace{e^{-\frac{i}{\hbar}p_i w_i t}}_{\substack{\text{translation}\\ \text{operator by}\\ -\vec{w}t}}\, \psi(\vec{r},t) = e^{\frac{i}{\hbar}(mw_i r_i - \frac{mw_i^2}{2}t)}\psi(\vec{r}-\vec{w}t,t)$$

$$(b)\quad [K_i, K_j] = [mr_i - p_i t, mr_j - p_j t] = 0$$

$$[K_i, p_j] = [mr_i, p_j] = i\hbar m\,\delta_{ij}$$

$$[K_i, H] = [mr_i, T] \underset{I.8.2}{=} i\hbar p_i$$

$$(c)\quad e^{\frac{i}{\hbar}\vec{K}\vec{w}_2}\, e^{\frac{i}{\hbar}\vec{K}\vec{w}_1} \underset{(b)}{=} e^{\frac{i}{\hbar}\vec{K}(\vec{w}_2+\vec{w}_1)}$$

$$e^{\frac{i}{\hbar}\vec{K}\cdot\vec{w}_1}\, e^{\frac{i}{\hbar}\vec{p}\cdot\vec{a}} = e^{\frac{i}{\hbar}(\vec{K}\cdot\vec{w}_1 + \vec{p}\cdot\vec{a} + \frac{i}{\hbar}w_{1j}\overbrace{[K_j, P_\ell]}^{i\hbar m\delta_{j\ell}}a_\ell/2)}$$

$$= \underbrace{e^{-\frac{i}{\hbar}\frac{m}{2}\vec{w}_1\vec{a}}}\, e^{\frac{i}{\hbar}(\vec{K}\cdot\vec{w}_1 + \vec{p}\cdot\vec{a})}$$

appearance of this phase factor means this is a projective representation.

Problem [4]

Ehrenfest's Theorem says:

$$\frac{m\,d^2}{dt^2}\langle\vec{r}\rangle = -\langle\nabla V(\vec{r})\rangle$$

Slowly varying $V(\vec{r})$: Taylor expand around $V(\langle\vec{r}\rangle)$.

$$V(\vec{r}) = V(\langle\vec{r}\rangle) + (r_i-\langle r_i\rangle)\frac{\partial V}{\partial r_i}(\langle\vec{r}\rangle) + \frac{1}{2!}(r_i-\langle r_i\rangle)(r_j-\langle r_j\rangle)\frac{\partial^2 V}{\partial r_i\partial r_j}(\langle\vec{r}\rangle)$$

$$+\frac{1}{3!}(r_i-\langle r_i\rangle)(r_j-\langle r_j\rangle)(r_k-\langle r_k\rangle)\frac{\partial^3 V}{\partial r_i\partial r_j\partial r_k} + \ldots$$

$$\left\langle\frac{\partial}{\partial r_e}V(\vec{r})\right\rangle = \frac{\partial V}{\partial r_e}(\langle\vec{r}\rangle) + \underbrace{\langle(r_i-\langle r_i\rangle)\rangle}_{=0}\frac{\partial^2 V}{\partial r_i\partial r_e}(\langle\vec{r}\rangle) + \frac{1}{2!}\underbrace{\langle(r_i-\langle r_i\rangle)(r_j-\langle r_j\rangle)\rangle}_{\substack{=0 \text{ for } i\neq j \\ =(\Delta r_i)^2 \text{ for } i=j}}\frac{\partial^3 V(\langle\vec{r}\rangle)}{\partial r_i\partial r_j\partial r_e}$$

$$= \frac{\partial V(\langle\vec{r}\rangle)}{\partial r_e} + \frac{1}{2!}(\Delta\vec{r})^2\frac{\partial}{\partial r_e}\Delta V(\langle\vec{r}\rangle)$$

$$\Rightarrow \frac{m\,d^2}{dt^2}\langle\vec{r}\rangle = -\nabla\left[V(\langle\vec{r}\rangle) + \frac{1}{2!}(\Delta\vec{r})^2\Delta V(\langle\vec{r}\rangle)\right]$$

Newton's Law

1st quantum correction vanishes for width $(\Delta\vec{r})^2$ of wave packet $\to 0$

[4] Define $\vec{A}' = \vec{A} + \nabla f$; $\phi' = \phi - \frac{\partial f}{\partial t}$; $\psi' = \psi e^{\frac{i}{\hbar} q f}$

Proof of invariance in two parts:

i) $i\hbar \frac{\partial \psi'}{\partial t} - q\phi'\psi' = \left(i\hbar \frac{\partial \psi}{\partial t}\right) e^{\frac{i}{\hbar}qf} + \cancel{\left(-q\frac{\partial f}{\partial t}\right)\psi e^{\frac{i}{\hbar}qf}} - q\phi\psi e^{\frac{i}{\hbar}qf} + \cancel{q\frac{\partial f}{\partial t}\psi e^{\frac{i}{\hbar}qf}}$

$= \left(i\hbar \frac{\partial \psi}{\partial t} - q\phi\psi\right) e^{\frac{i}{\hbar}qf}$

ii) $\left(-i\hbar\nabla - q\vec{A}'\right)^2 \psi' = \left(-i\hbar\nabla - q\vec{A}\right)^2 \psi e^{\frac{i}{\hbar}qf} + q^2(\nabla f)^2 \psi e^{\frac{i}{\hbar}qf} + \left(-i\hbar\nabla - q\vec{A}\right)\left(-q\nabla f\right)\psi e^{\frac{i}{\hbar}qf}$

$+ \left(-q\nabla f\right)\left(-i\hbar\nabla - q\vec{A}\right)\psi e^{\frac{i}{\hbar}qf}$

$= \left[\left(-i\hbar\nabla - q\vec{A}\right)^2\psi\right] e^{\frac{i}{\hbar}qf} + 2\left[\left(-i\hbar\nabla - q\vec{A}\right)\psi\right]\overbrace{\left(-i\hbar\nabla\right) e^{\frac{i}{\hbar}qf}}^{q\nabla f e^{\frac{i}{\hbar}qf}} + \left[\overbrace{\left(-i\hbar\nabla\right)^2 e^{\frac{i}{\hbar}qf}}^{q^2(\nabla f)^2 e^{\frac{i}{\hbar}qf} - i\hbar q \Delta f e^{\frac{i}{\hbar}qf}}\right]\psi$

$+ \cancel{q^2(\nabla f)^2\psi e^{\frac{i}{\hbar}qf}} + \cancel{i\hbar q \Delta f \psi e^{\frac{i}{\hbar}qf}} - \cancel{2q^2(\nabla f)^2 \psi e^{\frac{i}{\hbar}qf}} - \cancel{\left[2q\nabla f\cdot\left(-i\hbar\nabla - q\vec{A}\right)\psi\right] e^{\frac{i}{\hbar}qf}}$

$= \left[\left(-i\hbar\nabla - q\vec{A}\right)^2\psi\right] e^{\frac{i}{\hbar}qf}$

$\Rightarrow$ the transformed S.E. $i\hbar\frac{\partial\psi'}{\partial t} = \frac{1}{2m}\left(-i\hbar\nabla - q\vec{A}'\right)^2\psi' + q\phi'\psi'$

is identical to the original equation times an overall phase factor which can be dropped.

(b) $m\frac{d}{dt}\langle v_k\rangle = \frac{1}{i\hbar}\left\langle\left[p_k - qA_k, \frac{(\vec{P}-q\vec{A})^2}{2m} + q\phi\right]\right\rangle + m\left\langle\frac{\partial v_k}{\partial t}\right\rangle$ $\qquad k = 1,2,3$

$= \frac{1}{i\hbar}\left\langle (p_\ell - qA_\ell)\left[p_k - qA_k, p_\ell - qA_\ell\right]\frac{1}{2m} + \underbrace{\left[p_k - qA_k, p_\ell - qA_\ell\right]}_{i\hbar q\left(\frac{\partial}{\partial x_k}A_\ell - \frac{\partial}{\partial x_\ell}A_k\right)}(p_\ell - qA_\ell)\frac{1}{2m}\right\rangle$

$\underbrace{- q\left\langle\frac{\partial}{\partial x_k}\phi\right\rangle - q\left\langle\frac{\partial A_k}{\partial t}\right\rangle}_{= q\langle E_k\rangle}$

$= q\langle E_k\rangle + \frac{q}{2}\left\langle v_\ell\left(\frac{\partial}{\partial x_k}A_\ell - \frac{\partial}{\partial x_\ell}A_k\right) + \left(\frac{\partial}{\partial x_k}A_\ell - \frac{\partial}{\partial x_\ell}A_k\right)v_\ell\right\rangle$

on the other hand $\left[\vec{v}\times(\nabla\times\vec{A})\right]_k = \varepsilon_{k\ell m} v_\ell \varepsilon_{mno}\frac{\partial}{\partial x_n}A_o$

$= \left(\delta_{kn}\delta_{\ell o} - \delta_{ko}\delta_{\ell n}\right) v_\ell \frac{\partial}{\partial x_n}A_o = v_\ell\left(\frac{\partial}{\partial x_k}A_\ell - \frac{\partial}{\partial x_\ell}A_k\right)$

$\Rightarrow m\frac{d}{dt}\langle\vec{v}\rangle = q\langle\vec{E}\rangle + \frac{q}{2}\left\langle\vec{v}\times\vec{B} - \vec{B}\times\vec{v}\right\rangle$