Further Quantum Theory: Problem Sheet 4

Hilary Term 2020

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SAMPLE SOLUTIONS

4.1 Anharmonic oscillator WKB

Consider a (possibly anharmonic) oscillator in one dimension, with Hamiltonian

$$H = \tfrac{1}{2m}P^2 + \left(\tfrac{1}{2}m\omega^2 X^2\right)^k \ .$$

Derive the (integral) WKB quantization condition that implicitly determines the quantum energy levels of this system in the semi-classical approximation. By rescaling the integrand, show that the energy levels are given by

$$E_n = \left(\frac{\pi^{1/2}\Gamma(\frac{3k+1}{2k})}{2\Gamma(\frac{2k+1}{2k})}\hbar\omega(n+\tfrac{1}{2})\right)^{\frac{2k}{k+1}} \ ,$$

where you will need to utilize the integral formula

$$\int_{-1}^{1}\sqrt{1-x^{2k}} = \frac{\pi^{1/2}\Gamma(\frac{2k+1}{2k})}{\Gamma(\frac{3k+1}{2k})} \ .$$

Check the case $k=1$, which corresponds to the simple harmonic oscillator.

The quantization condition for energy levels is given by

$$\frac{1}{\hbar}\int_{x_1}^{x_2}\sqrt{2m(E-V(x))}dx = \pi(n+1/2) \ , \qquad n=0,1,2,\ldots \ ,$$

where x_1 and x_2 are the left and right classical turning points for a particle moving in the potential $V(x)$ with energy E. In the example at hand, we rescale by defining $y = (\frac{1}{2}m\omega^2)^{1/2}E^{-1/2k}x$, in terms of which our condition is

$$\frac{2E^{\frac{k+1}{2k}}}{\hbar\omega}\int_{-1}^{1}\sqrt{1-y^{2k}}dy = \pi(n+1/2) \ , \qquad n=0,1,2,\ldots \ .$$

Using the integral identity given in the problem, this gives the quantization condition

$$\frac{2E^{\frac{k+1}{2k}}}{\hbar\omega}\frac{\pi^{1/2}\Gamma(\frac{2k+1}{2k})}{\Gamma(\frac{3k+1}{2k})} = \pi(n+1/2) \ , \qquad n=0,1,2,\ldots \ .$$

Solving for E gives the expression given in the statement of the problem. Note that for $k=1$, this gives the exact result,

$$E_n = \left(\frac{\pi^{1/2}\Gamma(2)}{2\Gamma(\frac{3}{2})}\hbar\omega(n+\tfrac{1}{2})\right) = \hbar\omega(n+\tfrac{1}{2}) \ .$$

4.2 Spherical WKB approximation

Find the WKB approximation for stationary, spherically symmetric, bound states (*i.e.*, states with angular momentum $l=0$ and $E<0$) of an electron of mass m in a Coulomb potential, with the usual Hydrogen-like Hamiltonian,

$$E = \frac{P^2}{2m} - \frac{Zq_e{}^2}{r} \ .$$

(i) Imposing that the wave function is bounded at $r=0$ will lead to a Bohr-Sommerfeld-like quantization condition. Compare this to the exact answer for the Hydrogen energy levels.

(ii) Now analyze the case with angular momentum $l \neq 0$. Here there is both an inner and an outer turning point. Remember that the principle quantum number in the Hydrogen atom is given by $n = k + l + 1$, where k is the number of zeroes of the radial wavefunction. Compare your answer to the exact energy levels.

(iii) The *Langer correction* to the WKB analysis of the Hydrogen atom proceeds by replacing $l(l+1)$ in the centrifugal potential term with $(l + \frac{1}{2})^2$. This includes the case $l = 0$. Check that the WKB results improve dramatically upon including the Langer correction.

[*You will also need to be able to perform the integral*

$$\int_a^b \frac{\sqrt{(r-a)(b-r)}}{r} = \frac{\pi}{2}\left(a^{1/2} - b^{1/2}\right)^2 , \qquad a < b .$$

I've changed to denoting the charge of the electron as q_e *to avoid any ambiguity related to Euler's constant.*]

(i) The radial WKB wave function in the classically allowed region is given by

$$R(r) = \frac{a}{r\sqrt{p(r)}} \exp\left(\frac{i}{\hbar}\int_0^r p(s)ds\right) + \frac{b}{r\sqrt{p(r)}} \exp\left(\frac{-i}{\hbar}\int_0^r p(s)ds\right) .$$

The requirement that the function be bounded as $r \to 0$ means that the two complex exponentials must combine into a sin function,

$$R(r) = \frac{const.}{r\sqrt{p(r)}} \sin\left(\frac{1}{\hbar}\int_0^r p(s)ds\right) .$$

The WKB connection rules at the classical turning point $r = r_*$ require that the argument of the sine function be of the form $3\pi/4 + n\pi$ for $n = 0, 1, 2, \ldots$. Thus our quantization condition is given by

$$\tfrac{1}{\hbar}\int_0^{r_*} p(r)dr = \pi\left(\tfrac{3}{4} + n\right) .$$

Now for our case, with $V(r)$ given by a Coulomb-like potential, this becomes

$$\tfrac{\sqrt{-2mE}}{\hbar}\int_0^{r_*} \sqrt{-1 - \tfrac{Zq_e^2}{Er}}dr = \pi\left(\tfrac{3}{4} + n\right) .$$

Defining $r = -Zq_e^2 s/E$, this becomes (remember $E < 0$ for a bound state)

$$\tfrac{Zq_e^2\sqrt{2m}}{\sqrt{-E}}\int_0^1 (\tfrac{1}{s} - 1)^{\frac{1}{2}}dr = \pi\hbar\left(\tfrac{3}{4} + n\right) .$$

The integral is evaluated using the substitution $s = \sin^2\theta$, and we obtain

$$\tfrac{Zq_e^2\sqrt{m}}{\sqrt{-2E}} = \hbar\left(\tfrac{3}{4} + n\right) \quad \Longrightarrow \quad E_n = -\tfrac{Z^2 q_e^4 m}{2\hbar^2(n+\frac{3}{4})^2} = \tfrac{E_0}{(n+\frac{3}{4})^2} .$$

Requiring that $n = 1, 2, 3 \ldots$, we rewrite this as

$$E_n = \tfrac{E_0}{(n-\frac{1}{4})^2} ,$$

which should be compared with the exact result that doesn't have the shift by $-1/4$ in the denominator.

(ii) If we allow $\ell \neq 0$, then in the effective radial problem there is a centrifugal term that leads to an inner turning point as well. Thus we are in the more standard two-turning point scenario, and the Bohr-Sommerfeld quantization rule is

$$\tfrac{1}{\hbar}\int_{r_{in}}^{r_{out}} p(r)dr = \pi\left(\tfrac{1}{2} + k\right) , \quad k = 0, 1, 2, \ldots$$

With the Coulomb potential and centrifugal term contributing to an effective potential, this gives the condition

$$\tfrac{\sqrt{-2mE}}{\hbar}\int_{r_{in}}^{r_{out}} \left(-1 - \tfrac{Zq_e^2}{Er} + \tfrac{\hbar^2\ell(\ell+1)}{2mEr^2}\right)^{1/2} dr = \pi\left(\tfrac{1}{2} + k\right) , \quad k = 0, 1, 2, \ldots$$

which we can rewrite

$$\frac{\sqrt{-2mE}}{\hbar}\int_{r_{in}}^{r_{out}}\frac{\sqrt{(r-r_{in})(r_{out}-r)}}{r}dr = \pi\left(\tfrac{1}{2}+k\right) \ , \quad k=0,1,2,\dots$$

where we've used that r_{in} and r_{out} are the two roots to the quadratic under the radical. Using the integral formula given in the problem, we have

$$\frac{\sqrt{-2mE}}{\hbar}\frac{\pi}{2}\left(r_{in}+r_{out}-2\sqrt{r_{in}r_{out}}\right) = \pi\left(\tfrac{1}{2}+k\right) \ , \quad k=0,1,2,\dots$$

From the form of the quadratic, we see that

$$r_{in}+r_{out} = -\frac{Zq_e^2}{E} \ , \qquad r_{in}\times r_{out} = -\frac{\hbar^2\ell(\ell+1)}{2mE} \ ,$$

So our quantization condition simplifies to

$$\frac{\sqrt{m}Zq_e^2}{\sqrt{-2E}} - \hbar\sqrt{\ell(\ell+1)} = \hbar\left(\tfrac{1}{2}+k\right) \ , \quad k=0,1,2,\dots$$

which we solve for E,

$$E = -\frac{mZ^2q_e^4}{2\hbar^2\left(k+\frac{1}{2}+\sqrt{\ell(\ell+1)}\right)^2} \ , \quad k=0,1,2,\dots$$

Now the exact answer is given by

$$E = -\frac{mZ^2q_e^4}{2\hbar^2\left(k+\ell+1\right)^2} \ , \quad k=0,1,2,\dots$$

and the approximation is quite good for large values of k and/or ℓ.

(iii) If we make the (apparently *ad hoc*) replacement $\ell(\ell+1)\to(\ell+1/2)^2$ in the centrifugal term, then in the previous part we would have found the exact answer!

4.3 Quantum tunnelling with WKB

A particle is incident from the left upon a potential barrier of the form

$$V(x) = \begin{cases} 0 \ , & x<-a \ , \\ a^2-x^2 \ , & -a<x<a \ , \\ 0 \ , & x>a \ . \end{cases}$$

Set up a WKB approximation for the (non-normalizable) stationary wave function describing this system for both cases $E>a^2$ and $E<a^2$. For the latter case, determine the *transmission amplitude* through, and the *reflection amplitude* off of, the classical barrier as a function of the energy of the incident particle.

When $E>a^2$ there are no classical turning points, so the entire WKB wavefunction will represent right-moving particles:

$$\psi^{\rm WKB}(x) = \frac{1}{(2m(E-V(x)))^{1/4}}\exp\left(\frac{i}{\hbar}\int^x\sqrt{2m(E-V(x))}\right) \ .$$

To fix the overall constant, we start the integration at $x=-a$, and we have

$$\psi^{\rm WKB}(x) = \begin{cases} \frac{1}{(2mE)^{1/4}}\exp\left(\frac{i\sqrt{2mE}}{\hbar}x\right) & x<-a \\ \frac{1}{(2m(E-a^2+x^2))^{1/4}}\exp\left(\frac{i}{\hbar}\int_{-a}^x\sqrt{2m(E-a^2+x^2)}\right) & x\in[-a,a] \\ \frac{1}{(2mE)^{1/4}}\exp\left(\frac{i\sqrt{2mE}}{\hbar}(x-a)+i\phi\right) & x>a \end{cases} \ ,$$

where we have introduced the phase[1]

$$\phi = \frac{\sqrt{2m}}{\hbar}\int_{-a}^{a}(E - a^2 + x^2) = \frac{\sqrt{2m}}{\hbar}\left(aE^{1/2} + \tfrac{E-a^2}{2}\log\left(\tfrac{E^{1/2}+a}{E^{1/2}-a}\right)\right) \ .$$

At the level of the WKB approximation, here we have $T = 1$ and $R = 0$, so the WKB approximation is insensitive to quantum reflection off of a classically surmountable barrier. (In the exact solution, there is such an effect, and $R \neq 0$.)

Now turn to the case $E < a^2$, so we are studying quantum tunnelling through the barrier. In this case there are classical turning points at $x_\pm = \pm(a^2 - E)^{1/2}$, and we have to introduce WKB wave functions in the two classically allowed regions to the left and right and in the classically forbidden region in the middle.

$$\psi^{\rm WKB}(x) = \begin{cases} \frac{A_I}{p^{1/2}}\exp\left(-\frac{i}{\hbar}\int_x^{x_-}p(s)ds\right) + \frac{B_I}{p^{1/2}}\exp\left(\frac{i}{\hbar}\int_x^{x_-}p(s)ds\right) & x < -x_- \\ \frac{A_{II}}{q^{1/2}}\exp\left(\frac{1}{\hbar}\int_{x_-}^{x}q(s)ds\right) + \frac{B_{II}}{q^{1/2}}\exp\left(-\frac{1}{\hbar}\int_{x_-}^{x}q(s)ds\right) & x_- < x < x_+ \\ \frac{A_{III}}{p^{1/2}}\exp\left(\frac{i}{\hbar}\int_{x_+}^{x}p(s)ds\right) & x > x_+ \end{cases} \ ,$$

We will also write the wave-function in the forbidden region as

$$\frac{\tilde{A}_{II}}{q^{1/2}}\exp\left(-\frac{1}{\hbar}\int_x^{x_+}q(s)ds\right) + \frac{\tilde{B}_{II}}{q^{1/2}}\exp\left(\frac{1}{\hbar}\int_x^{x_+}q(s)ds\right) \ ,$$

where the coefficients are related according to $\tilde{A}_{II} = A_{II}\Gamma$ and $\tilde{B}_{II} = B_{II}\Gamma^{-1}$, where

$$\Gamma = \exp\left(\frac{1}{\hbar}\int_{x_-}^{x_+}q(s)ds\right) \ .$$

Now we need to use the WKB connection formulae to relate the coefficients in the different regions. At a turning point x_* where the classically allowed region is on the left, the relation between the WKB wave functions on the left and right is given by

$$\frac{2C}{p^{1/2}}\cos\left(\frac{1}{\hbar}\int_x^{x_*}p(s)ds - \frac{\pi}{4}\right) + \frac{D}{p^{1/2}}\cos\left(\frac{1}{\hbar}\int_x^{x_*}p(s)ds + \frac{\pi}{4}\right) \leftrightarrow \frac{C}{q^{1/2}}\exp\left(-\frac{1}{\hbar}\int_{x_*}^{x}q(s)ds\right) + \frac{D}{q^{1/2}}\exp\left(\frac{1}{\hbar}\int_{x_*}^{x}q(s)ds\right)$$

while at a turning point where the classically allowed region is on the right, the relation is given by

$$\frac{2C}{p^{1/2}}\cos\left(\frac{1}{\hbar}\int_{x_*}^{x}p(s)ds - \frac{\pi}{4}\right) + \frac{D}{p^{1/2}}\cos\left(\frac{1}{\hbar}\int_{x_*}^{x}p(s)ds + \frac{\pi}{4}\right) \leftrightarrow \frac{C}{q^{1/2}}\exp\left(-\frac{1}{\hbar}\int_x^{x_*}q(s)ds\right) + \frac{D}{q^{1/2}}\exp\left(\frac{1}{\hbar}\int_x^{x_*}q(s)ds\right)$$

Using the second set of relations, we can find the relationship between $(\tilde{A}_{II}, \tilde{B}_{II})$ and A_{III}. In particular, the wavefunction in region III can be expressed in terms of the coefficients in region II according to

$$\frac{\tilde{A}_{II}e^{-i\pi/4} + \tilde{B}_{II}e^{i\pi/4}/2}{p^{1/2}}\exp\left(\frac{i}{\hbar}\int_{x_+}^{x}p(s)ds\right) + \frac{\tilde{A}_{II}e^{i\pi/4} + \tilde{B}_{II}e^{-i\pi/4}/2}{p^{1/2}}\exp\left(-\frac{i}{\hbar}\int_{x_+}^{x}p(s)ds\right)$$

which, since the left-moving component must be zero, tells us that

$$\tilde{A}_{II}e^{i\pi/4} + \tilde{B}_{II}e^{-i\pi/4}/2 = 0 \ , \qquad \tilde{A}_{II}e^{-i\pi/4} + \tilde{B}_{II}e^{i\pi/4}/2 = A_{III} \ ,$$

which we solve to give us (after using the relation between (A_{II}, B_{II}) and $(\tilde{A}_{II}, \tilde{B}_{II})$):

$$A_{III} = 2\Gamma e^{-i\pi/4}A_{II} \ , \qquad B_{II} = -2i\Gamma^2 A_{II}.$$

Applying the first connection relations, we can then related these to A_I and B_I. The result is

$$A_I = e^{i\pi/4}A_{II}\left(-2i\Gamma^2 - \tfrac{i}{2}\right) \ , \qquad B_I = e^{-i\pi/4}A_{II}\left(-2i\Gamma^2 + \tfrac{i}{2}\right)$$

[1] Don't worry too much about getting this exactly, it's just a laborious integral.

We can now compute the reflection and transmission coefficients directly

$$R = \frac{|B_I|^2}{|A_I|^2} = \left(\frac{4\Gamma^2-1}{4\Gamma^2+1}\right)^2 \approx 1 \quad \text{for} \quad \Gamma \gg 1 \ ,$$
$$T = \frac{|A_{III}|^2}{|A_I|^2} = \frac{4\Gamma^2}{(2\Gamma^2+\frac{1}{2})^2} \approx \Gamma^{-2} \quad \text{for} \quad \Gamma \gg 1 \ ,$$

The approximate behaviour of T is what we would get from doing a very rough estimate of the tunnelling rate like we did for the model of α-decay in lectures.
To be complete, we can do the integral to compute Γ:

$$\sqrt{2m}\int_{x_-}^{x_+}\sqrt{(a^2-E)-x^2}dx = (a^2-E)\sqrt{2m}\int_{-1}^{1}\sqrt{1-y^2}dy = \pi(a^2-E)\sqrt{\tfrac{m}{2}} \ .$$

$$\Gamma = \exp\left(\frac{\pi m^{\frac{1}{2}}(a^2-E)}{\hbar\sqrt{2}}\right) \ .$$

When our particle is far from being able to classically overcome the barrier ($E \ll a^2$), then we see the expected exponential suppression of tunnelling.

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