CAS PY 452 — Quantum Physics II

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Date: Nov 9, 2022

Discussion Notes
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WKB wave-function and energies for the 'quantum bouncing ball'

Problem: Consider the 'quantum bouncing ball.' That is, consider the single-particle system governed by the Hamiltonian, $\hat{H} = \frac{\hat{p}^2}{2m} + V(x)$, where the potential is,

$$V(x) = \begin{cases} mgx & x > 0 \\ \infty & x \leq 0, \end{cases} \tag{1}$$

where $g > 0$. Find the WKB-approximation for the energies and wave-function. Make a plot of the wave-function and compare to the analytical solution.

Solution: First, we find the WKB-approximated energy. The semi-classical momentum when $x > 0$ is $p(x) = \sqrt{2m(E - mgx)}$. There is a turning point at $x_1 = 0$ because $V(0) \to \infty$. The other turning points occurs when,

$$p(x_2) = 0 \implies x_2 = E/mg. \tag{2}$$

The Bohr-Sommerfeld quantization condition is,

$$\int_0^{x_2} p(x)dx = \left(n - \frac{1}{4}\right)\pi\hbar \implies \sqrt{2m}\int_0^{E/mg} \sqrt{E - mgx}dx = -\frac{1}{gm}\sqrt{2m}\int_E^0 \sqrt{u}du = \frac{2\sqrt{2}}{3g\sqrt{m}}E^{3/2} = \left(n - \frac{1}{4}\right)\pi\hbar$$

$$E_n = \left(\frac{3\pi}{8\sqrt{2}}\hbar g(4n-1)\right)^{2/3} \tag{3}$$

To find the wave-function, we follow Griffiths section 9.2. In the classically-allowed region (region I) ($E_n > V(x)$), the wave-function is,

$$\psi_{\mathrm{I}}(x) = \frac{A}{[2m(E_n - V(x))]^{1/4}} \sin(\int_x^{x_2} \sqrt{2m(E_n - V(x'))}dx' + \pi/4). \tag{4}$$

We are free to add the factor of $\pi/4$ as a constant of integration; similarly, we chose the limit of integration x_2 arbitrarily. We choose a sine function with this phase-factor here because it will match the asymptotic expansions of the Airy functions. In the classically-disallowed region (region III) ($V(x) > E_n$),

$$\psi_{\mathrm{III}}(x) = \frac{B}{[2m(V(x) - E_n)]^{1/4}} \exp(-\int_{x_2}^{x} \sqrt{2m(V(x') - E_n)}dx'). \tag{5}$$

We need to deal with the 'patching' region (region II) next. We linearize the potential near the turning point: $V(x) \approx V(x_2) + (x - x_2)V'(x_2) = E_n + (x - x_2)V'(x_2)$. In this particular case, the approximation is exact because the potential is linear. Near the turning point, we want to solve the TISE:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (E_n + (x - x_2)V'(x_2))\psi = E_n\psi \implies \frac{\hbar^2}{2mV'(x_2)}\frac{d^2\psi}{dx^2} = (x - x_2)\psi. \tag{6}$$

By changing variables $\xi = (x - x_2)\alpha$, where $\alpha = [2mV'(x_2)/\hbar^2]^{1/3}$, this becomes,

$$\frac{d^2\psi}{d\xi^2} = \xi\psi(\xi), \tag{7}$$

which has solutions $\psi = C\mathrm{Ai}(\xi) + D\mathrm{Bi}(\xi)$.

The large positive ξ (i.e., $x \gg x_2$) asymptotic expansion is,

$$\mathrm{Ai}(\xi) \sim \frac{e^{-\frac{2\xi^{3/2}}{3}}}{2(\pi^2\xi)^{1/4}}, \qquad \mathrm{Bi}(\xi) \sim \frac{e^{\frac{2\xi^{3/2}}{3}}}{(\pi^2\xi)^{1/4}}. \tag{8}$$

To match to $\psi_{\text{III}}(x)$, we must have $D = 0$ and,

$$\frac{C}{2(\pi^2\xi)^{1/4}} = \frac{B}{(2m(V(x) - E_n))^{1/4}}. \tag{9}$$

The large negative ξ asymptotic expansion is,

$$\text{Ai}(\xi) \sim \frac{1}{\sqrt{\pi}(-\xi)^{1/4}} \sin(\frac{2}{3}(-\xi)^{3/2} + \pi/4). \tag{10}$$

This means that,

$$\frac{C}{\sqrt{\pi}(-\xi)^{1/4}} = \frac{A}{(2m(E_n - V(x)))^{1/4}}, \tag{11}$$

which gives us the relation between A, B, C. Specifically, it gives us A/C and B/C so that there is only one common constant: C, which is determined by normalization. Using all this, we can deduce the wave-function, but we have to choose the size of the 'patching region.' Note that the Bohr-Sommerfeld quantization condition for one 'vertical wall' was derived by requiring $\psi_I(0) = 0$, so we have already implicitly taken care of boundary conditions. The rest of the plotting and computation is continued in the attached *Mathematica* notebook. See figure 1 for the results.

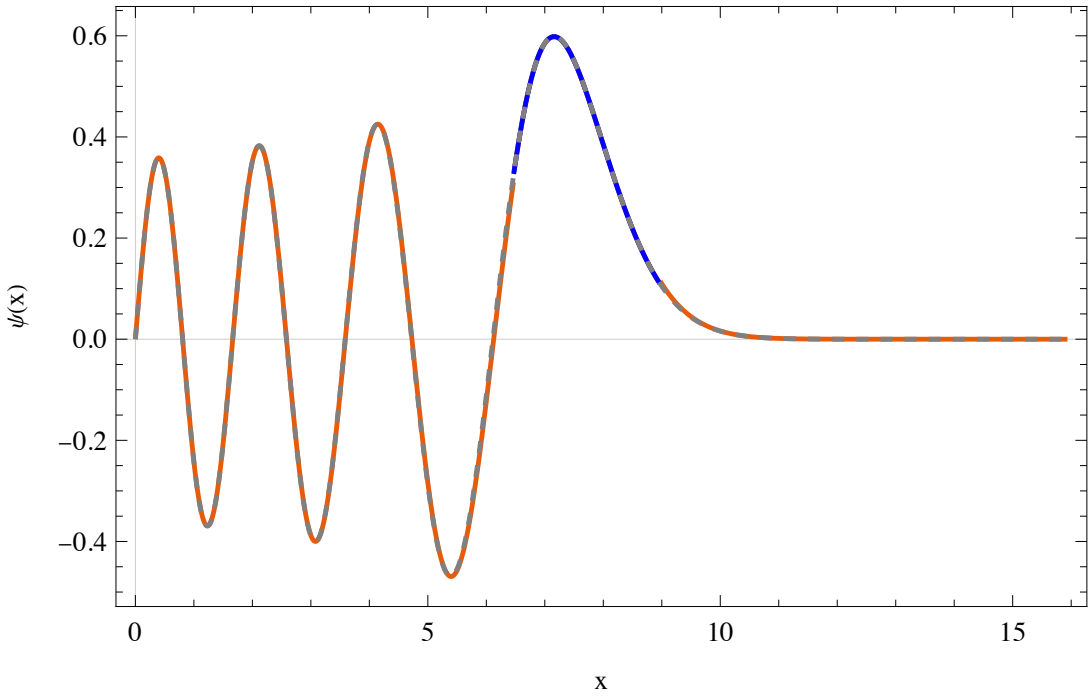

Figure 1: WKB compared to exact solution. Here, we show the exact solution using the gray-dotted line. The orange line represents the wave-function in region I and III. The blue line represents the patching region in region II. We see that are able to almost exactly replicate the exact solution.

The general (and numerical) approach to finding WKB energies

If we want to find WKB estimations for the energies, we need to solve the Bohr-Sommerfeld quantization condition for the energies. The process goes like this:

Write the semi-classical momentum $p(x, E) = \sqrt{2m[E - V(x)]}$**.** Here, we explicitly include write the energy E as part of the momentum to remind us that we do not yet know the energy.

Find the turning points. The turning points occur when $E = V(x)$ or equivalently $p(x, E) = 0$. This equation implicitly defines turning points $x_1(E)$ and $x_2(E)$ (where $x_1(E) < x_2(E)$) in terms of the so-far-unknown energy. If there are vertical walls within the range of the relevant E, one or both of these turning points might be trivial (i.e., at the vertical wall).

Identify and solve the Bohr-Sommerfeld quantization condition. To obtain the nth energy (starting at $n = 1$), we solve the equation:

$$\int_{x_1(E_n)}^{x_2(E_n)} p(x', E_n)dx' = \pi\hbar(n - \phi), \tag{12}$$

where $\phi = 0$ for two vertical walls at energy E, $\phi = \frac{1}{4}$ for one vertical wall at energy E, and $\phi = \frac{1}{2}$ for no vertical walls.

Numerically finding energies of the TISE

To find the exact eigenvalues for a quantum system that is discretized as $x_1, \ldots, x_n$ with spacing dx, we first define the 'discrete Laplacian:'

$$\Delta = \frac{1}{dx^2}\begin{pmatrix} -2 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & -2 \end{pmatrix}. \tag{13}$$

Note: the use of this form of the discrete Laplacian enforce 'Dirichlet boundary conditions,' meaning that it pins the numerically-found eigenstates to zero at x_1 and x_n; this could also be interpreted as inserting an infinite potential barrier at the points. The potential operator is,

$$\hat{V} = \begin{pmatrix} V(x_1) & 0 & \cdots & 0 & 0 \\ 0 & V(x_2) & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & V(x_{n-1}) & 0 \\ 0 & 0 & \cdots & 0 & V(x_n) \end{pmatrix}. \tag{14}$$

The total Hamiltonian is then a $n \times n$ matrix:

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + \hat{V}. \tag{15}$$

The eigenvalues of this operator are the energy eigenvalues and the eigenvectors are the stationary states.