1

For the finite square well

$$V = \begin{cases} 0 & |x| < a \\ V_0 & |x| > a \end{cases}, \tag{1}$$

1. Determine the odd parity eigenfunctions and their associated energy eigenvalues for this potential, and discuss limiting behaviour as $V_0 \to 0, V_0 \to \infty$.
2. FInd accurate numerical values for the boundstate energy eigenvalues of a particle in the aboe finite square well potential, in which the parameter

$$R \equiv \sqrt{\frac{2mV_0a^2}{\hbar^2}} = 4. \tag{2}$$

Find solutions graphically and numerically.

1. Odd parity

Lable region $\mathrm{I} : x \leftarrow a, \mathrm{II} : -a < x < a, \mathrm{III} : x > a$. From lecture: $\psi_{\mathrm{II}} = a \cos kx + B \sin kx$, $\psi_{\mathrm{I}} = De^{\kappa x}$, $\psi_{\mathrm{III}} = Fe^{\kappa x}$, with $k = \frac{\sqrt{2mE}}{\hbar}$, $\kappa = \frac{\sqrt{2m(V_0-E)}}{\hbar}$.

Imposing odd parity $\psi(-x) = -\psi(x)$, we have $A = 0, D = -F$. Imposing boundary condition of continuity and smoothness at $x = a$, we have

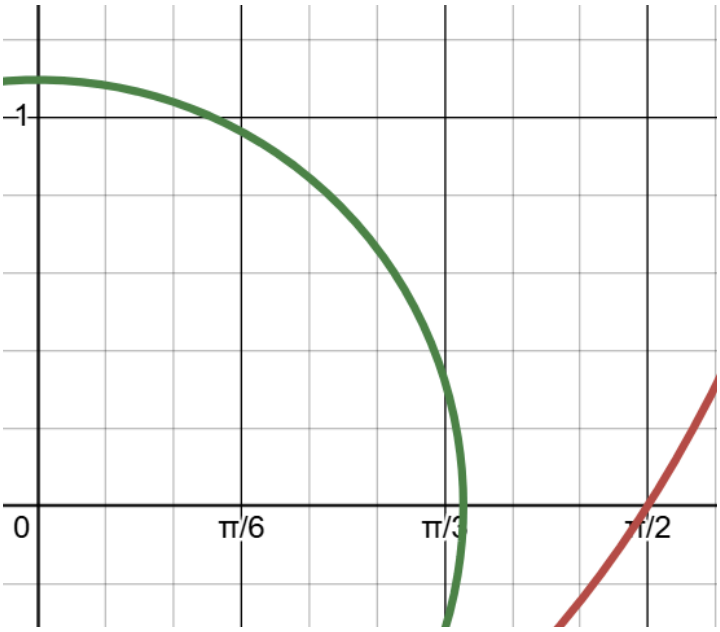
$$B \sin ka = Fe^{-\kappa a}, \quad B \cos ka = -\kappa Fe^{-\kappa a}. \tag{3}$$

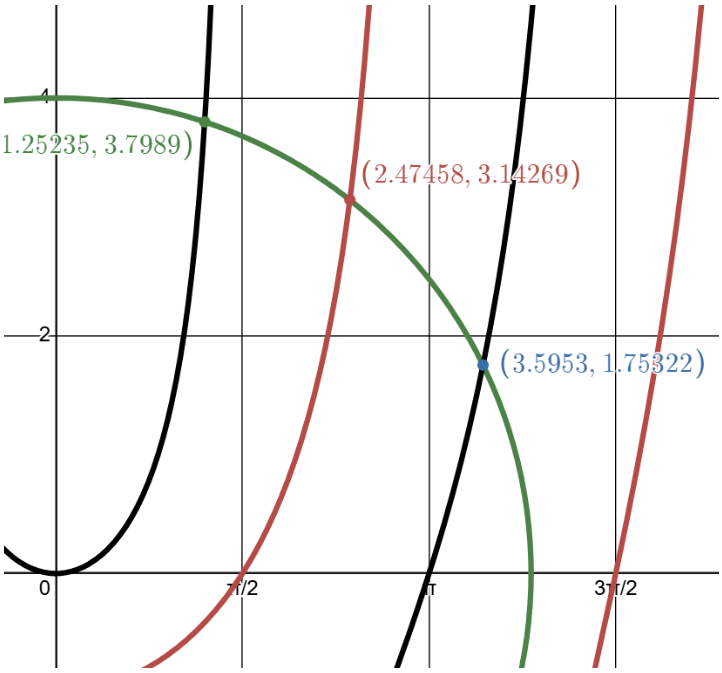
Dividing these and setting $\eta = \kappa a, \xi = ka$, we have

$$\xi \cot \xi = -\eta, \quad \xi^2 + \eta^2 = R^2. \tag{4}$$

Limiting behaviour:

- as $V_0 \to \infty, \eta \to \infty$ and $\cot \xi \to -\infty$ satisfied at $\eta = n\pi, n \in \mathbb{Z}$.
- as $V_0 \to 0, R \to 0$, but as seen below (LEFT) that $\xi \cot \xi = -\eta (\xi, \eta > 0)$ has solution only for $R \geq \frac{\pi}{2}$, the limit of $V_0 \to 0$ yields **no odd parity bound states.**)





2. Numerical and graphical

1. Graphically (ABOVE, RIGHT), The equations to solve are:

- Even States: $\xi \tan(\xi) = \eta$ (black)
- Odd States: $-\xi \cot(\xi) = \eta$ (red)

- Constraint: $\xi^2 + \eta^2 = 16$ (Green)

From a graphical analysis, we find three bound states:

- One intersection with the first branch of $\xi \tan(\xi)$ (even).
- One intersection with the first branch of $-\xi \cot(\xi)$ (odd).
- One intersection with the second branch of $\xi \tan(\xi)$ (even).

2

Show that for spinless particles moving in 1D, the energy spectrum of bound states is always non-degenrate.

Assume not: exists $\psi_i(x)$, $(i = 1, 2)$ s.t.

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_i}{\mathrm{d}x^2} + V(x)\psi_i = E\psi_i, \quad E = E_1 = E_2. \tag{5}$$

In particular, $\psi_1(x), \psi_2(x)$ are linear independent. This would imply that their wronskian

$$W(x) = \psi_1{\psi_2}' - \psi_2{\psi_1}' = 0 \tag{6}$$

However, we notice that

$$W'(x) = 2\frac{m}{\hbar^2}(\psi_1(V - E))\psi_2 - \psi_2(V - E)\psi_1) = 0 \tag{7}$$

so $W(x) = \text{const}$. Further, since ψ_1, ψ_2 are bound states,

$$\lim_{x \to \pm\infty} \psi_i(x) = 0 \Rightarrow W(\pm\infty) = 0 \Rightarrow W(x) = 0 \quad \forall x. \tag{8}$$

This contradicts the linear independence of ψ_1, ψ_2. Thus, the energy spectrum of bound states is always non-degenerate.

3

Use the Hermite generating function

$$g(y,t) = e^{-t^2+2ty} = \sum_{n=0}^{\infty} H_n(y)\frac{t^n}{n!} \tag{9}$$

1. To prove the following properties

$$\begin{gathered} H_n(y) = e^{\frac{y^2}{2}}\left(y - \frac{d}{d}y\right)^n e^{-\frac{y^2}{2}}, \\ H_n'(y) = 2nH_{n-1}(y) \\ H_{n+1}(y) = 2yH_n(y) - 2nH_{n-1}(y). \end{gathered} \tag{10}$$

2. Then evaluate

$$\int_{-\infty}^{\infty} \mathrm{d}y\, e^{-y^2} H_n(y) H_{n'}(y) \tag{11}$$

1

a

Recall that $H_n(y) = \left(\frac{\partial}{\partial t}\right)^n\Big|_{t=0} g(y,t)$. Let $u = t - y, \partial u = \partial t$. Then $g = e^{-u^2}e^{y^2}$. Then from definition,

$$H_n(y) = \left(\frac{\partial}{\partial u}\right)^n \left(e^{-u^2}e^{y^2}\right)\Big|_{u=-y} = e^{y^2}\left(\frac{\partial}{\partial u}\right)^n e^{-u^2}\Big|_{u=-y} = (-1)^n e^{y^2}\left(\frac{\partial}{\partial y}\right)^n e^{-y^2} \tag{12}$$

Notice the identity

$$\frac{\mathrm{d}}{\mathrm{d}y}\left(e^{-y^2/2}g\right) = -e^{-y^2/2}\left(y - \frac{\mathrm{d}}{\mathrm{d}y}\right)g, \tag{13}$$

we have

$$\left(\frac{\mathrm{d}}{\mathrm{d}y}\right)^n\left(e^{-y^2}\right) = \left(\frac{\mathrm{d}}{\mathrm{d}y}\right)^n\left(e^{-y^2/2}e^{-y^2/2}\right) = -e^{-y^2/2}\left(y - \frac{\mathrm{d}}{\mathrm{d}y}\right)^n e^{-y^2/2}. \tag{14}$$

And so

$$H_n(y) = (-1)^n e^{y^2}\left(\frac{\mathrm{d}}{\mathrm{d}y}\right)^n e^{-y^2} = (-1)^{2n} e^{y^2/2}\left(y - \frac{\mathrm{d}}{\mathrm{d}y}\right)^n e^{-y^2/2} = \boxed{e^{y^2/2}\left(y - \frac{\mathrm{d}}{\mathrm{d}y}\right)^n e^{-y^2/2}}, \tag{15}$$

as wanted.

b

Notice that

$$\frac{\partial g}{\partial t} = 2tg(y,t) = \sum_{n=0}^{\infty})\frac{2t^{n+1}}{n!}H_n(y) = \sum_{n=0}^{\infty}\underbrace{2(n+1)\frac{t^{n+1}}{(n+1)!}H_n(y)}_{*} = \sum_{n=0}^{\infty} H_n'\frac{(y)^{t^n}}{n!}. \tag{16}$$

But (*) is also

$$2nH_{n-1}(y)\frac{t^n}{n!}. \tag{17}$$

Therefore

$$H_n'(y) = 2nH_{n-1}(y). \tag{18}$$

as wanted.

c

$$\begin{aligned}\partial_t g = (2y-2t)g &= \sum_{n=0}^{\infty}\left(2yH_n(y)\frac{t^n}{n!} - 2H_n(y)\frac{t^{n+1}}{n!}\right)\\ &\underset{n:=n-1}{=} \sum_{n=0}^{\infty}\left(2yH_n(y)\frac{t^n}{n!} - 2nH_{n-1}(y)\frac{t^n}{n!}\right)\end{aligned} \tag{19}$$

But $\partial_t g$ is also

$$\sum_{n=0}^{\infty}\frac{t^{n-1}}{(n-1)!}H_n(y) = \sum_{n=0}^{\infty}\frac{t^n}{n!}H_{n+1}(y), \tag{20}$$

and so

$$H_{n+1}(y) = 2yH_n(y) - 2nH_{n-1}(y). \tag{21}$$

2.

Consider

$$\int_{-\infty}^{\infty} e^{-y^2} g(y,t)g(y,s)\,dy = e^{-(t^2+s^2)}\int_{-\infty}^{\infty} e^{-y^2+2(t+s)y}\,dy. \tag{22}$$

Complete the square in the exponent of the integrand: $-y^2+2(t+s)y = -(y-(t+s))^2+(t+s)^2$. Thus,

$$\int_{-\infty}^{\infty} e^{-(y-(t+s))^2+(t+s)^2}\,dy = e^{(t+s)^2}\int_{-\infty}^{\infty} e^{-u^2}\,du = e^{(t+s)^2}\sqrt{\pi}, \tag{23}$$

where $u = y-(t+s)$. Substituting back,

$$\int_{-\infty}^{\infty} e^{-y^2} g(y,t)g(y,s)\,dy = e^{-(t^2+s^2)}e^{(t+s)^2}\sqrt{\pi} = e^{-(t^2+s^2)+t^2+s^2+2ts}\sqrt{\pi} = e^{2ts}\sqrt{\pi}. \tag{24}$$

On the other hand, expanding the generating functions gives

$$g(y,t)g(y,s) = \sum_{m=0}^{\infty}\sum_{l=0}^{\infty}\frac{t^m}{m!}\frac{s^l}{l!}H_m(y)H_l(y), \tag{25}$$

so

$$\int_{-\infty}^{\infty} e^{-y^2} g(y,t)g(y,s)\,dy = \sum_{m=0}^{\infty}\sum_{l=0}^{\infty}\frac{t^m s^l}{m!l!}\int_{-\infty}^{\infty} e^{-y^2}H_m(y)H_l(y)\,dy. \tag{26}$$

Equating the two expressions yields

$$\sum_{m=0}^{\infty}\sum_{l=0}^{\infty}\frac{t^m s^l}{m!l!}\int_{-\infty}^{\infty} e^{-y^2}H_m(y)H_l(y)\,dy = \sqrt{\pi}\,e^{2ts}. \tag{27}$$

The Taylor expansion of the right-hand side is

$$e^{2ts} = \sum_{n=0}^{\infty}\frac{(2ts)^n}{n!} = \sum_{n=0}^{\infty}\frac{2^n t^n s^n}{n!}. \tag{28}$$

For the left-hand side to match, the double sum must reproduce this only when $m = l = n$, implying that the integral vanishes unless $m = l$. Specifically, the coefficient of $\frac{t^m s^l}{m!l!}$ on the right is $\sqrt{\pi}\,2^m\frac{m!}{m!}\delta_{ml}$ (zero otherwise), so

$$\int_{-\infty}^{\infty} e^{-y^2}H_m(y)H_l(y)\,dy = \sqrt{\pi}\,2^m m!\,\delta_{ml}. \tag{29}$$

4

Using wavefunctions, compute $\langle n'|p|n\rangle$for the eigenstates of the 1d SHO to show that

$$\langle n'|p|n\rangle = i\sqrt{\frac{m\omega\hbar}{2}}\left(\sqrt{n+1}\delta_{n',n+1} - \sqrt{n}\delta_{n',n-1}\right) \tag{30}$$

1

In the position representation, the momentum operator is $\hat{p} = -i\hbar\frac{d}{dx}$. The matrix element is therefore given by the integral:

$$\langle n'|\ p\ |\ n\rangle = \int_{-\infty}^{\infty} \psi^*_{n'}(x)\left(-i\hbar\frac{d}{dx}\right)\psi_n(x)\, dx \tag{31}$$

The normalized energy eigenfunctions are (from lecture)

$$\psi_n(x) = C_n H_n(y) e^{-y^2/2} \quad \text{with} \quad y = \frac{x}{b} = x\sqrt{\frac{m\omega}{\hbar}} \tag{32}$$

where $C_n = (m\omega/\pi\hbar)^{1/4}(2^n n!)^{-1/2} = (b\sqrt{\pi}2^k k!)^{-1/2}$ is the normalization constant.

First, consider:

$$\frac{d\psi_n(x)}{dx} = \frac{C_n}{b}\frac{d}{dy}\left(H_n(y)e^{-y^2/2}\right) = \frac{C_n}{b}\left(H_{(n)'}(y)e^{-y^2/2} - yH_n(y)e^{-y^2/2}\right) \tag{33}$$

Using P3:
1. $H_{(n)'}(y) = 2nH_{n-1}(y)$
2. $2yH_n(y) = H_{n+1}(y) + 2nH_{n-1}(y) \Longrightarrow yH_n(y) = \frac{1}{2}H_{n+1}(y) + nH_{n-1}(y)$

Then we have

$$\frac{d\psi_n(x)}{dx} = \frac{C_n}{b}e^{-y^2/2}\left(2nH_{n-1}(y) - \left[\frac{1}{2}H_{n+1}(y) + nH_{n-1}(y)\right]\right) = \frac{C_n}{b}e^{-y^2/2}\left(nH_{n-1}(y) - \frac{1}{2}H_{n+1}(y)\right) \tag{34}$$

Now $\langle n'|\ p\ |\ n\rangle$, with y ($dx = b\, dy$) becomes:

$$\langle n'|\ p\ |\ n\rangle = -i\hbar\int_{-\infty}^{\infty}\left(C_{n'}H_{n'}(y)e^{-y^2/2}\right)\left(\frac{C_n}{b}e^{-y^2/2}\left[nH_{n-1}(y) - \frac{1}{2}H_{n+1}(y)\right]\right)(b\, dy) \tag{35}$$

$$= -i\hbar C_{n'}C_n\int_{-\infty}^{\infty} e^{-y^2}H_{n'}(y)\left[nH_{n-1}(y) - \frac{1}{2}H_{n+1}(y)\right]dy \tag{36}$$

The integral splits into two terms. We use the orthogonality relation for Hermite polynomials, $\int_{-\infty}^{\infty} e^{-y^2}H_m(y)H_l(y)\, dy = \sqrt{\pi}\, 2^l l!\, \delta_{ml}$:
1. The first term is non-zero only if $n' = n - 1$:

$$n\int_{-\infty}^{\infty} e^{-y^2}H_{n-1}(y)H_{n-1}(y)\, dy = n\sqrt{\pi}2^{n-1}(n-1)! = \frac{\sqrt{\pi}}{2}2^n n! \tag{37}$$

2. The second term is non-zero only if $n' = n + 1$:

$$-\frac{1}{2}\int_{-\infty}^{\infty} e^{-y^2}H_{n+1}(y)H_{n+1}(y)\, dy = -\frac{1}{2}\sqrt{\pi}2^{n+1}(n+1)! \tag{38}$$

The matrix element is non-zero only for $n' = n \pm 1$.

- Case 1: $n' = n - 1$

$$\langle n-1\ |\ p\ |\ n\rangle = -i\hbar C_{n-1}C_n\left(\frac{\sqrt{\pi}}{2}2^n n!\right) \tag{39}$$

$$= -i\hbar \frac{1}{b\sqrt{\pi}\sqrt{2^{n-1}(n-1)!2^n n!}} \left(\frac{\sqrt{\pi}}{2} 2^n n! \right) = -i\hbar \frac{\sqrt{2^n n!}}{b\sqrt{2 \cdot 2^{n-1}(n-1)!}} = -i\hbar \frac{\sqrt{n}}{b\sqrt{2}} \tag{40}$$

Using $b = \sqrt{\hbar/m\omega}$, we get $\langle n-1 \mid p \mid n \rangle = -i\sqrt{\frac{m\omega\hbar}{2}}\sqrt{n}$.

- Case 2: $n' = n+1$,

$$\langle n+1 \mid p \mid n \rangle = -i\hbar C_{n+1} C_n \left(-\frac{1}{2}\sqrt{\pi} 2^{n+1}(n+1)! \right) \tag{41}$$

$$= i\hbar \frac{1}{b\sqrt{\pi}\sqrt{2^{n+1}(n+1)!2^n n!}} \left(\frac{\sqrt{\pi}}{2} 2^{n+1}(n+1)! \right) = i\hbar \frac{\sqrt{2^{n+1}(n+1)!}}{b\sqrt{2 \cdot 2^n n!}} = i\hbar \frac{\sqrt{2(n+1)}}{b\sqrt{2}} \tag{42}$$

Using $b = \sqrt{\hbar/m\omega}$, we get $\langle n+1 \mid p \mid n \rangle = i\sqrt{\frac{m\omega\hbar}{2}}\sqrt{n+1}$.

Combining these results using the Kronecker delta gives the final expression:

$$\boxed{\langle n' | \, p \mid n \rangle = i\sqrt{\frac{m\omega\hbar}{2}}\left(\sqrt{n+1}\delta_{n',n+1} - \sqrt{n}\delta_{n',n-1}\right)} \tag{43}$$

2

In the momentum representation,

$$\langle n' | \, p \mid n \rangle = \int_{-\infty}^{\infty} \phi^*_{n'}(p) \, p \, \phi_n(p) \, dp \tag{44}$$

The momentum-space eigenfunctions are (from lecture)

$$\phi_n(p) = (-i)^n D_n H_n(q) e^{-q^2/2} \quad \text{with} \quad q = \frac{p}{\sqrt{m\omega\hbar}} \tag{45}$$

where $D_n = (1/m\omega\pi\hbar)^{1/4}(2^n n!)^{-1/2}$ is the normalization constant.

The structure of this integral is mathematically identical to the calculation of the position matrix element $\langle n' | \, x \mid n \rangle$ in position space. The calculation proceeds in exactly the same way, using the Hermite polynomial identity for $qH_n(q)$.

$$\langle n' | \, p \mid n \rangle = \int_{-\infty}^{\infty} \left((-i)^{n'} D_{n'} H_{n'}(q) e^{-q^2/2} \right)^* \cdot p \cdot \left((-i)^n D_n H_n(q) e^{-q^2/2} \right) dp \tag{46}$$

$$= (i)^{n'} (-i)^n D_{n'} D_n \int_{-\infty}^{\infty} e^{-q^2} H_{n'}(q) H_n(q) \, p \, dp \tag{47}$$

Changing variables $p = q\sqrt{m\omega\hbar}$ and $dp = dq\sqrt{m\omega\hbar}$:

$$= (i)^{n'} (-i)^n D_{n'} D_n (m\omega\hbar) \int_{-\infty}^{\infty} e^{-q^2} H_{n'}(q)(qH_n(q)) dq \tag{48}$$

Using $qH_n(q) = \frac{1}{2}H_{n+1}(q) + nH_{n-1}(q)$ and the orthogonality relation, we again find that the integral is non-zero only for $n' = n \pm 1$.

- Case 1: $n' = n-1$, The phase factor is $(i)^{n-1}(-i)^n = i^{-1} = -i$. The integral gives $n\sqrt{\pi}2^{n-1}(n-1)!$.

$$\langle n-1 \mid p \mid n \rangle = (-i) D_{n-1} D_n (m\omega\hbar) \left(n\sqrt{\pi} 2^{n-1}(n-1)! \right) \tag{49}$$

The calculation for the constants is analogous to the position-space case, with the parameter $\sqrt{m\omega\hbar}$ replacing $1/b$.

$$\langle n-1 \mid p \mid n \rangle = (-i)\sqrt{\frac{m\omega\hbar}{2}}\sqrt{n} \tag{50}$$

- Case 2: $n' = n+1$, The phase factor is $(i)^{n+1}(-i)^n = i$. The integral gives $\frac{1}{2}\sqrt{\pi}2^{n+1}(n+1)!$.

$$\langle n+1 \mid p \mid n \rangle = (i) D_{n+1} D_n (m\omega\hbar) \left(\frac{1}{2}\sqrt{\pi} 2^{n+1}(n+1)! \right) \tag{51}$$

$$\langle n+1 \mid p \mid n \rangle = (i)\sqrt{\frac{m\omega\hbar}{2}}\sqrt{n+1} \tag{52}$$

Combining these gives the same final result

$$\boxed{\langle n' | \ p \mid n \rangle = i\sqrt{\tfrac{m\omega\hbar}{2}}\left(\sqrt{n+1}\delta_{n\prime,n+1} - \sqrt{n}\delta_{n\prime,n-1}\right)} \tag{53}$$

5

For 1. The ground state, and 2. The first excited state, calculate the probability that a particle of mass m in the 1d SHO with freq ω is farther from the origin than the classical turning points where $E = V$.