Introduction to Quantum Mechanics – Solutions to Problem sheet 7

1. An asymmetric square well. (Part of an exam question from 2013)

(a) Similar to the treatment of the finite well we consider the regions separately to find the general form of the bound state solutions:

$$\phi_E(x) = \begin{cases} 0, & x \le 0 \\ A\cos(kx) + B\sin(kx), & 0 < x \le L \\ C\mathrm{e}^{-\kappa x}, & x > L. \end{cases} ,$$

with $k = \sqrt{2mE}/\hbar$ and $\kappa = \sqrt{2m(V_0 - E)}/\hbar$.
From the continuity of the wavefunction at $x = 0$, we find

$$\phi_E(0) = 0 = A.$$

Using this together with the continuity condition at $x = L$ yields the condition

$$B\sin(kL) = C\mathrm{e}^{-\kappa L}. \tag{1}$$

Further, we know that the first derivative of $\phi_E(x)$ is continuous at $x = L$, which yields the condition

$$kB\cos(kL) = -\kappa C\mathrm{e}^{-\kappa L}. \tag{2}$$

Combining (1) and (2) we find the quantisation condition

$$\kappa = -k\cot(kL),$$

similar to the quantisation condition for the odd solutions of the symmetric finite square well. Again we can rewrite this in terms of the energy as

$$-\cot\left(\frac{\sqrt{2mE}L}{\hbar}\right) = \sqrt{\frac{V_0}{E} - 1}\,, \tag{3}$$

Here we use the quantisation condition in the form

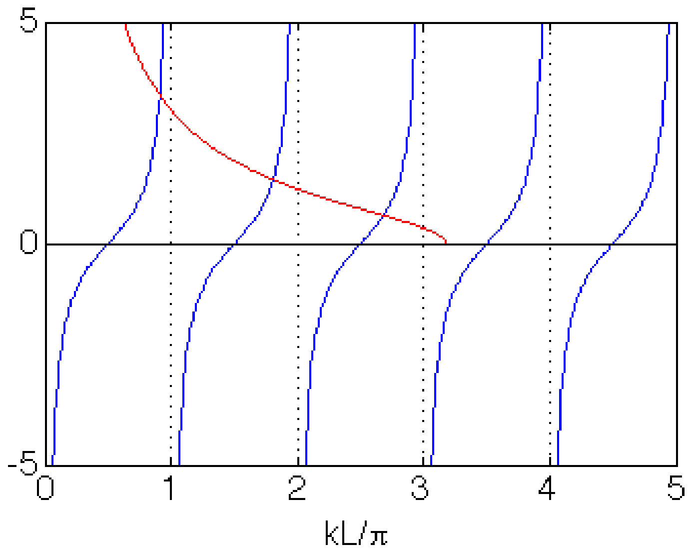
$$-\cot(Lk) = \sqrt{\frac{c^2}{(Lk)^2} - 1},$$

where we have defined $c = \sqrt{\frac{2mV_0L^2}{\hbar^2}}$. Thus, the possible values of Lk are those, at which the functions $-\cot(Lk)$ and $\sqrt{\frac{c^2}{(Lk)^2} - 1}$ intersect. In figure 1 we plot the cotangent in blue, and an example of the square root for the choice $c = 10$ in red.
There is no bound state if the square root reaches zero before the cotangent becomes positive for the first time, that is, for $c < \pi/2$. The minimum value of the potential for which there is a bound state is thus found from the condition

$$\sqrt{\frac{2mV_0L^2}{\hbar^2}} = \frac{\pi}{2},$$

which yields

$$V_0^{min} = \frac{\pi^2\hbar^2}{8mL^2}.$$



(b)

Figure 1: Example of the graphical solution of the quantisation condition. The blue line shows the negative cotangent, while the red line depicts the value of the square root as a function of kL for $c = 10$.

3. The variational method

Minimising $\langle H \rangle$ for a trial function with respect to some parameter. For a normalised state with $\phi(x)$ we have

$$E_0 \leq \int dx \phi^*(x) \hat{H} \phi(x).$$

With $\hat{H} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^4$ and the trial function

$$\phi(x) = \left(\frac{\lambda}{\pi}\right)^{\frac{1}{4}} e^{-\lambda x^2/2}$$

we have

$$\begin{aligned}\langle H \rangle &= \int dx \left(\frac{\lambda}{\pi}\right)^{\frac{1}{2}} e^{-\lambda x^2/2} \left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}x^4\right) e^{-\lambda x^2/2} \\ &= \int dx \left(\frac{\lambda}{\pi}\right)^{\frac{1}{2}} e^{-\lambda x^2/2} \left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} e^{-\lambda x^2/2}\right) + \int dx \left(\frac{\lambda}{\pi}\right)^{\frac{1}{2}} e^{-\lambda x^2/2} \left(\frac{1}{2}x^4\right) e^{-\lambda x^2/2} \\ &= \left(\frac{\lambda}{\pi}\right)^{\frac{1}{2}} \frac{1}{2} \int dx\ x^4 e^{-\lambda x^2} - \left(\frac{\lambda}{\pi}\right)^{\frac{1}{2}} \frac{1}{2} \int dx\ e^{-\lambda x^2/2} \left(\frac{\partial^2}{\partial x^2} e^{-\lambda x^2/2}\right).\end{aligned}$$

We have

$$\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x} e^{-\lambda x^2/2}\right) = (\lambda^2 x^2 - \lambda) e^{-\lambda x^2/2}$$

That is,

$$\begin{aligned}\langle H \rangle &= \left(\frac{\lambda}{\pi}\right)^{\frac{1}{2}} \left[\frac{1}{2}\int dx\ x^4 e^{-\lambda x^2} - \lambda^2 \int dx\ x^2 e^{-\lambda x^2/2} + \lambda \int dx\ e^{-\lambda x^2/2}\right] \\ &= \frac{1}{2}\left(\frac{3}{4\lambda^2} - \frac{\lambda}{2} + \lambda\right).\end{aligned}$$

Minimising this with respect to λ, we find for the possible extrema

$$\frac{d\langle H\rangle}{d\lambda} = \frac{1}{2}\left[\frac{3}{4}(-2)\frac{1}{\lambda^3} - \frac{1}{2} + 1\right] = 0,$$

which simplifies to

$$\lambda^3 = 3$$

That is, there is an extremum of the energy expectation value at

$$\lambda = 3^{1/3}.$$

+ Inserting this back into $\langle H\rangle$ we find

$$\begin{aligned}\langle H\rangle &= \frac{1}{2}\left(\frac{3}{4(3)^{2/3}} - \frac{3^{1/3}}{2} + 3^{1/3}\right)\\ &= 0.541\end{aligned}$$

Comparing this to the exact value, $E_0 = 0.530$, we find that indeed $\langle H\rangle \geq E_0$ is satisfied.

3. Number of bound states in a finite square well potential

The number of bound states in a finite square well potential depends on the parameters V_0 and L of the potential, the mass of the particle m, and Planck's constant $\hbar$, and is given by

$$N = \left[\frac{2c}{\pi}\right]_< + 1, \quad \text{where} \quad c := \sqrt{\frac{2mV_0L^2}{\hbar^2}}.$$

Now we have $V_0 = 2\text{eV}$, where $1\text{eV} \approx 1.60218 \times 10{-}19\text{J}$, further

$$L = 20\text{nm} = 2 \times 10^{-8}\text{m}, \quad \text{and} \quad \hbar \approx 1.054 \times 10^{-34}\text{Js}.$$

The mass of an electron is approximately

$$m_e \approx 9.109 \times 10^{-31}\text{kg},$$

and that of a proton is

$$m_p \approx 1.673 \times 10^{-27}\text{kg}.$$

Thus we have for an electron

$$c_e = \sqrt{\frac{2m_eV_0L^2}{\hbar^2}} \approx \sqrt{\frac{4 \times 1.60218 \times 9.109}{1.054^2 \times 10^{-2}}} \approx 72.49,$$

and for a proton

$$c_p = \sqrt{\frac{2m_pV_0L^2}{\hbar^2}} \approx 3106.65.$$

Thus, for an electron in the given potential we expect $N_e = 46 + 1 = 47$ bound states, and for a proton $N_p = 1977 + 1 = 1978$ bound states.