PHYS 606 – Spring 2015 – Homework IV – Solution

Problem [1]

(a) Merzbacher 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:

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

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

$$F \sum_{j=0}^{k-1} (-1)^j \binom{k-1}{j} F^{k-1-j} G F^j - \sum_{j=0}^{k-1} (-1)^j \binom{k-1}{j} F^{k-1-j} G F^j F$$

$$= \underbrace{F^k G}_{j=0\text{ term}} + \underbrace{\sum_{j=1}^{k-1} F^{k-j} G F^j (-1)^j \underbrace{\left[\binom{k-1}{j} + \binom{k-1}{j-1}\right]}_{\binom{k}{j}}}_{j\neq 0\text{ terms},\ j-1\text{ terms}} \underbrace{- G F^k (-1)^{k-1}}_{j=k-1\text{ term}}$$

$\square$

On the other hand

$$e^F G e^{-F} = \left(\sum_{k=0}^{\infty} \frac{1}{k!} F^k\right) G \left(\sum_{k'=0}^{\infty} (-1)^{k'} \frac{1}{k'!} F^{k'}\right)$$

$$= \sum_{k=0}^{\infty} \frac{1}{k!} \left(\sum_{j=0}^{k} F^{k-j} \frac{1}{(k-j)!} G F^j (-1)^j \frac{1}{j!} k! \right)$$

$$= \sum_{k=0}^{\infty} \frac{1}{k!} \underbrace{[F,\ldots,[F,G]]\ldots]}_{k\text{ times}}$$

$\square$

(b) Let's use the trick suggested by Merzbacher (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 $\frac{d}{dt} e^{tF} e^{tG} = e^{tF} F e^{tG} + \underbrace{e^{tF} G}_{} e^{tG} = \left(F + G + \frac{1}{2}[F,G]\right) e^{tF} e^{tG}$

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 $\frac{d\varphi}{dt} = \text{const} * \varphi$

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

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

Problem [2]

(a) $[\vec{r}\cdot\vec{p}, H] = p_i [\vec{r}\cdot\vec{p}, \frac{p_i}{2m}] + [\vec{r}\cdot\vec{p}, \frac{p_i}{2m}] p_i + r_i [p_i, V] + \overbrace{[r_i, V]}^{=0} p_i$

$= p_i r_j \underbrace{[p_j, \frac{p_i}{2m}]}_{=0} + p_i \underbrace{[r_j, \frac{p_i}{2m}]}_{\frac{i\hbar}{2m}\delta_{ij}} p_j + \underbrace{[r_j, \frac{p_i}{2m}]}_{\frac{i\hbar}{2m}\delta_{ij}} p_j p_i + \vec{r}\cdot(-i\hbar \nabla V)$

$= i\hbar \frac{p^2}{m} - i\hbar\, \vec{r}\cdot\nabla V = i\hbar\left(2T - \vec{r}\nabla V\right)$

$[\vec{p}\cdot\vec{r}, H] =$ ... completely analogous ... $= i\hbar(2T - \vec{r}\cdot\nabla V)$

(b) $[(\vec r\cdot\vec p)(\vec r\cdot\vec p), T] = (\vec r\cdot\vec p)\underbrace{[\vec r\cdot\vec p, T]}_{2i\hbar T}^{(a)} + \underbrace{[\vec r\cdot\vec p, T]}_{2i\hbar T}^{(a)}\vec r\cdot\vec p = 2i\hbar(\vec r\cdot\vec p\, T + T\,\vec r\cdot\vec p)$

$= 2i\hbar\{\vec r\cdot\vec p, T\}$

this sometimes denotes the <u>anti</u> commutator

$[(\vec r\cdot\vec p)(\vec p\cdot\vec r), T] = 2i\hbar(\vec r\cdot\vec p\, T + T\,\vec p\cdot\vec r)$

To see that both results are not the same apply these operators to test fcts. Here $\psi = e^{\frac{i}{\hbar}(\vec r\cdot\vec p - Et)}$ plane wave.

$T\psi = -\hbar^2\frac{\Delta\psi}{2m} = \frac{p^2}{2m}\psi$; $(\vec r\cdot\vec p)\psi = -i\hbar\,\vec r\cdot\nabla\psi = (\vec r\cdot\vec p)\psi$

$\vec p$ operator! $\vec p$ number, an eigenvalue of the operator $\vec p$!

$(\vec p\cdot\vec r)\psi = \vec p\cdot\vec r\,\psi - i\hbar\underbrace{(\nabla\vec r)}_{3}\psi$

operator number

one $\vec p$ in T applied to $\vec r\cdot\vec p$

$\Rightarrow [(\vec r\cdot\vec p)^2, T]\psi = 2i\hbar\left(\vec r\cdot\vec p\,\frac{p^2}{2m} + \frac{p^2}{2m}\vec r\cdot\vec p - 2i\hbar\frac{p^2}{2m}\right)\psi = \left(\frac{2i\hbar}{m}\vec r\cdot\vec p\, p^2 + \frac{2\hbar^2 p^2}{m}\right)\psi$

all numbers

$[(\vec r\cdot\vec p)(\vec p\cdot\vec r), T]\psi = 2i\hbar\left(\vec r\cdot\vec p\,\frac{p^2}{2m} + \frac{p^2}{2m}(\vec p\cdot\vec r - 3i\hbar)\underbrace{}_{-2i\hbar\frac{p^2}{2m}}\right)\psi = \left(\frac{2i\hbar}{m}(\vec r\cdot\vec p)p^2 + \frac{5\hbar^2}{m}p^2\right)\psi$

The two operators defined by the commutators are not the same.

c) $\{\vec r\cdot\vec p, H\} = \sum_{k=1}^{3}\left(p_k\underbrace{\frac{\partial H}{\partial p_k}}_{p_k/m} - r_k\underbrace{\frac{\partial H}{\partial r_k}}_{\partial V/\partial r_k}\right) = \frac{p^2}{m} - \vec r\cdot\nabla V = 2T - \vec r\cdot\nabla V$

$\{r_i, p_j\} = \sum_{k=1}^{3}(\delta_{ik}\delta_{jk} - 0) = \delta_{ij}$

So it seems $\underset{\text{operators}}{[A, B]} = i\hbar\underset{\text{cl. quantities}}{\{A, B\}}$

(d) $\{(\vec r\cdot\vec p)^2, T\} = \sum_{k=1}^{3}\left(2(\vec r\cdot\vec p)p_k\frac{p_k}{m} - 0\right) = 4\,\vec r\cdot\vec p\, T$

Caveat: obviously the order matters: $\frac{1}{i\hbar}[(\vec r\cdot\vec p)^2, H] = 4\cdot\frac{1}{2}(\vec r\cdot\vec p\, T + T\,\vec r\cdot\vec p) \neq 4\,\vec r\cdot\vec p\, T$ for operators

[3] (a) Hamilton-Jacobi: $\frac{\partial S}{\partial t} + \underbrace{\frac{1}{2m}\left(\nabla S - q\vec{A}\right)^2}_{H \text{ with } \vec{p} = \nabla S} + q\phi = 0$

Continuity equ.: $\frac{\partial \rho}{\partial t} + (\nabla \vec{v})\,\rho + \vec{v}\cdot\nabla\rho = 0 \Rightarrow \frac{\partial \rho}{\partial t} + \frac{\rho}{m}\nabla(\vec{p} - q\vec{A}) + \frac{1}{m}\nabla\rho\cdot(\vec{p} - q\vec{A}) = 0$
(I.5.3)

(b) Ansatz $\psi(\vec{r},t) = C e^{\frac{i}{\hbar}S}$ with C, S real into

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{1}{2m}\left(-i\hbar\nabla - q\vec{A}\right)^2 \psi + q\phi\psi$$

$$\Rightarrow \left(i\hbar \frac{1}{C}\frac{\partial C}{\partial t} - \frac{\partial S}{\partial t}\right)\psi = \frac{1}{2m}\Big(-\hbar^2\frac{\Delta C}{C} + (\nabla S)^2 - i\hbar\Delta S - i\hbar\frac{2}{C}\nabla C\cdot\nabla S + q^2A^2$$
$$+ i\hbar\frac{2}{C}q\vec{A}\cdot\nabla C - 2q\vec{A}\cdot\nabla S + i\hbar q\nabla\vec{A}\Big)\psi + q\phi\psi$$

Drop ψ from eq. and separate imaginary and real part:

Re: $0 = \frac{\partial S}{\partial t} + \frac{1}{2m}\Big((\nabla S)^2 - \underbrace{\hbar^2\frac{\Delta C}{C}}_{0 \text{ for } \hbar\to 0} - 2\nabla S\cdot(q\vec{A}) + (q\vec{A})^2\Big) + q\phi$

$$\Rightarrow 0 = \frac{\partial S}{\partial t} + \frac{1}{2m}\left(\nabla S - q\vec{A}\right)^2 + q\phi \qquad \text{Hamilton-Jacobi!}$$

Im: $\underbrace{2C\frac{\partial C}{\partial t}}_{\frac{\partial \rho}{\partial t}} = \frac{1}{2m}\Big(-\underbrace{2C^2}_{\rho}\underbrace{\Delta S}_{\nabla\vec{p}} - \underbrace{4C\nabla C}_{2\nabla\rho}\cdot\underbrace{\nabla S}_{\vec{p}} + \underbrace{4C(\nabla C)}_{2\nabla\rho}\cdot(q\vec{A}) + 2\underbrace{C^2}_{\rho}q\nabla\vec{A}\Big)$

where $\rho = C^2 = |\psi|^2$; $\Rightarrow \frac{\partial \rho}{\partial t} + \frac{\rho}{m}\nabla(\vec{p} - q\vec{A}) + \frac{1}{m}\nabla\rho\cdot(\vec{p} - q\vec{A}) = 0$

continuity equation.

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

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

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

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

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

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

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

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

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

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

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

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