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1 Shankar 5.2.2.

1.1 Expectation Value of Hamiltonian

For any normalized $|\psi\rangle$, the expectation value of the energy, $\langle\psi|\hat{H}|\psi\rangle$, is always greater than the lowest energy eigenvalue, E_0. To show this, start by expanding $|\psi\rangle$ in the energy eigenbasis. Let $|\psi_n\rangle$ be an eigenstate of the Hamiltonian operator, or total energy, such that

$$\hat{H}\,|\psi_n\rangle = E_n\,|\psi_n\rangle \ , \tag{1}$$

note that $E_n \geq E_0$ for any n. When the state $|\psi\rangle$ is expanded in this basis it becomes

$$|\psi\rangle = \sum_n a_n\,|\psi_n\rangle \ , \tag{2}$$

where the a_n's are constants that determine how much of $|\psi\rangle$ is projected onto each basis vector $|\psi_n\rangle$. The first step in finding the expectation value of energy is to have the Hamiltonian operator act on the state $|\psi\rangle$,

$$\hat{H}\,|\psi\rangle = \sum_n a_n\hat{H}\,|\psi_n\rangle = \sum_n a_nE_n\,|\psi_n\rangle \ . \tag{3}$$

Then take the inner product of $|\psi\rangle$ and $\hat{H}\,|\psi\rangle$,

$$\langle\psi|\hat{H}|\psi\rangle = \sum_{n'} a^*_{n'}\,\langle\psi_{n'}|\sum_n a_nE_n\,|\psi_n\rangle = \sum_n\sum_{n'} a^*_{n'}a_nE_n\,\langle\psi_{n'}|\psi_n\rangle \tag{4}$$

$$= \sum_n\sum_{n'} a^*_{n'}a_nE_n\delta_{nn'} = \sum_n |a_n|^2E_n \ , \tag{5}$$

which by the definition of E_0,

$$\sum_n |a_n|^2E_n \geq \sum_n |a_n|^2E_0 \ , \tag{6}$$

is true. Substituting in the expectation value of energy for the left side of the above equation, and rearranging the right side gives

$$\langle\psi|\hat{H}|\psi\rangle \geq E_0\sum_n |a_n|^2 \ . \tag{7}$$

The squared norm of each coefficient a_n determines the probability of measuring $|\psi\rangle$ in an energy eigenstate $|\psi_n\rangle$. The total probability of every state summed together must equal one, $\sum_n |a_n|^2 = 1$, which proves the statement postulated in the first sentence,

$$\langle\psi|\hat{H}|\psi\rangle \geq E_0 \ . \tag{8}$$

1.2 Bound States in One Dimensional Attractive Potentials

Every attractive potential in one dimension has at least one bound state ($E < 0$). Define an attractive potential such that the potential far out must be zero, $V(\infty) = 0$, so the wave functions can be normalized. This implies that $V(x) = -|V(x)|$ for all x. To prove that there always exists a bound state, consider the wavefunction

$$\psi_\alpha(x) = \left(\frac{\alpha}{\pi}\right)^{1/4}\exp[-\alpha x^2/2] \ . \tag{9}$$

Begin by calculating the energy of this state, $E(\alpha) = \langle\psi_\alpha|\hat{H}|\psi_\alpha\rangle$, using the Hamiltonian,

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - |V(x)| \ , \tag{10}$$

which yields

$$\langle\psi_\alpha|\hat{H}|\psi_\alpha\rangle = \int_{-\infty}^{\infty} \psi_\alpha(x)^* \hat{H}\psi_\alpha(x)dx \ . \tag{11}$$

This integral will be evaluated in steps. Start by determining $\hat{H}\psi_\alpha$,

$$\hat{H}\psi_\alpha = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}[\psi_\alpha] - |V(x)|\psi_\alpha \ , \tag{12}$$

which requires knowing the second derivative of ψ_α,

$$\begin{aligned}
\frac{d^2}{dx^2}[\psi_\alpha] &= \frac{d^2}{dx^2}\left[\left(\frac{\alpha}{\pi}\right)^{1/4}\exp[-\alpha x^2/2]\right] = \left(\frac{\alpha}{\pi}\right)^{1/4}\frac{d}{dx}\left[-\alpha x\exp(-\alpha x^2/2)\right] \\
&= -\alpha\left(\frac{\alpha}{\pi}\right)^{1/4}\left[\exp[-\alpha x^2/2] + x(-\alpha x)\exp[-\alpha x^2/2]\right] \\
&= -\alpha\left(\frac{\alpha}{\pi}\right)^{1/4}\left[(1-\alpha x^2)\exp[-\alpha x^2/2]\right] \ ,
\end{aligned}$$

which gives the result for $\hat{H}\psi_\alpha$,

$$\hat{H}\psi_\alpha = \frac{\alpha\hbar^2}{2m}\left(\frac{\alpha}{\pi}\right)^{1/4}\left[(1-\alpha x^2)\exp[-\alpha x^2/2]\right] - \left(\frac{\alpha}{\pi}\right)^{1/4}|V(x)|\exp[-\alpha x^2/2] \ . \tag{13}$$

Now multiply this by ψ_α^*, however $\psi_\alpha^* = \psi_\alpha$ because it is completely real, yielding

$$\psi_\alpha^*\hat{H}\psi_\alpha = \psi_\alpha\hat{H}\psi_\alpha = \left(\frac{\alpha}{\pi}\right)^{1/2}\exp[-\alpha x^2]\left[\frac{\alpha\hbar^2}{2m}(1-\alpha x^2) - |V(x)|\right] \ , \tag{14}$$

and taking the integral,

$$\begin{aligned}
\langle\psi_\alpha|\hat{H}|\psi_\alpha\rangle &= \left(\frac{\alpha}{\pi}\right)^{1/2}\int_{-\infty}^{\infty} dx\exp[-\alpha x^2]\left[\frac{\alpha\hbar^2}{2m}(1-\alpha x^2) - |V(x)|\right] &(15)\\
&= \left(\frac{\alpha}{\pi}\right)^{1/2}\left[\frac{\alpha\hbar^2}{2m}\int_{-\infty}^{\infty} dx\exp[-\alpha x^2](1-\alpha x^2) - \int_{-\infty}^{\infty} dx\exp[-\alpha x^2]|V(x)|\right] \ , &(16)
\end{aligned}$$

which using Mathematica to evaluate the first integral becomes

$$\begin{aligned}
E(\alpha) &= \left(\frac{\alpha}{\pi}\right)^{1/2}\left[\frac{\alpha\hbar^2}{2m}\frac{1}{2}\sqrt{\frac{\pi}{\alpha}} - \int_{-\infty}^{\infty} dx\exp[-\alpha x^2]|V(x)|\right] &(17)\\
&= \frac{\alpha\hbar^2}{4m} - \left(\frac{\alpha}{\pi}\right)^{1/2}\int_{-\infty}^{\infty} dx\exp[-\alpha x^2]|V(x)| \ . &(18)
\end{aligned}$$

Define a potential $I(\alpha)$ such that

$$I(\alpha) = \int_{-\infty}^{\infty} dx\exp[-\alpha x^2]|V(x)| \ , \tag{19}$$

so Equation 18 becomes

$$E(\alpha) = \frac{\alpha\hbar^2}{4m} - \left(\frac{\alpha}{\pi}\right)^{1/2} I(\alpha) \ . \tag{20}$$

For a bound state $E(\alpha) < 0$, so

$$0 > \frac{\alpha\hbar^2}{4m} - \left(\frac{\alpha}{\pi}\right)^{1/2} I(\alpha) \tag{21}$$

$$\left(\frac{\alpha}{\pi}\right)^{1/2} I(\alpha) > \frac{\alpha\hbar^2}{4m} \tag{22}$$

$$I(\alpha)^2 > \alpha\frac{\pi\hbar^2}{16m} \tag{23}$$

$$\alpha < I(\alpha)^2 \frac{16m}{\pi\hbar^4} \ . \tag{24}$$

In the limit that α goes to zero, the left side of the above equation falls linearly with α to zero. The limit, as $\alpha \to 0$, of the potential I is

$$\lim_{\alpha\to 0} I(\alpha) = \lim_{\alpha\to 0} \int_{-\infty}^{\infty} dx \exp[-\alpha x^2]|V(x)| = \int_{-\infty}^{\infty} dx|V(x)| = K \ , \tag{25}$$

where K is some positive constant, which depends on the potential. This makes the inequality,

$$0 < K^2 \frac{16m}{\pi\hbar^4} \ , \tag{26}$$

which is always true. Therefore for sufficiently small values of α there will always be a bound state.

2 Shankar 5.2.4.

The energy of a particle of mass m, in a state $|n\rangle$, in an infinite one dimensional square well of length L is given by Shankar Equation 5.2.17c,

$$E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2} \ . \tag{27}$$

If the walls of the well are slowly pushed in such that the particle remains in state $|n\rangle$, the force felt by the particle is

$$F = -\frac{\partial E_n}{\partial L} = -\frac{\partial}{\partial L}\left[\frac{\hbar^2\pi^2 n^2}{2mL^2}\right] = -\frac{\hbar^2\pi^2 n^2}{2m}\frac{\partial}{\partial L}[L^{-2}] = -\frac{\hbar^2\pi^2 n^2}{2m}(-2L^{-3}) = \frac{\hbar^2\pi^2 n^2}{mL^3} = \frac{2E_n}{L} \ . \tag{28}$$

In the classical analog to this problem, the energy of the particle E_n is constant in its collisions with the walls. Since there is no potential energy inside the square well, the velocity is

$$v = \pm\sqrt{\frac{2E_n}{m}} \ , \tag{29}$$

where the positive value is moving to the right (towards $x = L$) and the negative value is moving to the right (towards $x = 0$). From this the change in momentum of the particle from each collision can be found. Since no energy is lost (completely elastic collisions), the momenta before and after the collision have equal magnitudes, but in opposite directions. Consider a collision with the wall at $x = L$, where p_i is the particles momentum just before the collision and p_f is the momentum just after the collision,

$$\Delta p = p_i - p_f = m\sqrt{\frac{2E_n}{m}} - m\left(-\sqrt{\frac{2E_n}{m}}\right) = 2m\sqrt{\frac{2E_n}{m}} = \sqrt{8mE_n} \ . \tag{30}$$

To compare the average force felt by a classical particle to the quantum force, the value $\Delta p/\Delta t$ must be known. However $1/\Delta t$ is just the frequency f which is just the velocity of the particle divided by the distance it travels. The distance the particle travels between interactions with the *same* wall is twice the length of the box. The frequency is the same regardless of the direction the particle is travelling so choose the positive value. This gives the frequency

$$f = \frac{v}{2L} = \sqrt{\frac{2E_n}{m}}\frac{1}{2L} = \sqrt{\frac{E_n}{2mL^2}} \ , \tag{31}$$

which has units of inverse time. This gives the average force felt by the classical particle to be

$$\bar{F} = f\Delta p = \sqrt{\frac{E_n}{2mL^2}}\sqrt{8mE_n} = \sqrt{\frac{8mE_n^2}{2mL^2}} = \sqrt{\frac{4E_n^2}{L^2}} = \frac{2E_n}{L} \ , \tag{32}$$

which is the same force felt by the quantum particle.

3 Shankar 5.3.1

Consider a potential given by $V = V_r - iV_i$, where the imaginary part V_i is a constant. It is clear the Hamiltonian is not Hermitian with this potential because the definition of Hermiticity is $H = H^\dagger$,

$$H^\dagger = -\frac{\hbar^2}{2m}\nabla^2 + (V_r - (-i)V_i) \neq H \ . \tag{33}$$

It can be shown that the probability of finding a particle in this potential decreases exponentially with time. To prove this, the continuity equation for this potential is derived. For this potential the Schrödinger equation and its conjugate are

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + (V_r - iV_i)\psi \tag{34}$$

$$-i\hbar\frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + (V_r + iV_i)\psi^* \ , \tag{35}$$

multiplying Equation 34 by ψ^* and Equation 35 by ψ, then subtracting Equation 35 from Equation 34 gives

$$i\hbar\left(\psi^*\frac{\partial \psi}{\partial t} + \psi\frac{\partial \psi^*}{\partial t}\right) = -\frac{\hbar^2}{2m}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*) - 2iV_i\psi^*\psi \ . \tag{36}$$

Using the chain rule, the sum on the left hand side can be written as

$$\psi^*\frac{\partial \psi}{\partial t} + \psi\frac{\partial \psi^*}{\partial t} = \frac{\partial}{\partial t}\psi^*\psi = \frac{\partial}{\partial t}|\psi|^2 = \frac{\partial}{\partial t}P \ , \tag{37}$$

where P is the probability defined as $P = |\psi|^2$. This makes Equation 36 into

$$\frac{\partial}{\partial t}P = -\frac{\hbar^2}{2mi}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*) - \frac{2V_i}{\hbar}P \ , i \tag{38}$$

which using the definition of the probability current $\mathbf{j}$, can be written

$$\frac{\partial}{\partial t}P = -(\nabla \cdot \mathbf{j}) - \frac{2V_i}{\hbar}P \quad \Rightarrow \quad \frac{\partial}{\partial t}P + (\nabla \cdot \mathbf{j}) = -\frac{2V_i}{\hbar}P \ . \tag{39}$$

This expression can be integrated over all space which yields

$$\frac{d}{dt}\int Pd^3r + \int(\nabla \cdot \mathbf{j})d^3r = -\frac{2V_i}{\hbar}\int Pd^3r \ . \tag{40}$$

The middle integral can be shown to be zero using Gauss's law, as shown in Shankar Equation 5.3.3. Converting the volume integral over all space to a surface integral of a sphere with infinite radius S_∞ gives

$$\int(\nabla \cdot \mathbf{j})d^3r = \int_{S_\infty}\mathbf{j} \cdot dS \ , \tag{41}$$

which must be zero because for a normalizable wavefunction the probability of finding a particle at infinity must be zero. This must be true so that the integral over all space of the squared norm of the wavefunction is bounded. This allows Equation 40 to be written as

$$\int \frac{d}{dt}Pd^3r = \int\left(-\frac{2V_i}{\hbar}\right)Pd^3r \ , \tag{42}$$

but because the integral is over the same volume, the integrand of each side must also be equal,

$$\frac{d}{dt}Pd^3r = -\frac{2V_i}{\hbar}Pd^3r \ , \tag{43}$$

which is trivial to solve for $P(t)$. It may be bothersome that this equation is not equivalent to Equation 38, but the P in that equation is the probability of finding the particle at a specific location as a function of time. The P in the above equation is the probability of finding the particle anywhere in all space as a function of time. The solution to the above differential equation is an exponential of the form

$$P(t) = e^{-2V_i t/\hbar} \ , \tag{44}$$

which decays exponentially with time, proving the statement claimed at the onset of the problem.

4 Problem #4: Matrix Hamiltonian.

Consider the following one-dimensional Hamiltonian:

$$H_1 = -\frac{d^2}{dx^2} + V_1(x) \ , \text{ where } V_1(x) = \begin{cases} -1 & 0 < x < \pi \\ \infty & else \end{cases} \ , \tag{45}$$

for simplicity, we have set $\hbar = 2m = 1$. To solve this, define $\beta = \sqrt{E - V_1}$, which makes the time independent Schr\'odinger equation

$$H_1 \psi^{(1)} = E\psi^{(1)} \quad \Rightarrow \quad \frac{d^2}{dx^2}\psi^{(1)} = -\beta^2 \psi^{(1)} \ , \tag{46}$$

which has a solution of the form $\psi^{(1)}(x) = A\cos(\beta x) + B\sin(\beta x)$. The constants A and B can be determined by enforcing that the wavefunction goes to zero when the potential is infinite, i.e. when $x = 0$ and $x = \pi$. Applying the boundary conditions gives

$$\psi^{(1)}(0) = 0 = A\cos(0) + B\sin(0) \quad \Rightarrow \quad A = 0 \tag{47}$$

$$\psi^{(1)}(\pi) = 0 = B\sin(\beta\pi) \quad \Rightarrow \quad \beta = n \text{ where } n = 1, 2, 3 \ldots \tag{48}$$

making the wavefunction $\psi^{(1)}(x) = B\sin nx$ for integer values of n. To find B, the normalization requirement must be satisfied,

$$1 = \int_0^\pi \psi_n^{(1)*}\psi_n^{(1)} dx = B^2 \int_0^\pi \sin^2(nx) dx = B^2 \frac{\pi}{2} \ , \tag{49}$$

which makes the wavefunction

$$\psi^{(1)}(x) = \sqrt{\frac{2}{\pi}}\sin(nx) \ , \tag{50}$$

where n must be an integer. The energy can be found noting that, from Equation 48, $\beta = n$, which can be solved for energy by using the definition of β,

$$E_n^{(1)} = n^2 + V_1 \quad \Rightarrow \quad E_n^{(1)} = n^2 - 1 \ , \tag{51}$$

after substituting in the value of V_1. The ground and first excited states are given by $n = 1, 2$, respectively. However, when $n = 1$, the energy is zero, which normally implies there is no particle, but because the potential is negative, the particle still has kinetic energy that makes its total energy zero. The lowest two energy states are

$$\psi_1^{(1)}(x) = \sqrt{\frac{2}{\pi}}\sin(x) \qquad E_1^{(1)} = 0 \tag{52}$$

$$\psi_2^{(1)}(x) = \sqrt{\frac{2}{\pi}}\sin(2x) \qquad E_2^{(1)} = 3 \ . \tag{53}$$

Define the function $W(x)$ which is given by

$$W(x) = -\frac{\psi_1^{(1)'}(x)}{\psi_1^{(1)}(x)} = -\frac{\cos x}{\sin x} \ , \tag{54}$$

where $\psi_1^{(1)'}(x)$ denotes the first derivative with respect to x. This function allows the following operators to be defined:

$$A = \frac{d}{dx} + W(x), \quad A^\dagger = -\frac{d}{dx} + W(x) \ . \tag{55}$$

The products of these operators can be examined. Consider the product $A^\dagger A$,

$$A^\dagger A = \left(-\frac{d}{dx} + W(x)\right)\left(\frac{d}{dx} + W(x)\right) = -\frac{d^2}{dx^2} + W^2 - \frac{d}{dx}W + W\frac{d}{dx} \tag{56}$$

$$= -\frac{d^2}{dx^2} + W^2 - \left[\frac{dW}{dx} + W\frac{d}{dx}\right] + W\frac{d}{dx} \tag{57}$$

$$= -\frac{d^2}{dx^2} + W^2 - \frac{dW}{dx} \tag{58}$$

$$= -\frac{d^2}{dx^2} + \frac{\cos^2 x}{\sin^2 x} + \frac{d}{dx}\frac{\cos x}{\sin x} \tag{59}$$

$$= -\frac{d^2}{dx^2} + \frac{\cos^2 x}{\sin^2 x} - \frac{1}{\sin^2 x} \tag{60}$$

$$= -\frac{d^2}{dx^2} + \frac{\cos^2 x - (\cos^2 x + \sin^2 x)}{\sin^2 x} = -\frac{d^2}{dx^2} + \frac{\cos^2 x - \cos^2 x}{\sin^2 x} - \frac{\sin^2 x}{\sin^2 x} \tag{61}$$

$$= -\frac{d^2}{dx^2} - 1 = -\frac{d^2}{dx^2} + V_1 = H_1 \ . \tag{62}$$

Therefore the product of $A^\dagger$ and A is the Hamiltonian H_1. Now, consider the Hamiltonian $H_2 = AA^\dagger$,

$$H_2 = A^\dagger A = \left(\frac{d}{dx} + W(x)\right)\left(-\frac{d}{dx} + W(x)\right) = -\frac{d^2}{dx^2} + W^2 + \frac{d}{dx}W - W\frac{d}{dx} \tag{63}$$

$$= -\frac{d^2}{dx^2} + W^2 + \frac{dW}{dx} = -\frac{d^2}{dx^2} + \frac{\cos^2 x}{\sin^2 x} + \frac{1}{\sin^2 x} \tag{64}$$

$$= -\frac{d^2}{dx^2} + \frac{\cos^2 x + (\cos^2 x + \sin^2 x)}{\sin^2 x} \tag{65}$$

$$= -\frac{d^2}{dx^2} + \frac{1 + \cos^2 x}{\sin^2 x} \ . \tag{66}$$

This gives the form of the potential for this Hamiltonian,

$$V_2 = \frac{1 + \cos^2 x}{\sin^2 x} \ . \tag{67}$$

From the definitions of H_1 and H_2, it is easy to show

$$AH_1 = H_2 A \quad \Rightarrow \quad AH_1 |\psi_n^{(1)}\rangle = H_2 A |\psi_n^{(1)}\rangle \ , \tag{68}$$

which when applying the H_1 operator becomes

$$AE_n^{(1)} |\psi_n^{(1)}\rangle = H_2 A |\psi_n^{(1)}\rangle \quad \Rightarrow \quad H_2 A |\psi_n^{(1)}\rangle = E_n^{(1)} A |\psi_n^{(1)}\rangle \,, \tag{69}$$

which implies that the eigenstates of H_2 are the eigenstates of H_1 operated on by A, with the same eigenvalues,

$$|\psi_n^{(2)}\rangle = A |\psi_n^{(1)}\rangle \qquad E_n^{(2)} = E_n^{(1)} \ . \tag{70}$$

This allows the entire spectrum of H_2 to be found. Using the ground state of H_1, the corresponding state of H_2 can be calculated,

$$|\psi_1^{(2)}\rangle = A\,|\psi_1^{(1)}\rangle = \left(\frac{d}{dx} - \frac{\cos x}{\sin x}\right)\sqrt{\frac{2}{\pi}}\sin(x) \tag{71}$$

$$= \sqrt{\frac{2}{\pi}}\left(\frac{d}{dx}\sin(x) - \frac{\cos x}{\sin x}\sin(x)\right) \tag{72}$$

$$= \sqrt{\frac{2}{\pi}}\,(\cos x - \cos x) = 0\ , \tag{73}$$

which says there is no particle because the wavefunction is zero (and so must be the energy), therefore the ground state of H_2 does not correspond to the ground state of H_1. The ground state wavefunction of H_2 is not $n = 1$, as in the spectrum of H_1, but $n = 2$. Therefore, the ground state of H_2 is

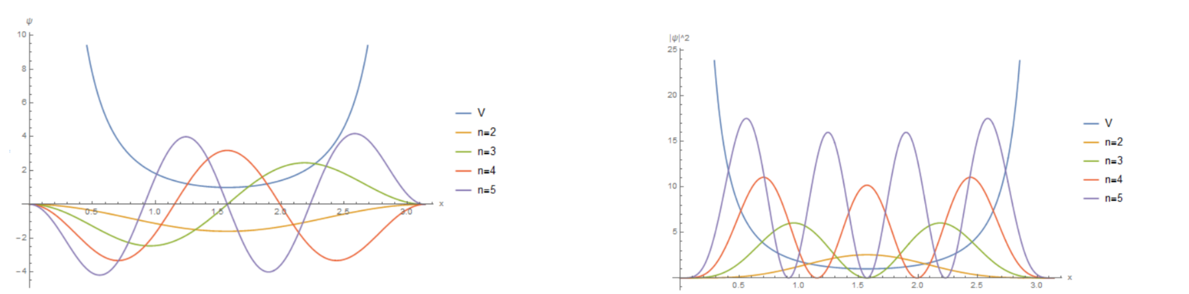
$$|\psi_2^{(2)}\rangle = A\,|\psi_2^{(1)}\rangle = \left(\frac{d}{dx} - \frac{\cos x}{\sin x}\right)\sqrt{\frac{2}{\pi}}\sin(2x) \tag{74}$$

$$= \sqrt{\frac{2}{\pi}}\left(\frac{d}{dx}\sin(2x) - \frac{\cos x}{\sin x}\sin(2x)\right) = \sqrt{\frac{2}{\pi}}\left(2\cos(2x) - \frac{\cos x}{\sin x}\sin(2x)\right) \tag{75}$$

$$= \sqrt{\frac{2}{\pi}}\left(2\cos(2x) - \frac{\cos x}{\sin x}2\sin(x)\cos(x)\right) \tag{76}$$

$$= 2\sqrt{\frac{2}{\pi}}[\cos(2x) - \cos^2(x)]\ , \tag{77}$$

which has energy $E_2^{(2)} = E_2^{(1)} = 3$. The $|\psi_n^{(2)}\rangle$ for each n satisfies the same boundary conditions imposed for V_1, see Figure 1.



(a) Wavefunctions of H_2 for multiple values of n. (b) Probability densities of H_2 for some values of n.

Figure 1: Plots showing that the behavior of the eigenstates of H_2 obey the necessary boundary conditions for all n.