PHYS 606 – Spring 2015 – Homework VII – Solution

Problem [1]

(a) $$\frac{\partial W}{\partial t} = \frac{1}{(2\pi\hbar)^3}\int \frac{\partial\psi^*}{\partial t}(\vec{r}-\tfrac{\vec{r}'}{2},t)\,\psi(\vec{r}+\tfrac{\vec{r}'}{2},t)\,e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}'}d^3r'$$

$$+\frac{1}{(2\pi\hbar)^3}\int \psi^*(\vec{r}-\tfrac{\vec{r}'}{2},t)\,\frac{\partial\psi}{\partial t}(\vec{r}+\tfrac{\vec{r}'}{2},t)\,e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}'}d^3r'$$

$$=\frac{1}{(2\pi\hbar)^3}\int \frac{i}{\hbar}H\psi^*(\vec{r}-\tfrac{\vec{r}'}{2},t)\,\psi(\vec{r}+\tfrac{\vec{r}'}{2},t)\,e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}'}d^3r'$$

$$+\frac{1}{(2\pi\hbar)^3}\int \psi^*(\vec{r}-\tfrac{\vec{r}'}{2},t)\left(-\frac{i}{\hbar}\right)H\psi(\vec{r}+\tfrac{\vec{r}'}{2},t)\,e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}'}d^3r' \qquad (*)$$

$H = T+V$ First consider only kinetic part $T=-\frac{\hbar^2}{2m}\Delta$

$$\frac{1}{(2\pi\hbar)^3}\left(-\frac{\hbar^2}{2m}\right)\int \frac{i}{\hbar}\Big(\underbrace{\nabla^k_{\vec{r}-\frac{\vec{r}'}{2}}}_{=-2\nabla_{\vec{r}'}}\nabla^k_{\vec{r}-\frac{\vec{r}'}{2}}\psi^*(\vec{r}-\tfrac{\vec{r}'}{2})\Big)\psi(\vec{r}+\tfrac{\vec{r}'}{2})\,e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}'}d^3r'$$

$$-\int\frac{i}{\hbar}\psi^*(\vec{r}-\tfrac{\vec{r}'}{2})\Big(\underbrace{\nabla^k_{\vec{r}+\frac{\vec{r}'}{2}}}_{=+2\nabla_{\vec{r}'}}\nabla^k_{\vec{r}+\frac{\vec{r}'}{2}}\psi(\vec{r}+\tfrac{\vec{r}'}{2})\Big)e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}'}d^3r'$$

$$\underset{\text{part. int.}}{=}\frac{1}{(2\pi\hbar)^3}\frac{-i\hbar}{2m}\Bigg[\int 2\Big(\underbrace{\nabla^k_{\vec{r}-\frac{\vec{r}'}{2}}}_{-2\nabla_{\vec{r}'}}\psi^*(\vec{r}-\tfrac{\vec{r}'}{2})\Big)\Big(\nabla^k_{\vec{r}'}\psi(\vec{r}+\tfrac{\vec{r}'}{2})\Big)e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}'}d^3r'$$

$$+\int 2\Big(\underbrace{\nabla^k_{\vec{r}-\frac{\vec{r}'}{2}}}_{=\nabla^k_{\vec{r}}}\psi^*(\vec{r}-\tfrac{\vec{r}'}{2})\Big)\psi(\vec{r}+\tfrac{\vec{r}'}{2})\left(-\frac{i}{\hbar}p^k\right)e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}'}d^3r'$$

$$-\int(-2)\Big(\nabla^k_{\vec{r}'}\psi^*(\vec{r}-\tfrac{\vec{r}'}{2})\Big)\Big(\underbrace{\nabla^k_{\vec{r}+\frac{\vec{r}'}{2}}}_{2\nabla^k_{\vec{r}'}}\psi(\vec{r}+\tfrac{\vec{r}'}{2})\Big)e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}'}d^3r'$$

$$-\int(-2)\,\psi^*(\vec{r}-\tfrac{\vec{r}'}{2})\Big(\underbrace{\nabla^k_{\vec{r}+\frac{\vec{r}'}{2}}}_{=\nabla^k_{\vec{r}}}\psi(\vec{r}+\tfrac{\vec{r}'}{2})\Big)\left(-\frac{i}{\hbar}p^k\right)e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}'}d^3r'\Bigg]$$

$$=-\frac{1}{2m}p^k\frac{2}{(2\pi\hbar)^3}\Bigg[\int\Big(\nabla^k_{\vec{r}}\psi^*(\vec{r}-\tfrac{\vec{r}'}{2})\Big)\psi(\vec{r}+\tfrac{\vec{r}'}{2})\,e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}'}d^3r$$

$$+\int\psi^*(\vec{r}-\tfrac{\vec{r}'}{2})\Big(\nabla^k_{\vec{r}}\psi(\vec{r}+\tfrac{\vec{r}'}{2})\Big)e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}'}d^3r$$

$$= -\frac{\vec{p}}{m}\cdot\nabla_{\vec{p}} W(\vec{r},\vec{p},t)$$

$\Rightarrow$ For free particles $\frac{\partial W}{\partial t} + \frac{\vec{p}}{m}\cdot\nabla W = 0$

(b) Need to consider the potential energy term in (*) (1-D only)

$$\frac{1}{2\pi\hbar}\frac{i}{\hbar}\int \psi^*(x-\tfrac{x'}{2})\Big[\underbrace{V(x-\tfrac{x'}{2})}_{\sum_{\ell=0}^{\infty}\frac{1}{\ell!}(-\frac{x'}{2})^{\ell}\frac{d^{\ell}V}{dx^{\ell}}}-\underbrace{V(x+\tfrac{x'}{2})}_{\sum_{\ell=0}^{\infty}\frac{1}{\ell!}(\frac{x'}{2})^{\ell}\frac{d^{\ell}V}{dx^{\ell}}}\Big]\psi(x+\tfrac{x'}{2})\,e^{-\frac{i}{\hbar}px'}\,dx'$$

$$= \frac{1}{2\pi\hbar}\int \psi^*(x-\tfrac{x'}{2})\psi(x+\tfrac{x'}{2})\,\frac{2i}{\hbar}\sum_{\ell=0}^{\infty}\frac{1}{(2\ell+1)!}\left(\frac{i\hbar}{2}\right)^{2\ell+1}\frac{d^{2\ell+1}V}{dx^{2\ell+1}}\frac{d^{2\ell+1}}{dp^{2\ell+1}}e^{-\frac{i}{\hbar}px'}\,dx'$$

$$= -\frac{2}{i\hbar}\sum_{\ell=0}^{\infty}\frac{1}{(2\ell+1)!}\left(-\frac{i\hbar}{2}\right)^{2\ell+1}\frac{d^{2\ell+1}V}{dx^{2\ell+1}}\frac{\partial^{2\ell+1}W}{\partial p^{2\ell+1}}$$

$$\Rightarrow \frac{\partial W}{\partial t} = -\frac{p}{m}\frac{\partial W}{\partial x} - \frac{2}{i\hbar}\sum_{\ell=0}^{\infty}\frac{1}{(2\ell+1)!}\left(-\frac{i\hbar}{2}\right)^{2\ell+1}\frac{d^{2\ell+1}V}{dx^{2\ell+1}}\frac{\partial^{2\ell+1}W}{\partial p^{2\ell+1}} \qquad (**)$$

On the other hand:

$$-\{\{W,H\}\} = -\frac{2}{i\hbar}W\sum_{\ell=0}^{\infty}\frac{1}{(2\ell+1)!}\left(\frac{i\hbar}{2}\right)^{2\ell+1}\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p}-\frac{\overleftarrow{\partial}}{\partial p}\frac{\overrightarrow{\partial}}{\partial x}\right)^{2\ell+1}\left(\frac{p^2}{2m}+V(x)\right)$$

• all mixed terms $\frac{\overrightarrow{\partial}^k}{\partial p^k}\frac{\overrightarrow{\partial}^n}{\partial x^n}$ $k>1, n>1$ vanish when acting on $H=\frac{p^2}{2m}+V$

• all terms $\left(\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial p}\right)^{2\ell+1}=0$ except for $\ell=0$ since $\frac{\partial^k}{\partial p^k}H=0$ for $k\geq 3$

$$= -\frac{2}{i\hbar}\sum_{\ell=0}^{\infty}\frac{1}{(2\ell+1)!}\left(-\frac{i\hbar}{2}\right)^{2\ell+1}\left(\frac{\partial^{2\ell+1}}{\partial p^{2\ell+1}}W\right)\left(\frac{d^{2\ell+1}}{dx^{2\ell+1}}V\right) - \frac{\partial W}{\partial x}\underbrace{\frac{\partial H}{\partial p}}_{p/m} \qquad (***)$$

same as (**)!

(c) Keep only $\ell=0,1$ terms in (***):

$$\frac{\partial W}{\partial t} + \frac{p}{m}\frac{\partial W}{\partial x} \underbrace{- \frac{dV}{dx}}_{=+F \text{ "force"}}\frac{\partial W}{\partial p} = -\frac{\hbar^2}{4}\frac{d^3V}{dx^3}\frac{\partial^3 W}{\partial p^3} + O(\hbar^4)$$

Problem [2]

(a) $E > V_0 \Rightarrow$ plane waves everywhere. General solution

$$\psi(x) = \begin{cases} A e^{ikx} + B e^{-ikx} & \text{f. } x < -a \\ C e^{ik'x} + D e^{-ik'x} & \text{f. } -a < x < a \\ E e^{ikx} + F e^{-ikx} & \text{f. } x > a \end{cases} \qquad k = \frac{1}{\hbar}\sqrt{2mE} \qquad k' = \frac{1}{\hbar}\sqrt{2m(E-V_0)}$$

Matching: @ $x = -a$: $A e^{-ika} + B e^{+ika} = C e^{-ik'a} + D e^{+ik'a}$ (1)

$$ik\left(A e^{-ika} - B e^{+ika}\right) = ik'\left(C e^{-ik'a} - D e^{+ik'a}\right) \qquad (2)$$

$\Rightarrow ik(1)+(2)$: $A = \frac{1}{2k} e^{ika}\left[C(k+k')e^{-ik'a} + D(k-k')e^{ik'a}\right]$ (1')

$ik(1)-(2)$: $B = \frac{1}{2k} e^{-ika}\left[C(k-k')e^{-ik'a} + D(k+k')e^{ik'a}\right]$ (2')

@ $x = +a$: $C e^{ik'a} + D e^{-ik'a} = E e^{ika} + F e^{-ika}$ (3)

$$ik'\left(C e^{ik'a} - D e^{-ik'a}\right) = ik\left(E e^{ika} - F e^{-ika}\right) \qquad (4)$$

$\Rightarrow C = \frac{1}{2k'} e^{-ik'a}\left[E(k'+k)e^{ika} + F(k'-k)e^{-ika}\right]$ (3')

$D = \frac{1}{2k'} e^{ik'a}\left[E(k'-k)e^{ika} + F(k'+k)e^{-ika}\right]$ (4')

Eliminate C, D from (1') through (4'):

$$A = \frac{1}{4kk'} E\left[(k+k')^2 e^{2i(k-k')a} - (k-k')^2 e^{2i(k+k')a}\right]$$

$$+ \frac{1}{4kk'} F\left[(k'^2-k^2)e^{-2ik'a} - (k'^2-k^2)e^{2ik'a}\right]$$

$$= E e^{2ika}\left[\frac{k^2+k'^2}{4kk'} 2i\sin(-2k'a) + \frac{2kk'}{4kk'} 2\cos(-2k'a)\right]$$

$$+ F \frac{k'^2-k^2}{4kk'} 2i\sin(-2k'a)$$

$$B = \frac{1}{4kk'} E\left[(k^2-k'^2)\, e^{-2ik'a} - (k^2-k'^2)\, e^{+2ik'a}\right] + \frac{1}{4kk'} F\left[(k-k')^2 e^{-2i(k+k')a} + (k+k')^2 e^{2i(k'-k)a}\right]$$

$$= E\,\frac{k^2-k'^2}{4kk'}\, 2i\sin(-2k'a) + F e^{-2ika}\left[\frac{k^2+k'^2}{4kk'}\, 2i\sin 2k'a + \frac{2kk'}{4kk'}\, 2\cos 2k'a\right]$$

$\Rightarrow \begin{pmatrix} A \\ B \end{pmatrix} = M \begin{pmatrix} E \\ F \end{pmatrix}$ with M-matrix with $\varepsilon' = \frac{k'}{k} + \frac{k}{k'} = \frac{k^2+k'^2}{kk'}$

$\eta' = \frac{k'}{k} - \frac{k}{k'} = \frac{k'^2-k^2}{kk'}$

$$M = \begin{pmatrix} \left(\cos 2k'a - i\frac{\varepsilon'}{2}\sin 2k'a\right) e^{2ika} & -\frac{i\eta'}{2}\sin 2k'a \\ \frac{i\eta'}{2}\sin 2k'a & \left(\cos 2k'a + i\frac{\varepsilon'}{2}\sin 2k'a\right) e^{-2ika} \end{pmatrix}$$

$T = \left|\frac{E}{A}\right|^2 = |M_{11}|^2 = \cos^2 2k'a + \frac{\varepsilon'^2}{4}\sin^2 2k'a$, $R = 1 - T$

$T \to 1$ for $k' \to k$, i.e. $E \gg V_0$

(b) Situation obviously exactly the same as (a) just replace

$k' = \frac{1}{\hbar}\sqrt{2m(E+V_0)}$.

Problem [3]

$$-\frac{\hbar^2}{2m}\Delta\phi + V\phi = E\phi$$

$$V(x) = \begin{cases} \infty & \text{for } x<0 \\ \frac{1}{2}m\omega^2 x^2 & \text{for } x>0 \end{cases} \Rightarrow \phi(x) \sim \begin{cases} 0 & \text{for } x<0 \\ \psi_n(x) & \text{for } x>0 \end{cases}$$

$\underbrace{\psi_n}_{\text{"full"}}$ harm. osc. solutions

$\psi(x)=0$ @ $V(x)=\infty$ clear from finiteness of energy

Matching condition from continuity equation $\psi(x\to 0^-) = \psi(x\to 0^+)$

$\Rightarrow$ only $\psi_n(x)$ with $\psi_n(x)=0$ allowed $\Rightarrow$ <u>odd n</u> solutions.

$\Rightarrow$ Energy eigenvalues $\quad E_n = \left(n+\frac{1}{2}\right)\hbar\omega \quad$ with $n = 1, 3, 5, \ldots$

i.e. $E_1 = \frac{3}{2}\hbar\omega, \quad E_3 = \frac{7}{2}\hbar\omega, \ldots$

Eigenfcts. $\phi_n(x) = \begin{cases} 0 & \text{for } x<0 \\ 2^{-\frac{n}{2}+1}\frac{1}{\sqrt{n!}}\left(\frac{m\omega}{\hbar\pi}\right)^{1/4} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-\frac{m\omega}{2\hbar}x^2} & \text{for } x>0 \end{cases}$

Normalization adjustments: $\int_{\mathbb{R}}|\phi_n|^2dx = \int_0^\infty \underbrace{|\psi_n|^2}_{\text{even fct. in } x}dx = \frac{1}{2}\int_0^\infty|\psi_n|^2dx = \frac{1}{2}$

$\Rightarrow$ add'l factor $\sqrt{2}$ needed for proper normalization

Problem [4]

Let $\varphi(x)$ be an extremum of $S[\varphi]$ and $\varphi(x,\alpha) = \varphi(x) + \alpha\,\eta(x)$ a 1-parameter curve through it with $\eta(x) = 0$ on the boundary $\partial\Gamma$

$\varphi(x,\alpha)$ for small α then is a variation around $\varphi(x)$ and <u>any</u> allowed variation can be written as an $\varphi(x,\alpha)$ with some suitable $\eta(x)$.

Then for variation $\varphi(x,\alpha)$

$$\delta S = \frac{\partial S}{\partial \alpha}\delta\alpha = \int_\Gamma \left(\frac{\partial \mathcal{L}}{\partial \varphi}\frac{\partial \varphi}{\partial \alpha} + \sum_{i=1}^{N} \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \varphi}{\partial x_i}\right)} \underbrace{\frac{\partial\left(\frac{\partial \varphi}{\partial x_j}\right)}{\partial \alpha}}_{=\frac{\partial}{\partial x_j}\frac{\partial \varphi}{\partial \alpha}} \right) d^N x \; \delta\alpha$$

$$\overset{\text{part. int.}}{=} \int_\Gamma \left(\frac{\partial \mathcal{L}}{\partial \varphi} - \sum_{j=1}^{N} \frac{\partial}{\partial x_j}\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \varphi}{\partial x_j}\right)} \right) \underbrace{\frac{\partial \varphi}{\partial \alpha}}_{\eta(x)} \delta\alpha \; dx \; + \text{boundary term}$$

($\frac{\partial \varphi}{\partial \alpha} = 0$ on $\partial\Gamma$ since $\eta = 0$ on $\partial\Gamma$)

Thus $\frac{\partial \mathcal{L}}{\partial \varphi} - \sum_{j=1}^{N} \frac{\partial}{\partial x_j}\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \varphi}{\partial x_j}\right)} = 0 \Rightarrow \delta S = 0$

Conversely, if $\delta S = 0$ for <u>any</u> allowed choice of $\eta(x)$ then $\frac{\partial \mathcal{L}}{\partial \varphi} - \sum_{j=1}^{N} \frac{\partial}{\partial x_j}\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \varphi}{\partial x_j}\right)} = 0$