

PHYS 606 - Spring 2014 - HW III Solution

[1] We have  $i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = -\frac{\hbar^2}{2m} \Delta \psi(\vec{r}, t) + V(\vec{r}) \psi(\vec{r}, t)$

Using the Fourier transformation  $\psi(\vec{r}, t) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \phi(\vec{p}, t) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3 p$

we get

$$\frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \left[ i\hbar \frac{\partial}{\partial t} \phi(\vec{p}, t) \right] e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \phi(\vec{p}, t) \left[ \underbrace{\left(-\frac{\hbar^2}{2m} \Delta\right) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}}_{= \frac{p^2}{2m} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}} + \underbrace{V(\vec{r}) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}}_{V(-\frac{i}{\hbar} \nabla_p) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}}$$

partial integration in the last term:  $\int \phi \nabla_p e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3 p =$

after repeated application to the power series expansion of  $V$ :

$$= \int (-\nabla_p \phi) e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3 p + \text{boundary term } (\rightarrow 0)$$

from a power series  
 $e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} = \left(-\frac{i}{\hbar} \nabla_p\right)^n e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}}$   
 $k=1,2,3; n \in \mathbb{N}$

$$\frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \left[ i\hbar \frac{\partial}{\partial t} \phi(\vec{p}, t) - \frac{p^2}{2m} \phi(\vec{p}, t) - V\left(\frac{i}{\hbar} \nabla_p\right) \phi(\vec{p}, t) \right] e^{\frac{i}{\hbar} \vec{p} \cdot \vec{r}} d^3 p = 0$$

$\Rightarrow$  Expression in bracket  $[...] = 0$  (apply inverse FT!)

[2] (a) Induction: eqs (2)+(3) obviously true for  $n=1$ ; suppose they are true for  $n-1$

$$\begin{aligned} \text{then } \left\{ \begin{aligned} [F, G^n] &= G^{n-1} [F, G] + [F, G^{n-1}] G = G^{n-1} [F, G] + (n-2) G^{n-2} [F, G] G \\ [F^n, G] &= F^{n-1} [F, G] + [F^{n-1}, G] F = F^{n-1} [F, G] + (n-2) F^{n-2} [F, G] F \end{aligned} \right\} \\ &\quad \uparrow \qquad \qquad \qquad \uparrow \\ &\quad \text{Product rule} \qquad \qquad \qquad \text{Product rule} \end{aligned}$$

$$= \begin{cases} (n-1) G^{n-1} [F, G] \\ (n-1) F^{n-1} [F, G] \end{cases}$$

Direct calculation is also possible.

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$$(b) [F, [G, H]] = [F, GH] - [F, HG] = G[F, H] + [F, G]H - H[F, G] - [F, H]G$$

Product rule

$$= [G, [F, H]] - [H, [F, G]] = -[H, [F, G]] - [G, [H, F]]$$

[3] (a) In  $\vec{p}$ -space:  $[\vec{L}, T] = [i\hbar \nabla_p \times \vec{p}, \frac{p^2}{2m}]$

x-component:  $[i\hbar (\frac{\partial}{\partial p_x} p_z - \frac{\partial}{\partial p_z} p_x), \frac{\sum p_i^2}{2m}] = \frac{i\hbar}{2m} \left( \frac{\partial}{\partial p_x} \underbrace{[\sum p_i^2]}_{=0} + \underbrace{[\frac{\partial}{\partial p_x} \sum p_i^2]}_{2p_x} p_x - \frac{\partial}{\partial p_z} \underbrace{[\sum p_i^2]}_{=0} - \underbrace{[\frac{\partial}{\partial p_z} \sum p_i^2]}_{2p_z} p_z \right) = 0$

Similar for y- and z- components.

In  $\vec{r}$ -space:  $[\vec{L}, T] = [\vec{r} \times (-i\hbar \nabla_r), -\frac{\hbar^2}{2m} \Delta]$

x-component:  $[-i\hbar (y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y}), -\frac{\hbar^2}{2m} \Delta]$

$$= \frac{i\hbar^3}{2m} \left( y \underbrace{[\frac{\partial}{\partial z}, \Delta]}_{=0} + \underbrace{[y, \Delta]}_{2 \frac{\partial}{\partial y}} \frac{\partial}{\partial z} - z \underbrace{[\frac{\partial}{\partial y}, \Delta]}_{=0} - \underbrace{[z, \Delta]}_{2 \frac{\partial}{\partial z}} \frac{\partial}{\partial y} \right) = 0$$

(b)  $\frac{d}{dt} \langle \vec{L} \rangle = \int_{\mathbb{R}^3} \frac{\partial \psi^*}{\partial t} \vec{L} \psi d^3r + \int_{\mathbb{R}^3} \psi^* \frac{\partial \vec{L}}{\partial t} \psi d^3r + \int_{\mathbb{R}^3} \psi^* \vec{L} \frac{\partial \psi}{\partial t} d^3r$

Schr. equ.  $\int_{\mathbb{R}^3} \underbrace{-\frac{i}{\hbar} (H\psi^*)}_{\text{partial integr.}} \vec{L} \psi d^3r + \int_{\mathbb{R}^3} \psi^* \vec{L} H \psi d^3r = \int_{\mathbb{R}^3} \frac{1}{i\hbar} \psi^* [\vec{L}, H] \psi d^3r$

$\int \Delta \psi^* \vec{L} \psi = \int \psi^* \Delta \vec{L} \psi + \text{boundary terms}$

(a)  $\frac{1}{i\hbar} \langle [\vec{L}, V] \rangle = -\langle [\vec{r} \times \nabla, V] \rangle = \langle \vec{r} \times \vec{F} \rangle$



[4] (a) Herzbacher p 39 has an elegant proof. Here let's try brute force math.

After looking at the first couple of nested commutators of type  $[F, G], [F, [F, G]], [F, [F, [F, G]]]$  etc. the following formula suggests itself:

$$\underbrace{[F, [F, \dots, [F, G] \dots]]}_{k \text{ commutators with } F} = \sum_{j=0}^k (-1)^j \binom{k}{j} F^{k-j} G F^j$$

Proof by induction:  $k=1$  clear; if formula holds for  $k-1$  we have for  $k$ :

$$\begin{aligned} & F \sum_{j=0}^{k-1} (-1)^j \binom{k-1}{j} F^{k-1-j} G F^j - \sum_{i=0}^{k-1} (-1)^i \binom{k-1}{i} F^{k-1-i} G F^i F \\ & \begin{array}{cccc} \swarrow j=0 \text{ term} & \swarrow j \neq 0 \text{ terms} & \swarrow j-i \text{ terms} & \swarrow j=k-1 \text{ term} \\ = F^k G & + \sum_{j=1}^{k-1} F^{k-j} G F^j (-1)^j \underbrace{\left[ \binom{k-1}{j} + \binom{k-1}{j} \right]}_{\binom{k}{j}} & - G F^k (-1)^{k-1} & \square \end{array} \end{aligned}$$

On the other hand

$$\begin{aligned} e^F G e^{-F} &= \left( \sum_{k=0}^{\infty} \frac{1}{k!} F^k \right) G \left( \sum_{k'=0}^{\infty} (-1)^{k'} \frac{1}{k'!} F^{k'} \right) \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \left( \sum_{j=0}^k F^{k-j} \frac{1}{(k-j)!} G F^j (-1)^j \frac{1}{j!} k! \right) \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \underbrace{[F, \dots, [F, G] \dots]}_{k \text{ times}} \square \end{aligned}$$

(b) Let's use the trick suggested by Herzbacher (other ways, e.g. calculating

$\log(e^F e^G)$  using the series for the logarithm can be found in the literature.)

For  $t \in \mathbb{R}$

Consider  $\frac{d}{dt} e^{tF} e^{tG} = e^{tF} F e^{tG} + e^{tF} G e^{tG} = (F + G + \frac{1}{2}[F, G]) e^{tF} e^{tG}$

usual product rule  
or explicitly via power series

$= (G + \frac{1}{2}[F, G]) e^{tF}$   
According to (a)!  
higher order commutators vanish

This is a diff. equation  $\frac{d\psi}{dt} = \text{const} * \psi$

with  $\psi = e^{tF} e^{tG}$ . The solution must be of the form  $e^{t * \text{const}}$ .

$\Rightarrow e^{tF} e^{tG} = e^{t(F+G+\frac{1}{2}[F, G])}$ . Now set  $t=1$ .