Deriving the Bohr-Sommerfield quantization using the WKB approximation[1]

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The goal is to derive the Bohr-Sommerfield quantization condition i.e.,

$$\oint p\, dx = n\ h\ , \qquad \text{for } n \in \mathbb{Z}_{>0}\ ,$$

for bound states in one-dimensional quantum systems. We use this formula in Statistical Physics to obtain semi-classical expression for the density of states. The integral is an area in phase space and the number of bound states associated is given by the area divided by h.

1 The details

The Hamiltonian of interest is

$$H = \frac{p^2}{2m} + V(x)\ ,$$

where $V(x)$ is a unimodal function that goes to ∞ at $x = \pm\infty$. Let E be an energy value such that $E > V(x)$ for $x \in [x_1, x_2]$ – (x_1, x_2) are the classical turning points.

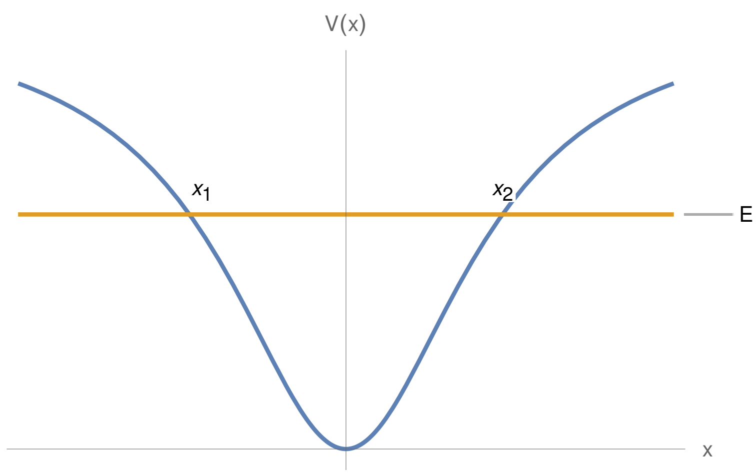

Figure 1: A typical potential for a bound state

Define region I is given by $x < x_1$, region II is given by $x_1 < x < x_2$ and region

[1]This is pretty standard material and so I don't claim any originality here.

III is $x > x_2$. The wavefunction in the WKB approximation is given by

$$\begin{aligned}
\psi_I(x) &= \frac{\alpha}{2\sqrt{\pi\kappa(x)}}\ \exp\Big(-\int_x^{x_1}\kappa(x)\,dx\Big)\\
\psi_{II}(x) &= \frac{A}{\sqrt{\pi k(x)}}\cos\left(\int_{x_1}^{x}k(x)\,dx-\frac{\pi}{4}\right)+\frac{B}{\sqrt{\pi k(x)}}\sin\left(\int_{x_1}^{x}k(x)\,dx-\frac{\pi}{4}\right)\\
\psi_{III}(x) &= \frac{\beta}{\sqrt{\pi\kappa(x)}}\ \exp\Big(-\int_{x_2}^{x}\kappa(x)\,dx\Big)
\end{aligned}$$

where $k(x) = \sqrt{2m(E-V(x)}$ and $\kappa(x) = \sqrt{2m(V(x)-E)}$ The Schrödinger equation near $x = x_1$ takes the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E-V(x))\,\psi \simeq g(x-x_1)\,\psi\ ,$$

where $g = -dV/dx|_{x=x_1}$. Defining $u =:= (x_1-x)/L$ where $L = (\hbar^2/2mg)^{1/3}$, the differential equation becomes the Airy differential equation

$$\frac{d^2\psi}{du^2} - u\,\psi = 0\ .$$

This equation has two solutions that are conventionally denoted by $\mathrm{Ai}(u)$ and $\mathrm{Bi}(u)$. From `https://dlmf.nist.gov/9.7`, we see that they have the following asymptotic behaviour ($\zeta = \frac{2}{3}|u|^{3/2}$)

$$\mathrm{Ai}(u) \sim \begin{cases} \dfrac{e^{-\zeta}}{2\sqrt{\pi}u^{1/4}}\ , & u \gg 1\\ \dfrac{\cos(\zeta-\frac{\pi}{4})}{\sqrt{\pi}|u|^{1/4}}\ , & u \ll -1 \end{cases} \tag{1}$$

$$\mathrm{Bi}(u) \sim \begin{cases} \dfrac{e^{\zeta}}{\sqrt{\pi}u^{1/4}}\ , & u \gg 1\\ \dfrac{-\sin(\zeta-\frac{\pi}{4})}{\sqrt{\pi}|u|^{1/4}}\ , & u \ll -1 \end{cases} \tag{2}$$

Exercise: Show that one has

$$\int_x^{x_1}\kappa(x)dx = \int_{x_1}^{x}k(x)dx = \zeta$$

and $\sqrt{\kappa(x)} = \sqrt{k(x)} = \sqrt{\eta}\,|u|^{1/4}$. Matching at $x = x_1$ via the Airy function, we get

$$\boxed{A = \alpha \quad \text{and} \quad B = 0}\ . \tag{3}$$

We see that the solution near $x = x_1$ is given by $\psi^{(x_1)}(x) = A\sqrt{L}\ \mathrm{Ai}(u_1)$, where $u_1 = (x_1-x)/L$, We rewrite $\psi_{II}(x)$ in a manner that is suitable for matching conditions at $x = x_2$.

$$\begin{aligned}
\psi_{II}(x) &= \frac{A}{\sqrt{\pi k(x)}} \cos\left(\int_{x_1}^{x} k(x)\,dx - \frac{\pi}{4}\right) + \frac{B}{\sqrt{\pi k(x)}} \sin\left(\int_{x_1}^{x} k(x)\,dx - \frac{\pi}{4}\right) \\
&= \frac{A}{\sqrt{\pi k(x)}} \cos\left(\int_{x}^{x_2} k(x)\,dx - \frac{\pi}{4} - \Delta\right) - \frac{B}{\sqrt{\pi k(x)}} \sin\left(\int_{x}^{x_2} k(x)\,dx - \frac{\pi}{4} - \Delta\right)
\end{aligned}$$

where

$$\Delta := \int_{x_1}^{x_2} k(x)dx - \frac{\pi}{2} \ .$$

Matching at $x = x_2$ via the Airy function, we see that since $B = 0$, the only way $\psi_{II}(x)$ will match with $\psi_{III}(x)$ if

$$\Delta = n\pi \implies \boxed{\int_{x_1}^{x_2} k(x)dx = \left(n + \tfrac{1}{2}\right)\pi} \quad n = 0, 1, 2, \ldots \tag{4}$$

For each value of n, we find a solution and the energy of that solution is determined by this condition. Then one has a matching provided we set

$$\boxed{\beta = (-1)^n A = (-1)^n \alpha} \ .$$

We see that the solution near $x = x_2$ is given by $\psi^{(x_2)}(x) = A\sqrt{L}\ \mathrm{Ai}(u_2)$, where $u_1 = (x - x_2)/L$.

The Bohr-Sommerfeld quantisation condition follows from the boxed part of Eq. (3). Multiplying it by $\hbar$ and setting $\hbar k(x) = p(x)$, we obtain

$$\boxed{\oint p\,dx = 2\int_{x_1}^{x_2} p(x)dx = \left(n + \tfrac{1}{2}\right) h \ .} \tag{5}$$

The $\frac{1}{2}$ is called the Maslov correction.