Physics 742 – Graduate Quantum Mechanics 2

Solutions to Chapter 12

3. [15] Joe isn't getting any smarter. He is attempting to find the ground state energy of an infinite square well with allowed region $-a < x < a$ using the trial wave function (in the allowed region) $\psi(x) = 1 - x^2/a^2 + B(1 - x^4/a^4)$, where B is a variational parameter. Estimate the ground state energy and compare to the exact value.

Since there is no potential, we need to calculate only the normalization and kinetic terms, which are

$$\langle \psi | \psi \rangle = \int_{-a}^{a} \left[1 - x^2/a^2 + B\left(1 - x^4/a^4\right)\right]^2$$

$$= 2\int_0^a \left[1 - 2x^2/a^2 + x^4/a^4 + 2B\left(1 - x^2/a^2 - x^4/a^4 + x^6/a^6\right) + B^2\left(1 - 2x^4/a^4 + x^8/a^8\right)\right] dx$$

$$= 2a\left[1 - \tfrac{2}{3} + \tfrac{1}{5} + 2B\left(1 - \tfrac{1}{3} - \tfrac{1}{5} + \tfrac{1}{7}\right) + B^2\left(1 - \tfrac{2}{5} + \tfrac{1}{9}\right)\right] = a\left(\tfrac{16}{15} + \tfrac{256}{105}B + \tfrac{64}{45}B^2\right),$$

$$\langle \psi | P^2 | \psi \rangle = \left\| P|\psi\rangle \right\|^2 = \int_{-a}^{a} \left| -i\hbar \frac{d}{dx}\left[1 - x^2/a^2 + B\left(1 - x^4/a^4\right)\right]\right|^2 dx = 2\hbar^2 \int_0^a \left(2x/a^2 + 4Bx^3/a^4\right)^2 dx$$

$$= 2\hbar^2 \int_0^a \left(4x^2/a^4 + 16Bx^4/a^6 + 16B^2x^6/a^8\right) dx = 8\hbar^2\left(\tfrac{1}{3} + \tfrac{4}{5}B + \tfrac{4}{7}B^2\right)\Big/a.$$

The expectation value of the energy, as a function of B, is therefore

$$E(B) = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\hbar^2 \langle \psi | P^2 | \psi \rangle}{2m\langle \psi | \psi \rangle} = \frac{8\hbar^2}{2ma^2 16} \cdot \frac{\tfrac{1}{3} + \tfrac{4}{5}B + \tfrac{4}{7}B^2}{\tfrac{1}{15} + \tfrac{16}{105}B + \tfrac{4}{45}B^2} = \frac{3\hbar^2}{4ma^2} \cdot \frac{60B^2 + 84B + 35}{28B^2 + 48B + 21}.$$

To minimize this, we set the derivative equal to zero, which yields

$$0 = \frac{\left(28B^2 + 48B + 21\right)\left(120B + 84\right) - \left(60B^2 + 84B + 35\right)\left(56B + 48\right)}{\left(28B^2 + 48B + 21\right)^2},$$

$$0 = 528B^2 + 560B + 84 = 16\left(33B^2 + 35B + \tfrac{21}{4}\right),$$

$$B = \frac{-35 \pm \sqrt{35^2 - 4 \cdot 33 \cdot \tfrac{21}{4}}}{2 \cdot 33} = \frac{-35 \pm \sqrt{532}}{66} = -0.1808 \quad \text{or} \quad -0.8798.$$

We now substitute each of these into the expression for $E(B)$, to yield

$$E(-0.1808) = \frac{3\hbar^2}{4ma^2} \cdot \frac{60(-0.1808)^2 + 84(-0.1808) + 35}{28(-0.1808)^2 + 48(-0.1808) + 21} = \frac{1.233719\hbar^2}{ma^2},$$

$$E(-0.8798) = \frac{3\hbar^2}{4ma^2} \cdot \frac{60(-0.8798)^2 + 84(-0.8798) + 35}{28(-0.8798)^2 + 48(-0.8798) + 21} = \frac{12.76628\hbar^2}{ma^2}.$$

We are trying to minimize the energy, which clearly corresponds to the first case, not the second (which is a maximum).

Since the well has width $2a$, the exact energy is

$$E = \frac{\pi^2\hbar^2}{2m(2a)^2} = \frac{\pi^2\hbar^2}{8ma^2} \approx \frac{1.233701\hbar^2}{ma^2} \quad ,$$

or a difference of about 15 parts per million. Not bad, for a simple polynomial estimate!

4. [10] A particle lies in one dimension with Hamiltonian $H = P^2/2m + F|X|$. Using the WKB method, our goal is to find the eigenenergies of this Hamiltonian.

(a) [2] For energy *E*, find the classical turning points *a* and *b*.

We first find the classical turning points, which are solutions to $E = F|x|$. The solutions are $|x| = E/F$, $x = \pm E/F$, so $a = -E/F$ and $b = E/F$.

(b)[4] Perform the integral required by the WKB method.

The WKB formula for the energy is

$$\pi\hbar\left(n+\tfrac{1}{2}\right) = \int_a^b \sqrt{2m\left[E - V(x)\right]}\,dx = \int_{-E/F}^{E/F} \sqrt{2m\left(E - F|x|\right)}\,dx$$

$$= 2\int_0^{E/F} \sqrt{2m(E - Fx)}\,dx = -\frac{2}{2mF}\cdot\frac{2}{3}\left[2m(E - Fx)\right]^{\frac{3}{2}}\Big|_0^{E/F} = \frac{2(2mE)^{3/2}}{3mF}.$$

(c) [4] Solve the resulting equation for E_n

Solving for E, we have

$$(2mE)^{3/2} = \tfrac{3}{2}\pi\hbar\left(n+\tfrac{1}{2}\right)mF,$$

$$E_n = \frac{\left[\tfrac{3}{2}\pi\hbar\left(n+\tfrac{1}{2}\right)mF\right]^{2/3}}{2m} = \left[\frac{3\pi\hbar\left(n+\tfrac{1}{2}\right)F}{4\sqrt{2m}}\right]^{2/3}.$$

5. **[10] We never completed a discussion of how to normalize the WKB wave function, given by eq. (12.29b).**

   (a) [3] Treating the average value of $\sin^2 \to \frac{1}{2}$, and including only the wave function in the classically allowed region $a < x < b$, write an integral equation for *N*.

In general, we must demand that the integral of the wave function squared equal one. This wave function is only appropriate in the classically allowed region, so

$$1 = \int_a^b |\psi(x)|^2 \, dx = \int_a^b \frac{N^2 dx}{\sqrt{E - V(x)}} \sin^2\left[\frac{1}{\hbar}\int_a^x dx' \sqrt{2m[E - V(x)]} + \gamma\right] \approx \frac{N^2}{2}\int_a^b \frac{dx}{\sqrt{E - V(x)}},$$

$$\frac{2}{N^2} = \int_a^b \frac{dx}{\sqrt{E - V(x)}}.$$

   (b) [2] We are now going to find a simple formula for *N* in terms of the *classical* period *T*, the time it takes for the particle to get from point *a* to *b* and back again. As a first step, find an expression for the velocity $v(x) = dx/dt$ as a function of position. This is purely a classical problem!

We use the classical formula for the total energy, which is kinetic energy plus potential energy, $E = \frac{1}{2}mv^2 + V(x)$. Solving for the speed *v*, we have

$$v = \sqrt{\frac{2[E - V(x)]}{m}}.$$

   (c) [3] Use the equation in part (b) to get an integral expression for the time it takes to go from *a* to *b*. Double it to get an expression for *T*.

The time for the period is

$$T = 2\int_{x=a}^{x=b} dt = 2\int_{x=a}^{x=b} \frac{dx}{dx/dt} = \int_a^b \frac{2dx}{\sqrt{2[E - V(x)]/m}} = \sqrt{2m}\int_a^b \frac{dx}{\sqrt{E - V(x)}}.$$

   (d) [2] Relate your answers in parts (a) and (c) to get a NON-integral relationship between the normalization *N* and the classical period *T*.

It is obvious that the integrals in the two parts are very similar. Solving for the integral in (c), we see that

$$\frac{T}{\sqrt{2m}} = \int_a^b \frac{dx}{\sqrt{E - V(x)}} = \frac{2}{N^2},$$

$$N^2 T = 2\sqrt{2m}.$$