Quantum Mechanics II HW 2

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1. (a) For the 1d Schrödinger equation with potential V(x), use the standard WKB expansion

$$\psi(x) = \exp\left[\frac{i}{\hbar}(S_0 + \hbar S_1 + \hbar^2 S_2 + \hbar^3 S_3 + ...)\right]$$

to find expressions for S_0 , S_1 , S_2 and S_3 , and show that both S_1 and S_3 are in fact total derivatives.

Denoting S(x) as

$$S(x) = S_0(x) + \hbar S_1(x) + \hbar^2 S_2(x) + h^3 S_3(x) + \dots$$

and $\psi(x)$ as

$$\psi(x) = \exp\left[\frac{i}{\hbar}S(x)\right]$$

(no loss of generality for S(x) complex), our TISE reads

$$-(S')^{2} + i\hbar S'' + [p(x)]^{2} = 0$$
(1)

where

$$p(x) \equiv \sqrt{E - V(x)}.$$

If we now substitute the expansion of S(x) into (1), keeping terms up to $\mathcal{O}(\hbar^3)$ we have

$$0 = [p(x)]^{2} - (S'_{0})^{2}$$

$$+ \hbar [-2S'_{0}S'_{1} + iS''_{0}]$$

$$+ \hbar^{2} [-2S'_{0}S'_{2} + iS''_{1} - (S'_{1})^{2}]$$

$$+ \hbar^{3} [-2S'_{0}S'_{3} - 2S'_{1}S'_{2} + iS''_{2}]$$

As another power series in \hbar , we equate each "coefficient" of \hbar to zero identically. Thus

$$[p(x)]^2 = (S'_0)^2$$

 $\to S_0(x) = \pm \int^x dx' \ p(x')$

$$2S_0'S_1' = iS_0''$$

$$S'_{1} = \frac{i}{2} \frac{p'}{p}$$

$$\rightarrow S'_{1} = \left[\frac{i}{2} \ln p\right]'$$

$$2S'_{0}S'_{2} = iS''_{1} - (S'_{1})^{2}$$

$$S'_{2} = \frac{1}{2S'_{0}} \left[iS''_{1} - (S'_{1})^{2}\right]$$

$$\rightarrow S'_{2} = \frac{1}{4p} \left[\frac{3}{2} \left(\frac{p'}{p}\right)^{2} - \frac{p''}{p}\right]$$

$$2S'_{0}S'_{3} = -2S'_{1}S'_{2} + iS''_{2}$$

$$S'_{3} = \frac{1}{2S'_{0}} \left[-2S'_{1}S'_{2} + iS''_{2}\right]$$

$$S'_{3} = \frac{3i}{4} \left[\frac{p'p''}{p^{4}} - \frac{p'^{3}}{p^{5}} - \frac{1}{6}\frac{p'''}{p^{3}}\right]$$

$$\rightarrow S'_{3} = \frac{i}{16} \left[\frac{3p'^{2} - 2pp''}{p^{4}}\right]'$$

We see that S_1 and S_3 can be written in explicit form (in terms of V(x) and its higher derivatives) while S_0 and S_2 are given as integral forms.

(b) Now make a different expansion, writing

$$\psi(x) = A(x) \exp\left[\frac{i}{h}W(x)\right]$$

where the amplitude function A(x) and phase function W(x) are both real. Separate the Schrodinger equation into real and imaginary parts to find an expression for the amplitude A(x) in terms of the phase W(x).

Writing the TISE as

$$\left[\frac{d^2}{dx^2} + \left(\frac{p(x)}{\hbar} \right)^2 \right] \psi = 0$$

we substitute $\psi(x) = A(x) \exp\left[\frac{i}{\hbar}W(x)\right]$ to arrive at

$$i\hbar[2A'W' + AW''] + [Ap^2 - A(W')^2 + \hbar^2 A''] = 0.$$

Now setting the imaginary and real parts equal to zero, we get two equations:

$$2A'W' + AW'' = 0 (2)$$

$$Ap^2 - AW'^2 + \hbar^2 A'' = 0 (3)$$

We can express (2) in terms of the total derivative

$$\left[\ln(A^2W')\right]' = 0.$$

Hence an equation for A(x) in terms of W(x) goes as

$$A(x) = \frac{C}{\sqrt{W'(x)}}.$$

(c) Show that the resulting equation for W(x) can be solved by an expansion of the form

$$W(x) = W_0 + \hbar^2 W_2 + \hbar^4 W_4 + \dots$$

involving only terms with even powers of \hbar .

First, we form the differential equation for W(x) by substituting $A(x) = C/\sqrt{W'(x)}$ into (4)

$$\frac{p^2}{\sqrt{W'}} - (W')^{3/2} + \hbar^2 \left[\frac{3}{4} \frac{(W'')^2}{(W')^{5/2}} - \frac{W'''}{2(W')^{3/2}} \right] = 0.$$

We may simplify by multiplying through by $(W')^{5/2}$

$$p^{2}(W')^{2} - (W')^{4} + \hbar^{2} \left[\frac{3}{4} (W'')^{2} - \frac{1}{2} W' W''' \right] = 0.$$
 (4)

If we now substitute the even expansion of W(x) up to $\mathcal{O}(\hbar^4)$ and equate each "coefficient" of \hbar to zero, we have

$$\mathcal{O}(\hbar^0): \quad p^2 W_0'^2 = W_0'^4$$

 $\to W_0(x) = \int^x dx' \ p(x')$

$$\mathcal{O}(\hbar^2): 8p^2 W_0' W_2' - 16(W_0')^3 W_2' + 3(W_0')^2 - 2W_0' W_0'' = 0$$
$$-8p^3 W_2' + 3(p')^2 - 2pp'' = 0$$
$$\rightarrow W_2'(x) = \frac{1}{4p} \left[\frac{3}{2} \left(\frac{p'}{p} \right)^2 - \frac{p''}{p} \right]$$

$$\begin{split} \mathcal{O}(\hbar^4): \quad & 4p^2(W_2')^2 - 24(W_0')^2(W_2')^2 + 8p^2W_0'W_4' - 16(W_0')^3W_4' \\ & \quad + 6W_0''W_2'' - 2W_2'W_0''' - 2W_0'W_2''' = 0 \\ & \quad - 8p^3W_2' + 3(p')^2 - 2pp'' = 0 \\ & \quad \rightarrow W_4'(x) = -\frac{297}{128}\frac{(p')^4}{p^7} + \frac{99}{32}\frac{(p')^2p''}{p^6} - \frac{13}{32}\frac{(p'')^2}{p^5} - \frac{5}{8}\frac{p'p^{(3)}}{p^5} + \frac{1}{16}\frac{p^{(4)}}{p^4} \end{split}$$

If we desired, we could continue calculating even higher order terms of \hbar^{2n} . Thus we can see that an expansion of W(x) in even powers of \hbar presents a solution to (4).

(d) Show that your expressions for $W_0(x)$ and $W_2(x)$, and the corresponding expression for A(x) to this order, are consistent with your results for $S_0(x)$, $S_1(x)$, and $S_2(x)$ in (a), to $\mathcal{O}(\hbar^2)$.

The wavefunction can be expressed in terms of A(x) and W(x) as

$$\psi(x) = A(x) \exp\left[\frac{i}{\hbar}W(x)\right]$$

$$\simeq \exp\left[\frac{i}{\hbar}(W_0 + \hbar^2 W_2) + \ln[(W_0' + \hbar^2 W_2')^{-1/2}]\right].$$

Alternatively, we may express it in terms of S(x) as

$$\psi(x) \simeq \exp\left[\frac{i}{\hbar}(S_0 + \hbar S_1 + \hbar^2 S_2)\right].$$

For our results to be consistent, we must equate the arguments in the exponentials

$$\frac{i}{\hbar}(W_0 + \hbar^2 W_2) + \ln[(W_0' + \hbar^2 W_2')^{-1/2}] = \frac{i}{\hbar}(S_0 + \hbar S_1 + \hbar^2 S_2)$$

or

$$F = G$$

where F denotes the LHS and G the RHS. For F we have

$$F = \frac{i}{\hbar}W_0 + i\hbar W_2 - \frac{1}{2} \left[\ln(p + \hbar^2 W_2') \right]$$

while for G

$$G = \frac{i}{\hbar}S_0 + i\hbar S_2 - \frac{1}{2}\ln p.$$

If we note from earlier that $S_0 = W_0$ and $S_2 = W_2$ and then keep terms up to $\mathcal{O}(\hbar^2)$ such that

$$\ln(p + \hbar^2 W_2') \to \ln p$$
.

then we can conclude that F = G, thus showing consistency between results.

**As an aside, perhaps a better way to show the last step would be

$$\ln(W_0' + \hbar^2 W_2') = \ln(W_0') + \ln\left(1 + \hbar^2 \frac{W_2'}{W_0'}\right)$$
$$\approx \ln(W_0') + \hbar^2 \frac{W_2'}{W_0'} + \dots$$

where, when we multiply both F and G by an overall \hbar and take up to $\mathcal{O}(\hbar^2)$ only $\ln(p)$ remains.**

2. (a) Use WKB for bound states the estimate the energy for the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \lambda x^{2N}$$

where $\lambda > 0$ and N is an integer. Comment on the limit $N \to \infty$.

For a bound state with two turning points, the WKB estimation for energy can used

$$k \int_{x_1}^{x_2} dx \sqrt{1 - \frac{V(x)}{E}} = \left(n + \frac{1}{2}\right) \pi \quad (n = 0, 1, 2, 3, ..)$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}.$$

For this problem, the two turning points are located at

$$x = \pm \left(\frac{E}{\lambda}\right)^{\frac{1}{2N}}$$

thus our energy estimation will be

$$2k \int_0^{\left(\frac{E}{\lambda}\right)^{\frac{1}{2N}}} dx \sqrt{1 - \frac{\lambda x^{2N}}{E}} = \left(n + \frac{1}{2}\right) \pi.$$

This yields energies

$$E = \left(\frac{\hbar^2 \pi}{2m}\right)^{\frac{N}{N+1}} \left(\frac{\Gamma\left[\frac{1}{2}\left(3 + \frac{1}{N}\right)\right]}{\Gamma\left[\frac{1}{2}\left(2 + \frac{1}{N}\right)\right]}\right)^{\frac{2N}{N+1}} \lambda^{\frac{1}{N+1}} \left(n + \frac{1}{2}\right)^{\frac{2N}{N+1}}.$$

For N=2 and $\lambda=m\omega^2/2$ we get the familiar harmonic oscillator

$$E = \hbar\omega \left(n + \frac{1}{2} \right).$$

In the limit of $N \to \infty$

$$E = \frac{\hbar^2 \pi^2 n^2}{8m} \quad (n = 1, 2, 3..)$$

which is precisely the energy spectrum of the infinite square well with width L=1.

(b) Use WKB to estimate the transmission probability for scattering from the potential

$$V = -\lambda x^{2N}$$

where $\lambda > 0$ and N is an integer, and for energies **below** the top of the barrier.

For a single barrier, the relation for the transmission probability is

$$T = \exp(-\gamma)$$

where

$$\gamma \equiv \frac{2}{\hbar} \int_{x_1}^{x_2} \sqrt{2m(V(x) - E)}$$

and $(x_2 - x_1)$ represents the tunneling region. The points of entry/exit for this potential are located at

$$x = \pm \left(\frac{|E|}{\lambda}\right)^{\frac{1}{2N}}$$

thus

$$\gamma = 4k \int_0^{\left(\frac{|E|}{\lambda}\right)^{\frac{1}{2n}}} dx \sqrt{1 + \frac{\lambda x^{2N}}{E}}$$
$$= 2k\sqrt{\pi} \left(\frac{|E|}{\lambda}\right)^{\frac{1}{2N}} \frac{\Gamma\left[\frac{1}{2}\left(2 + \frac{1}{N}\right)\right]}{\Gamma\left[\frac{1}{2}\left(3 + \frac{1}{N}\right)\right]}$$

where

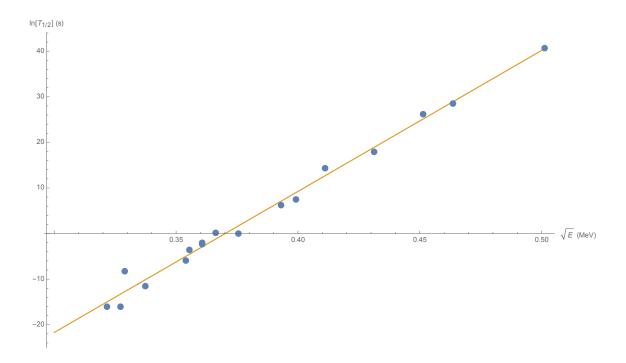
$$k = \frac{\sqrt{2m|E|}}{\hbar}.$$

Therefore the probability of transmission is

$$T = \exp\left[2k\sqrt{\pi} \left(\frac{|E|}{\lambda}\right)^{\frac{1}{2N}} \frac{\Gamma\left[\frac{1}{2}\left(2 + \frac{1}{N}\right)\right]}{\Gamma\left[\frac{1}{2}\left(3 + \frac{1}{N}\right)\right]}\right].$$

Since $\gamma \propto |E|$, the transmission probability increases as you approach the top of the barrier.

3. (a) Using the data for Thorium in the attached table, make a plot of $\ln T_{1/2}$ versus $1/\sqrt{E}$



(b) Your answer in (a) should show approximately linear behavior, over a huge range of energies. Use WKB to find a rough estimate for the slope coefficient. [Note that thorium has Z = 90, and the mass of an α particle is approximately 3724 Mev/ c^2]. How good is the WKB estimate?

We may use the tunneling probability to find half life of Thorium. In utilizing the WKB in three dimensions, we can use an effective potential that includes the angular momentum barrier such that

$$\gamma = \frac{2}{\hbar} \int_{r_0}^{r_1} dr \sqrt{2m(V_{eff}(r) - E)}$$

where

$$V_{eff}(r) = \frac{\hbar^2}{2m} \frac{(l + \frac{1}{2})^2}{r^2} + \frac{2(Z - 2)e^2}{r}.$$

Here we have used the Langer substitution along with a repulsive (Z-2) Coulomb potential representing the nuclear force after emission of an alpha particle. Gamma then becomes

$$\gamma = 2 \int_{r_0}^{r_1} dr \, \frac{1}{r} \left[\left(l + \frac{1}{2} \right)^2 + \frac{2m}{\hbar^2} \left[2(Z - 2)e^2r - Er^2 \right] \right]^{1/2}.$$

The first turning point may be approximated by

$$r_0 \approxeq (1.0 \text{ fm}) A^{1/3}$$

with A being the number of neutrons and protons. Then, r_1 may be found by solving for the positive root in the quadratic equation for

$$E = V_{eff}(r)$$

If we now set

$$m = 3724 \text{ MeV}/c^2$$

$$l = 0$$

$$Z = 90,$$

we may get an estimation for $\gamma(E)$. Then, the lifetime can be found using

$$\tau = \frac{1}{R}$$

where

$$R = \frac{[2m(E + V_0)]^{1/2}}{2mr_0} \exp(-\gamma).$$

Then we should be able to find the slope using

$$\frac{d}{d\left(\frac{1}{\sqrt{E}}\right)} \left(\ln[T_{1/2}(\tau(1/\sqrt{E}))] \right).$$