Physics 731: Assignment #3, Solutions

1. (a) The odd parity eigenfunctions of the finite square well potential for regions I ($x < -a$), region II ($-a < x < a$), and region III ($x > a$) take the form

$$\psi_{\rm I} = -Fe^{\kappa x}, \quad \psi_{\rm II} = B\sin kx, \quad \psi_{\rm III}(x) = Fe^{-\kappa x},$$

in which $k = \sqrt{2mE}/\hbar$ and $\kappa = \sqrt{2m(V_0 - E)}/\hbar$. Building in the continuity of the wavefunction, we can write

$$\psi_{\rm I} = -B'\sin ka\, e^{\kappa x}, \quad \psi_{\rm II} = B'\sin kx\, e^{-\kappa a}, \quad \psi_{\rm III}(x) = B'\sin ka\, e^{-\kappa x}.$$

Continuity of $d\psi/dx$ at $x = a$ leads to the condition

$$-\kappa a = ka\cot ka.$$

Defining as usual $\xi = ka$ and $\eta = \kappa a$, we have the conditions

$$\eta = -\xi\cot\xi, \quad \eta^2 + \xi^2 = R^2,$$

in which $R = \sqrt{2mV_0 a^2/\hbar^2}$. It is straightforward to see that for there are no solutions for $R < \pi/2$ (*i.e.*, $V_0 < \pi^2\hbar^2/(8ma^2)$), there is one solution for $\pi/2 < R < 3\pi/2$, and there are two solutions for $3\pi/2 < R < 5\pi/2$, and so on. Therefore, as $V_0 \to 0$, there are no odd parity bound states. For $V_0 \to \infty$, there are an infinite number of bound states, with $k = n\pi/(2a)$ for even values of n, as expected for the infinite square well.

(b) We are asked to analyze the bound states of the above finite square well potential with specific values of the parameter

$$R = \left(\frac{2mV_0 a^2}{\hbar^2}\right)^{\frac{1}{2}} = 4.$$

The bound states, which have $E < V_0$, can be classified by even/odd parity. For the even parity states, the conditions which determines the bound state energies are

$$\xi\tan\xi = \eta, \quad \xi^2 + \eta^2 = R^2 = \frac{2mV_0 a^2}{\hbar^2},$$

where $\xi = ka = \sqrt{2mEa^2/\hbar^2}$ and $\eta = \kappa a = \sqrt{2m(V_0 - E)a^2/\hbar^2}$, while for the odd parity states, we have

$$-\xi\cot\xi = \eta, \quad \xi^2 + \eta^2 = R^2 = \frac{2mV_0 a^2}{\hbar^2}.$$

For $R = 4$, there are three solutions (two even parity solutions and one odd parity solution). Using the above constraints, we find $\xi_1 = 1.2524$, $\xi_2 = 2.4746$, and $\xi_3 = 3.5953$ (to 4 figures, perhaps a bit of overkill). The energies are then, respectively,

$$\frac{E_n}{V_0} = \frac{\xi_n^2}{R^2} = \frac{\xi_n^2}{16},$$

such that

$$E_1 = 0.0980V_0, \qquad E_2 = 0.3827V_0, \qquad E_3 = 0.8079V_0.$$

The graphical solution is given in Figure 1.

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(* Finite square well *)

In[74]:= Plot[{ξ Tan [ξ], -ξ Cot[ ξ], Sqrt[16 - ξ^2]},
  {ξ, 0, 2 Pi}, PlotRange → { {0, 2 Pi}, {0, 5}},
  AspectRatio → Automatic, PlotStyle → {Red, Dashed, Blue}]
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Out[74]=

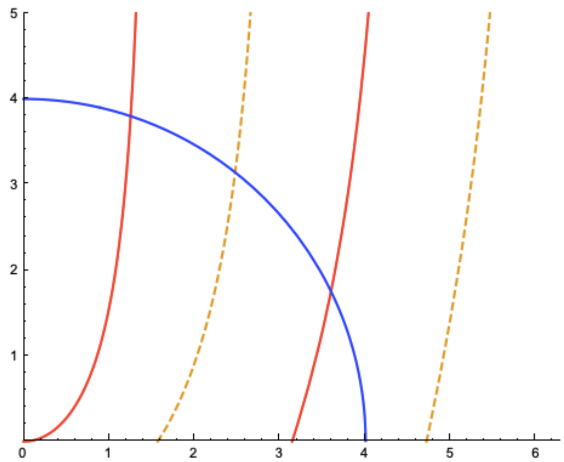

Figure 1: Graphical solution for the even parity (red) and odd parity (orange-dashed) solutions for the finite square well with $R = 4$.

2. Assume that opposite is true. Let $\psi_1(x)$ and $\psi_2(x)$ be two linearly-independent eigenfunctions with the same energy eigenvalue E. Using the equations

$$\psi_1'' + \frac{2m}{\hbar^2}(E - V)\psi_1 = 0, \quad \psi_2'' + \frac{2m}{\hbar^2}(E - V)\psi_2 = 0$$

we can write

$$\frac{\psi_1''}{\psi_1} = \frac{\psi_2''}{\psi_2},$$

which can be expressed as

$$(\psi_1'\psi_2)' - (\psi_2'\psi_1)' = 0.$$

Integrating this differential equation we obtain

$$\psi_1'\psi_2 - \psi_2'\psi_1 = \text{constant}.$$

The constant is zero since both wavefunctions vanish at infinity for bound states. Therefore, we have

$$\frac{\psi_1'}{\psi_1} - \frac{\psi_2'}{\psi_2} = 0,$$

such that

$$\frac{d \ln \psi_1}{dx} - \frac{d \ln \psi_2}{dx} = 0.$$

Integrating once more we obtain

$$\ln \psi_1 = \ln \psi_2 + \text{another constant},$$

such that

$$\psi_1 = (\text{yet another constant}) \times \psi_2$$

which violates the original assumption.

3. (a) To prove

$$H_n(y) = e^{y^2/2}\left(y - \frac{d}{dy}\right)^n e^{-y^2/2},$$

first note that

$$H_n(y) = \frac{\partial^n}{\partial t^n} g(y,t)|_{t=0} = \frac{\partial^n}{\partial t^n} e^{-t^2+2ty}|_{t=0}.$$

Rewriting $g(t, y)$ as follows:

$$g(t,y) = e^{-t^2+2ty} = e^{y^2} e^{-(t-y)^2},$$

we see that

$$\frac{d}{dt} e^{y^2} e^{-(t-y)^2} = -e^{y^2} \frac{d}{dy} e^{-(t-y)^2}.$$

Therefore,

$$H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n} e^{-y^2}.$$

In addition, note that for any function $F(y)$,

$$-\frac{d}{dy}\left[e^{-y^2/2} F(y)\right] = e^{-y^2/2}\left(y - \frac{d}{dy}\right) F(y).$$

Putting these results together, we obtain the desired result:

$$H_n(y) = e^{y^2}\left(-\frac{d}{dy}\right)^n \left[e^{-y^2/2} e^{-y^2/2}\right] = e^{y^2/2}\left(y - \frac{d}{dy}\right)^n e^{-y^2/2}.$$

To prove the identity

$$H'_n(y) = 2nH_{n-1}(y),$$

note that

$$\frac{\partial g(t,y)}{\partial y} = 2tg(y,t).$$

Hence,

$$\sum_{n=0}^{\infty} H'_n(y) \frac{t^n}{n!} = 2t \sum_{n=0}^{\infty} H_n(y) \frac{t^n}{n!}.$$

By equating powers of t, we see that

$$H'_n(y) = 2nH_{n-1}(y).$$

Finally, to prove

$$H_{n+1}(y) = 2yH_n(y) - 2nH_{n-1}(y),$$

consider

$$\frac{\partial g(t,y)}{\partial t} = 2(y-t)g(y,t).$$

Therefore,

$$\sum_{n=0}^{\infty} H_n(y)\frac{t^{n-1}}{(n-1)!} = 2(y-t)\sum_{n=0}^{\infty} H_n(y)\frac{t^n}{n!},$$

and again by equating powers of t, it is straightforward to see that

$$H_{n+1}(y) = 2yH_n(y) - 2nH_{n-1}(y).$$

(b) Consider the expression

$$\int_{-\infty}^{\infty} e^{-y^2} g(y,t)g(y,s)dy = \int_{-\infty}^{\infty} e^{-y^2} e^{-t^2+2ty} e^{-s^2+2sy} dy.$$

We have

$$\begin{aligned}\int_{-\infty}^{\infty} e^{-y^2} e^{-t^2+2ty} e^{-s^2+2sy} dy &= e^{2ts}\int_{-\infty}^{\infty} e^{-(y-t-s)^2} dy = \sqrt{\pi}e^{2ts} = \sqrt{\pi}\sum_{n=0}^{\infty}\frac{(2ts)^n}{n!} \\ &= \sum_{nn'}\left[\int_{-\infty}^{\infty} e^{-y^2} H_n(y)H_{n'}(y)dy\right]\frac{t^n s^{n'}}{n!n'!}.\end{aligned}$$

Therefore, we see that

$$\int_{-\infty}^{\infty} e^{-y^2} H_n(y)H_{n'}(y)dy = \sqrt{\pi}2^n n!\delta_{nn'}.$$

4. The position space eigenfunction of the nth energy level is given by

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right).$$

Therefore, we have

$$\begin{aligned}\langle n'|p|n\rangle &= \sqrt{\frac{m\omega}{\pi\hbar}}\frac{-i\hbar}{\sqrt{2^n 2^{n'} n!n'!}}\int_{-\infty}^{\infty} dy\, e^{-y^2/2}H_{n'}(y)\frac{d}{dy}(e^{-y^2/2}H_n(y)) \\ &= -i\sqrt{\frac{m\omega\hbar}{\pi}}\frac{1}{\sqrt{2^n 2^{n'} n!n'!}}\int_{-\infty}^{\infty} dy\, e^{-y^2}(-H_{n'}(y)yH_n(y) + H_{n'}(y)H_n'(y)).\end{aligned}$$

Using the identities derived above,

$$\begin{aligned}\langle n'|p|n\rangle &= -i\sqrt{\frac{m\omega\hbar}{\pi}}\frac{1}{\sqrt{2^n 2^{n'} n!n'!}}\int_{-\infty}^{\infty} dy\, e^{-y^2}(-\frac{1}{2}H_{n'}H_{n+1} + nH_{n'}H_{n-1}) \\ &= -i\sqrt{\frac{m\omega\hbar}{\pi}}\frac{1}{\sqrt{2^n 2^{n'} n!n'!}}\sqrt{\pi}(-\frac{1}{2}2^{n'}n'!\delta_{n',n+1} + n2^{n'}n'!\delta_{n',n-1}),\end{aligned}$$

which then takes the form

$$\begin{aligned}\langle n'|p|n\rangle &= i\sqrt{m\omega\hbar}\left(\frac{2^{n+1}(n+1)!}{2\sqrt{2^{2n+1}(n+1)!n!}}\delta_{n',n+1}-\frac{n2^{n-1}(n-1)!}{\sqrt{2^{2n-1}(n-1)!n!}}\delta_{n',n-1}\right)\\ &= i\sqrt{\frac{m\omega\hbar}{2}}(\sqrt{n+1}\delta_{n',n+1}-\sqrt{n}\delta_{n',n-1}).\end{aligned}$$

In momentum space, we have

$$\phi_n(p)=(-i)^n\left(\frac{1}{\pi m\omega\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}e^{-p^2/(2m\omega\hbar)}H_n(p/\sqrt{m\omega\hbar}).$$

Therefore, defining $\tilde{p}=p/\sqrt{m\omega\hbar}$, we have

$$\begin{aligned}\langle n'|p|n\rangle &= \frac{(i)^{n'}(-i)^n}{\sqrt{2^n2^{n'}n!n'!}}\sqrt{\frac{m\omega\hbar}{\pi}}\int_{-\infty}^{\infty}d\tilde{p}e^{-\tilde{p}^2}H_{n'}(\tilde{p})\tilde{p}H_n(\tilde{p})\\ &= \frac{(i)^{n'}(-i)^n}{\sqrt{2^n2^{n'}n!n'!}}\sqrt{\frac{m\omega\hbar}{\pi}}\int_{-\infty}^{\infty}d\tilde{p}e^{-\tilde{p}^2}H_{n'}(\tilde{p})(\frac{1}{2}H_{n+1}(\tilde{p})+nH_{n-1}(\tilde{p}))\\ &= \sqrt{m\omega\hbar}\frac{(i)^{n'}(-i)^n}{\sqrt{2^n2^{n'}n!n'!}}\left(\frac{1}{2}2^{n'}n'!\delta_{n',n+1}+n2^{n'}n'!\delta_{n',n-1}\right)\\ &= \sqrt{m\omega\hbar}\left(\frac{i^{n+1}(-i)^n2^{n+1}(n+1)!}{\sqrt{2^{2n+1}(n+1)!n!}}\delta_{n',n+1}+\frac{i^{n-1}(-i)^n2^{n-1}n!}{\sqrt{2^{2n-1}(n-1)!n!}}\delta_{n',n-1}\right)\\ &= \sqrt{\frac{m\omega\hbar}{2}}\left(i\sqrt{n+1}\delta_{n',n+1}+\frac{1}{i}\sqrt{n}\delta_{n',n-1}\right)\\ &= i\sqrt{\frac{m\omega\hbar}{2}}(\sqrt{n+1}\delta_{n',n+1}-\sqrt{n}\delta_{n',n-1}).\end{aligned}$$

5. (i) For the ground state,

$$\psi_0(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left[-\frac{m\omega x^2}{2\hbar}\right].$$

Since $E_0=\hbar\omega/2$, the classical turning point x_c is given by

$$x_c=\sqrt{\frac{2E_0}{m\omega^2}}=\sqrt{\frac{\hbar}{m\omega}}\equiv b.$$

The probability that the particle is beyond the classical turning point is

$$P(|x|>x_c)=2\int_{x_c}^{\infty}|\psi_0|^2dx=\frac{2}{\sqrt{\pi}}\int_1^{\infty}e^{-y^2}dy=1-\mathrm{erf}(1),$$

where $\mathrm{erf}(z)=\frac{2}{\sqrt{\pi}}\int_0^z e^{-y^2}dy$ is the error function. Evaluating it (tables, Mathematica, etc.) yields $P(|x|>x_c)=0.157$.
(ii) For the first excited state,

$$\psi_1(x)=\left(\frac{m\omega}{4\pi\hbar}\right)^{1/4}\exp\left[-\frac{m\omega x^2}{2\hbar}\right]2\left(\sqrt{\frac{m\omega}{\hbar}}x\right),$$

and

$$x_c = \sqrt{\frac{2E_0}{m\omega^2}} = \sqrt{\frac{3\hbar}{m\omega}}.$$

Hence, we have

$$P(|x| > x_c) = 2\int_{x_c}^{\infty} |\psi_1|^2 dx = \frac{4}{\sqrt{\pi}} \int_{\sqrt{3}}^{\infty} e^{-y^2} y^2 dy = 1 - \mathrm{erf}(\sqrt{3}) + \frac{2\sqrt{3}}{\sqrt{\pi} e^3} = .112.$$

6. There are multiple ways to show that

$$\langle 0|e^{ikx}|0\rangle = e^{-k^2\langle 0|x^2|0\rangle/2} = e^{-\hbar k^2/(4m\omega)},$$

in which we have used

$$\langle 0|x^2|0\rangle = \frac{\hbar}{2m\omega}\langle 0|(a+a^\dagger)^2|0\rangle = \frac{\hbar}{2m\omega}\langle 0|aa + a^\dagger a^\dagger + 2a^\dagger a + 1|0\rangle = \frac{\hbar}{2m\omega} = e^{-\hbar k^2/(4m\omega)}.$$

A straightforward method is to use position space wavefunctions to evaluate $\langle 0|e^{ikx}|0\rangle$. This yields

$$\begin{aligned} \langle 0|e^{ikx}|0\rangle &= \int_{-\infty}^{\infty} dx\, \psi_0^*(x) e^{ikx} \psi_0(x) = \sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} dx\, e^{ikx} e^{-m\omega x^2/\hbar} \\ &= \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\hbar k^2/(4m\omega)} \int_{-\infty}^{\infty} dx\, e^{-m\omega(x - i\hbar k/(2m\omega))/\hbar} = e^{-\hbar k^2/(4m\omega)}. \end{aligned}$$

It can of course also be shown using creation and annihilation operators, or using momentum space eigenfunctions. For the operator method, a useful result is that

$$\langle 0|(a+a^\dagger)^n|0\rangle = \begin{cases} 0 & n \text{ odd} \\ (n-1)!! & n \text{ even.} \end{cases}$$