PHYS 606 – Spring 2014 – HW VIII Solution

[1] (a) $H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + C\,\delta(x)$, $C>0$; Solve $H\psi = E\psi$

Ansatz $$\psi(x) = \begin{cases} A e^{ikx} + B e^{-ikx} & \text{for } x<0 \\ E e^{ikx} + F e^{-ikx} & \text{for } x>0 \end{cases}$$

Recall: for finite discontinuities in $V(x)$ we have conditions $\psi(x)$, $\psi'(x)$ continuous

for infinite discontinuities in $V(x)$ we have $\psi(x)$ continuous, but $\psi'(x)$ might not be.

Thus at $x=0$: $A+B = E+F$ (1)

For behavior of ψ' integrate S.E. over range $(-\varepsilon, \varepsilon)$ with $\epsilon \to 0$:

$$\underbrace{\int_{-\varepsilon}^{+\varepsilon}\left(-\frac{\hbar^2}{2m}\right)\frac{d^2}{dx^2}\psi(x)dx}_{\left(-\frac{\hbar^2}{2m}\right)\left[\psi'(\varepsilon)-\psi'(-\varepsilon)\right]} + \underbrace{C\int_{-\varepsilon}^{+\varepsilon}\delta(x)\,\psi(x)\,dx}_{C\psi(0)} = \underbrace{E\int_{-\varepsilon}^{+\varepsilon}\psi(x)\,dx}_{2\varepsilon E\psi(0)\to 0} \qquad \left(\psi' = \frac{d\psi}{dx}\right)$$

$$\Rightarrow -ik(A-B-E+F)\left(-\frac{\hbar^2}{2m}\right) + C(A+B) = 0 \qquad (2)$$

From (1): $B = E+F-A \overset{(2)}{\Rightarrow} -ik\frac{\hbar^2}{2m}(2A-2E) \overset{(1)}{=} C(E+F) \Rightarrow A = i\frac{mC}{\hbar^2 k}(E+F) + E$

$$\Rightarrow B = -i\frac{mC}{\hbar^2 k}(E+F) + F$$

$$\Rightarrow M = \begin{pmatrix} 1 + i\frac{m}{\hbar^2 k}C & +i\frac{m}{\hbar^2 k}C \\ -i\frac{m}{\hbar^2 k}C & 1 - i\frac{m}{\hbar k}C \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} A \\ B \end{pmatrix} = M\begin{pmatrix} E \\ F \end{pmatrix}$$

Coefficient of transmission

$$T = \frac{|E|^2}{|A|^2} = |M_{11}|^{-2} = \frac{1}{1 + \frac{m^2}{\hbar^4 k^2}C^2}$$

$$R = 1 - T = \frac{\frac{m^2}{\hbar^4 k^2}C^2}{1 + \frac{m^2}{\hbar^4 k^2}C^2}$$

(2)

(b) The rectangular barrier $\sqcap$ with width $2a$ and height V_0 is a representation of $C'\delta(x)$ for $a \to 0$, $V_0 \to \infty$ with $2aV_0 = C'$ fixed

The last condition is necessary so that $\int_{\mathbb{R}} \sqcap * f(x)\,dx \xrightarrow[V_0\to\infty]{a\to 0} C' f(0) = \int_{\mathbb{R}} \delta(x) f(x)\,dx$

II.2.2, case $E < V_0$: $M_{barrier} = \begin{pmatrix} \left(\cosh 2\kappa a + \frac{i\varepsilon}{2}\sinh 2\kappa a\right)e^{2ika} & +\frac{i\eta}{2}\sinh 2\kappa a \\ -\frac{i\eta}{2}\sinh 2\kappa a & \left(\cosh 2\kappa a - \frac{i\varepsilon}{2}\sinh 2\kappa a\right)e^{-2ika} \end{pmatrix}$

$\kappa = \frac{1}{\hbar}\sqrt{2m(V_0 - E)} \to \infty$ and $\kappa a \sim \sqrt{V_0}\,a \to 0 \quad \Rightarrow \cosh 2\kappa a \to 1$

$\varepsilon = \frac{\kappa}{k} - \frac{k}{\kappa} \Rightarrow \frac{i\varepsilon}{2}\sinh 2\kappa a = \frac{i\kappa}{2k} 2\kappa a + O(a^2) \approx \frac{i}{\hbar^2 k} 2mV_0 a \to i\frac{mC'}{\hbar^2 k}$

similarly: $\frac{i\eta}{2}\sinh 2\kappa a \to i\frac{mC'}{\hbar^2 k}$

$\Rightarrow M_{barrier} \to \begin{pmatrix} 1 + i\frac{mC}{\hbar^2 k} & i\frac{mC}{\hbar^2 k} \\ -i\frac{mC'}{\hbar^2 k} & 1 - i\frac{mC'}{\hbar^2 k} \end{pmatrix}$ as in (a)

[2] 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 $\varphi(x,\alpha)$

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

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

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

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

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

[3](a) $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi + b|x|\psi = E\psi$

symmetric pot. energy $\Rightarrow$ H commutes with parity operator $\Rightarrow$ energy eigenfcts. can be chosen even or odd

Thus it is sufficient to solve $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + bx\psi = E\psi$ for $x>0$

Substitution: define $z = \left(\frac{2mb}{\hbar^2}\right)^{1/3}\left(x - \frac{E}{b}\right) \Rightarrow \frac{d^2}{dx^2} = \left(\frac{2mb}{\hbar^2}\right)^{2/3}\frac{d^2}{dz^2}$

$\Rightarrow \frac{d^2\psi}{dz^2} - z\psi = 0$

$\Rightarrow$ Physical solution (regular) Airy fct. $Ai(z)$

(b) From (a) for eigenvalue E_n the eigenfct. is (for $x>0$)

$\psi_n(x) = C_n\, Ai\left(\left(\frac{2mb}{\hbar^2}\right)^{1/3}\left(x - \frac{E_n}{b}\right)\right)$ and C_n determined by $\int_{\mathbb{R}} |\psi_n|^2 dx = 1$

$\psi_n(x) = \psi_n(-x)$ for $x<0$ for ~~od~~ even eigenfcts.

$\psi_n(x) = -\psi_n(-x)$ for $x<0$ for odd eigenfcts.

Even eigenfcts. require $\frac{d}{dx}\psi_n(0) = 0$

Odd eigenfcts. require $\psi_n(0) = 0$

$\Rightarrow$ "odd eigenvalues" given by zeros of $Ai\left(-\left(\frac{2mb}{\hbar^2}\right)^{1/3}\frac{E_n}{b}\right)$, "even eigenvalues" given by zeros of $\frac{d}{dx}Ai\left(-\left(\frac{2mb}{\hbar^2}\right)^{1/3}\frac{E_n}{b}\right)$

Smallest zeros (absolute value) of Ai and Ai' are $-2.33811 =: -a_1$

and $-1.01879 =: -a_0$ resp.

$$\Rightarrow \quad E_0 = a_0 \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3} \qquad \text{(even)}$$

$$E_1 = a_1 \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3} \qquad \text{(odd)}$$

[4] (a) Trial fct. $\psi(x) = \left(\frac{2\alpha^2}{\pi}\right)^{1/4} e^{-\alpha^2 x^2}$ (i.e. $\int_{\mathbb{R}} |\psi|^2 dx = 1$ for all $\alpha \in \mathbb{R}$)

$$\langle H \rangle = \int_{\mathbb{R}} -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}\psi(x) + b|x|\psi(x)\, dx$$

$$= -\frac{\hbar^2}{2m}\left(\frac{2\alpha^2}{\pi}\right)^{1/2} \int_{\mathbb{R}} (-2\alpha^2 + 4\alpha^4 x^2)\, e^{-2\alpha^2 x^2} dx + 2b \int_0^\infty x e^{-2\alpha^2 x^2} dx \left(\frac{2\alpha^2}{\pi}\right)^{1/2}$$

$$= -\frac{\hbar^2}{2m}\left(-2\alpha^2 + 4\alpha^4 \frac{1}{4\alpha^2}\right) + 2b \frac{1}{4\alpha^2}\sqrt{\frac{2}{\pi}}\,\alpha = \frac{\hbar^2 \alpha^2}{2m} + \frac{b}{\sqrt{2\pi}\,\alpha}$$

$$\frac{\partial \langle H \rangle}{\partial \alpha} = 0 \Rightarrow \frac{\hbar^2 \alpha}{m} - \frac{b}{\sqrt{2\pi}\,\alpha^2} = 0 \Rightarrow \alpha = \left(\frac{bm}{\sqrt{2\pi}\,\hbar^2}\right)^{1/3}$$

$$\Rightarrow \langle H \rangle = \frac{(\hbar b)^{2/3}}{m^{1/3}} \frac{1}{2(2\pi)^{1/3}} + \frac{(\hbar b)^{2/3}}{m^{1/3}} \frac{1}{(2\pi)^{1/3}} = \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3} \frac{3}{2\pi^{1/3}}$$

$$\approx 1.024 \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3} \quad \text{vs} \quad E_0 = 1.019 \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3}$$

(b) Odd trial fct. $\psi(x) = 2a^{3/2}\left(\frac{2}{\pi}\right)^{1/4} x\, e^{-\alpha^2 x^2}$ ($\int_{\mathbb{R}} |\psi|^2 dx = 1$ with this prefactor)

$$\langle H \rangle = -\frac{\hbar^2}{2m} 4a^3 \left(\frac{2}{\pi}\right)^{1/2} \int (-6\alpha^2 x^2 + 4\alpha^4 x^4)\, e^{-2\alpha^2 x^2} + 2b\, 4a^3 \left(\frac{2}{\pi}\right)^{1/2} \int_0^\infty x^3 e^{-2\alpha^2 x^2} dx$$

$$= \frac{3\hbar^2 \alpha^2}{2m} + \frac{2b}{\sqrt{2\pi}\,\alpha}$$

$$\frac{\partial \langle H \rangle}{\partial \alpha} = 0 \Rightarrow \frac{3\hbar^2 \alpha}{m} - \frac{2b}{\sqrt{2\pi}\,\alpha^2} = 0 \Rightarrow \alpha = \left(\frac{\frac{2}{3} bm}{\sqrt{2\pi}\,\hbar^2}\right)^{1/3}$$

$$\Rightarrow \langle H \rangle = \left(\frac{\hbar^2 b^2}{2m}\right)^{1/3} \left(\frac{3}{2}\left(\frac{2^2}{3^2 \pi}\right)^{1/3} + \frac{2\, 3^{1/3}}{(2\pi)^{1/3}}\right) = \left(\frac{\hbar^2 b}{2m}\right)^{1/3} 3\left(\frac{3}{2\pi}\right)^{1/3}$$

$$\approx 2.3448 \left(\frac{\hbar^2 b}{2m}\right)^{1/3} \quad \text{vs} \quad E_0 = 2.3381 \left(\frac{\hbar^2 b}{2m}\right)^{1/3}.$$

(c) This is a bad trial fct. since the first derivative is discontinuous. Nevertheless one can calculate $\langle H \rangle$. $\psi(x) = e^{-\beta|x|}$ (not normalized)

$\Rightarrow \psi(x) = e^{-\beta x}\Theta(x) + e^{\beta x}\Theta(-x)$ $\qquad \Theta$: Heaviside step fct.

$$\langle T \rangle = -\frac{\hbar^2}{2m} \int_{\mathbb{R}} \frac{d}{dx}\left[e^{-\beta x}\delta(x) - e^{\beta x}\delta(x) - \beta e^{-\beta x}\Theta(x) + \beta e^{\beta x}\Theta(-x)\right] dx$$

$$= -\frac{\hbar^2}{2m}\left[\dots\right]_{+\infty}^{-\infty} = 0$$

$$\langle V \rangle = 2b \int_0^\infty x e^{-\beta x} dx = \frac{2b}{\beta^2} \qquad \Rightarrow \langle H \rangle = \frac{2b}{\beta^2} \quad \text{no local extrema.}$$