PH 451/551 **Solutions of HW #1** **Winter 2026**

(due January 14, 2026)

1. **McIntyre 2.17**.

We are given a spin-1 particle in an arbitrary state.

a) The possible results of a measurement of the spin component S_z are always $+1\hbar, 0\hbar, -1\hbar$ for a spin-1 particle. The probabilities are

$$\wp_{\hbar} = \left|\langle 1|\psi\rangle\right|^2 = \left| \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \tfrac{1}{\sqrt{30}} \begin{pmatrix} 1 \\ 2 \\ 5i \end{pmatrix} \right|^2 = \left|\tfrac{1}{\sqrt{30}}1\right|^2 = \frac{1}{30}$$

$$\wp_{0} = \left|\langle 0|\psi\rangle\right|^2 = \left| \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \tfrac{1}{\sqrt{30}} \begin{pmatrix} 1 \\ 2 \\ 5i \end{pmatrix} \right|^2 = \left|\tfrac{1}{\sqrt{30}}2\right|^2 = \frac{4}{30}$$

$$\wp_{-\hbar} = \left|\langle -1|\psi\rangle\right|^2 = \left| \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \tfrac{1}{\sqrt{30}} \begin{pmatrix} 1 \\ 2 \\ 5i \end{pmatrix} \right|^2 = \left|\tfrac{1}{\sqrt{30}}5i\right|^2 = \frac{25}{30}$$

The expectation value of S_z is

$$\langle S_z\rangle = \wp_{\hbar}\hbar + \wp_{0}0 + \wp_{-\hbar}(-\hbar) = \frac{1}{30}\hbar + \frac{4}{30}0 + \frac{25}{30}(-\hbar) = -\frac{24}{30}\hbar = -\frac{4}{5}\hbar$$

b) The expectation value of S_x is

$$\langle S_x\rangle = \langle\psi|S_x|\psi\rangle = \frac{1}{\sqrt{30}} \begin{pmatrix} 1 & 2 & -5i \end{pmatrix} \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \frac{1}{\sqrt{30}} \begin{pmatrix} 1 \\ 2 \\ 5i \end{pmatrix}$$

$$= \frac{1}{30}\frac{\hbar}{\sqrt{2}} \begin{pmatrix} 1 & 2 & -5i \end{pmatrix} \begin{pmatrix} 2 \\ 1+5i \\ 2 \end{pmatrix} = \frac{1}{30}\frac{\hbar}{\sqrt{2}}\left(2 + 2(1+5i) - 5i\times 2\right) = \frac{\sqrt{2}}{15}\hbar$$

2. **McIntyre 5.11**.

We are given an initial wave function, which corresponds to that of the ground state of a box of size L. Hence the initial state is

$$\psi_{initial}(x) = \begin{cases} 0 & x<0, x>L \\ \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right) & 0<x<L \end{cases}.$$

If the box is expanded "suddenly," it means the wave function remains unaltered, at least for a short time after the expansion. Now we want the probabilities that the particle in the expanded box is in the ground state and first excited state of the expanded box. The probability that the initial state $\left|\psi_{initial}\right\rangle \square\ \psi_{initial}(x)$ is measured to be in the final state $\left|\psi_{final}\right\rangle \square\ \psi_{final}(x)$ is the square of the projection of the two states:

$$\begin{aligned}\wp_{i\to f} &= \left|\left\langle \psi_{final} \middle| \psi_{initial} \right\rangle\right|^2 \\ &= \left|\int_{-\infty}^{\infty} \psi^*_{final}(x)\,\psi_{initial}(x)\,dx\right|^2\end{aligned}$$

The energy eigenfunctions of the <u>expanded</u> box are

$$\varphi_n(x) = \sqrt{\frac{2}{3L}}\sin\left(\frac{n\pi x}{3L}\right)$$

between 0 and $3L$.

(i) We are interested in the term with $n = 1$; this is the ground state of the new box. Break the integral over the new box into two pieces, with one piece being zero:

$$\begin{aligned}\wp_{i\to n=1} &= \left|\int_{-\infty}^{\infty} \varphi_1^*(x)\,\psi_{initial}(x)\,dx\right|^2 \\ &= \left|\int_0^L \sqrt{\frac{2}{3L}}\sin\left(\frac{\pi x}{3L}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)dx + \int_L^{3L}\sqrt{\frac{2}{3L}}\sin\left(\frac{\pi x}{3L}\right)\cdot 0\,dx\right|^2 \\ &= \left|\frac{2}{\sqrt{3}L}\int_0^L \sin\left(\frac{\pi x}{3L}\right)\sin\left(\frac{\pi x}{L}\right)dx\right|^2 = \left|\frac{2\sqrt{3}}{\pi}\left[\cos\left(\frac{\pi x}{3L}\right)\sin\left(\frac{\pi x}{3L}\right)^3\right]_0^L\right|^2 \\ &= \left|\frac{9}{8\pi}\right|^2 = \frac{81}{64\pi^2} \cong 0.13\end{aligned}$$

There is a 13% chance that the particle is measured in the ground state of the expanded box.

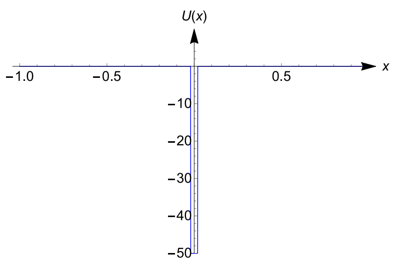
(ii) Now the $n = 2$ state:

$$\begin{aligned}P_{i\to n=2} &= \left|\int_{-\infty}^{\infty} \varphi_2^*(x)\,\psi_{initial}(x)\,dx\right|^2 \\ &= \left|\int_0^L \sqrt{\frac{2}{3L}}\sin\left(\frac{2\pi x}{3L}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)dx + \int_L^{3L}\sqrt{\frac{2}{3L}}\sin\left(\frac{2\pi x}{3L}\right)\cdot 0\,dx\right|^2 \\ &= \left|\frac{2}{\sqrt{3}L}\int_0^L \sin\left(\frac{2\pi x}{3L}\right)\sin\left(\frac{\pi x}{L}\right)dx\right|^2 = \left|\left[\frac{4\sqrt{3}}{5\pi}\left(3+2\cos\left(\frac{2\pi x}{3L}\right)\right)\sin\left(\frac{\pi x}{3L}\right)^3\right]_0^L\right|^2 \\ &= \left|\frac{9}{5\pi}\right|^2 = 0.33\end{aligned}$$

There is a 33% chance of finding the particle in the second state. This seems reasonable because the second state of the bigger box is a better match to the first state of the smaller box.

3. Solve the energy eigenvalue equation analytically to find the bound state energy eigenvalue and eigenfunction (there is only one bound state) of the potential energy $U(x) = -\lambda\delta(0)$ where λ is a positive constant.

(a)-(b) The constant λ has dimensions of [energy * length]. In particular:



The delta function has dimensions of the reciprocal of its argument, in this case length. The reason is that $\int_{-\infty}^{\infty} \delta(x)dx = 1$. So for $\lambda\delta(0)$ to have the dimensions of energy, λ must have dimensions of [energy*length].

(c) "Bound state" means that $E < 0$, *i.e.* it is less than the energy of the top of the well.

The delta function well is a limiting case of the finite well, just infinitely thin and infinitely deep. It is interesting because it admits only one bound state.

Energy eigenvalue equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} - \lambda\delta(0)\psi(x) = E\psi(x)$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m\lambda}{\hbar^2}\delta(0)\psi(x) = -\frac{2m}{\hbar^2}E\psi(x)$$

Because $\boldsymbol{E < 0}$,

$$\frac{d^2\psi(x)}{dx^2} = +\frac{2m}{\hbar^2}|E|\psi(x)$$

Notice that, away from zero but even arbitrarily close to it, the solution is the sum of exponentially decaying and growing functions. To ensure that the function goes to zero at ±infinity, reject the exponentially growing solution. Introduce constants *A* and *B*.

$$\psi(x) = \begin{cases} Ae^{-\sqrt{\frac{2m|E|}{\hbar^2}}x} & x > 0 \\ Be^{\sqrt{\frac{2m|E|}{\hbar^2}}x} & x < 0 \end{cases}$$

and continuity at $x = 0$ requires $A = B$.

We will need the derivative:

$$\frac{d\psi(x)}{dx} = \begin{cases} -\sqrt{\frac{2m|E|}{\hbar^2}}Ae^{-\sqrt{\frac{2m|E|}{\hbar^2}}x} & x > 0 \\ \sqrt{\frac{2m|E|}{\hbar^2}}Ae^{\sqrt{\frac{2m|E|}{\hbar^2}}x} & x < 0 \end{cases}$$

Integrate the equation across $x = 0$ where the delta function has its singularity, and let ε->0.

$$\int_{-\varepsilon}^{\varepsilon} \frac{d^2\psi(x)}{dx^2}dx + \frac{2m\lambda}{\hbar^2}\underbrace{\int_{-\varepsilon}^{\varepsilon}\delta(0)\psi(x)dx}_{\to\psi(0)=A} = -\underbrace{\int_{-\varepsilon}^{\varepsilon}\frac{2mE}{\hbar^2}\psi(x)dx}_{\to 0}$$

(i) The wave function is continuous, but its derivative is not necessarily continuous if the potential is infinite, as we see here. The integral of the second derivative is the first derivative. Evaluate the first derivative at values slightly greater than zero (where the first derivative is negative) and at values lightly less than zero (where it is positive).

(ii) The integral of the delta function gives the value of the wave function at the position of the delta function.

(iii) The integral over the wave function is whatever it is, but the difference in the value on either side of zero is infinitesimal and goes to zero as ε->0.

$$\left.\frac{d\psi(x)}{dx}\right|_{-\varepsilon}^{\varepsilon} + \frac{2m\lambda}{\hbar^2}\psi(0) = 0$$

$$\frac{d\psi(0^+)}{dx} - \frac{d\psi(0^-)}{dx} = -\frac{2m\lambda}{\hbar^2}\psi(0)$$

Use the form of the wave function: $-\sqrt{\frac{2m|E|}{\hbar^2}}A - \sqrt{\frac{2m|E|}{\hbar^2}}A = -\frac{2m\lambda}{\hbar^2}A$

Find that

$$-2\sqrt{\frac{2m|E|}{\hbar^2}} = -\frac{2m\lambda}{\hbar^2}$$

$$|E| = \frac{m^2\lambda^2}{\hbar^4}\frac{\hbar^2}{2m} \Rightarrow E = -\frac{m\lambda^2}{2\hbar^2}$$

(recall that $E<0$ for a bound state)

Normalization gives the value of A:

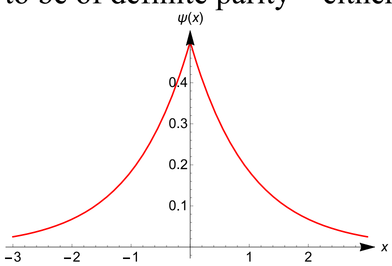
$$\int_{-\infty}^{\infty}|\psi(x)|^2 dx = 1 \qquad 2\int_0^{\infty}|A|^2 e^{-2\sqrt{\frac{2m|E|}{\hbar^2}}x}dx = 1$$

$$|A|^2 = \frac{1}{2}\left[\int_0^{\infty} e^{-2\sqrt{\frac{2mE}{\hbar^2}}x}dx\right]^{-1} = \frac{1}{2}\left[\frac{e^{-\infty}-e^0}{-2\sqrt{\frac{2m|E|}{\hbar^2}}}\right]^{-1} = \sqrt{\frac{2m|E|}{\hbar^2}}$$

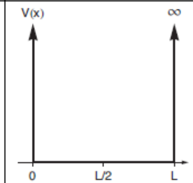
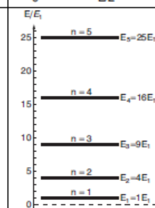
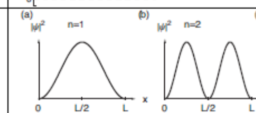
Substitute for $|E|$: $\frac{2m|E|}{\hbar^2} = \frac{2m^2\lambda^2}{2\hbar^4}$ $\qquad A = \left(\frac{2mE}{\hbar^2}\right)^{1/4} = \left(\frac{2m^2\lambda^2}{2\hbar^4}\right)^{1/4} = \frac{\sqrt{m\lambda}}{\hbar}$

$$\psi(x) = \begin{cases} \frac{\sqrt{m\lambda}}{\hbar} e^{-\frac{m\lambda}{\hbar^2}x} & x > 0 \\ \frac{\sqrt{m\lambda}}{\hbar} e^{\frac{m\lambda}{\hbar^2}x} & x < 0 \end{cases} \quad ; \qquad E = \frac{m\lambda^2}{2\hbar^2}$$

(d) The wave function is continuous but has a cusp corresponding to the discontinuous first derivative. As the wave function approaches 0 at large x, this is a bound state. Note that the wave function is even – the wave functions of symmetric potentials are expected to be of definite parity – either even or odd – which is supported by this observation.



4. Fill in the table that describes the different representations of the operators, eigenvalues, eigenstates *etc*. for a quantum particle subject to a 1-dimensional infinite square well potential energy (p. 2).

Infinite well pot. energy	Ket Representation	Matrix Representation	Wave Function Representation	Graphical Rep.
Hamiltonian	H or $\hat{H}$	$H \doteq \begin{pmatrix} E_1 & 0 & 0 & \cdots \\ 0 & E_2 & 0 & \cdots \\ 0 & 0 & E_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$	$H \doteq -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \quad 0<x<L$	
Eigenvalues of Hamiltonian	$E_n = \frac{\pi^2\hbar^2}{2mL^2}n^2$	$E_n = \frac{\pi^2\hbar^2}{2mL^2}n^2$	$E_n = \frac{\pi^2\hbar^2}{2mL^2}n^2$	
Normalized eigenstates of Hamiltonian	$\vert n\rangle$	$\vert 1\rangle \doteq \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad \vert 2\rangle \doteq \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \ldots$	$\vert n\rangle \doteq \psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)$	
Coefficient of n^{th} energy eigenstate	$c_n = \langle n\vert\psi\rangle$	$c_n = \begin{pmatrix} 0 & \cdots & 1 & \cdots \end{pmatrix}\begin{pmatrix} c_1 \\ \vdots \\ c_n \\ \vdots \end{pmatrix}$	$c_n = \int_0^L \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)\psi(x)dx$	Depends on $\psi(x)$, but can graph integrand
Probability of measuring E_n	$\mathcal{P}_{E_n} = \vert c_n\vert^2 = \vert\langle n\vert\psi\rangle\vert^2$	$\mathcal{P}_{E_n} = \vert c_n\vert^2 = \left\vert \begin{pmatrix} 0 & \cdots & 1 & \cdots \end{pmatrix}\begin{pmatrix} c_1 \\ \vdots \\ c_n \\ \vdots \end{pmatrix}\right\vert^2$	$\mathcal{P}_{E_n} = \vert c_n\vert^2 = \left\vert \int_0^L \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)\psi(x)dx\right\vert^2$	Depends on $\psi(x)$
Expectation value of Hamiltonian	$\langle\psi\vert H\vert\psi\rangle = \sum_n \mathcal{P}_{E_n}E_n = \sum_n \vert c_n\vert^2 E_n$	$\langle\psi\vert H\vert\psi\rangle = \begin{pmatrix} c_1^* & c_2^* & \cdots \end{pmatrix}\begin{pmatrix} E_1 & 0 & \cdots \\ 0 & E_2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}$	$\langle\psi\vert H\vert\psi\rangle = \int_0^L \psi^*(x)\hat{H}\psi(x)\,dx$	Depends on $\psi(x)$