Phys 125
Boyda

Solutions to the second midterm.

1. Particle in a box, $-1 \le x \le 1$.

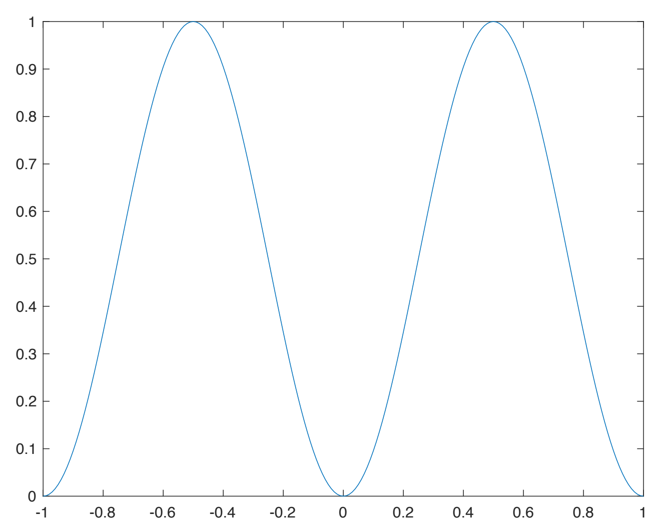
   (a) Normalization. Use the substituion $u = \pi x$ to integrate $\sin^2(\cdot)$ and be sure to include factor $dx = du/\pi$:

   $$1 = |N|^2 \int_{-1}^{1} dx \sin^2 \pi x = |N|^2 \int_{-\pi}^{\pi} \frac{du}{\pi} \sin^2 u = \frac{|N|^2}{\pi} \left(\frac{u}{2} - \frac{\sin 2u}{4} \right)\Big|_{-\pi}^{\pi} = |N|^2.$$

   Up to choice of overall phase, $N = 1$.

   (b) The probability density is $|\psi(x)|^2 = \sin^2 \pi x$. (The probability is the probability density integrated over some interval in x.) In the spirit of MatLab plotting,

   $$>>x = -1 : 1/100 : 1;$$
   $$>>y = (sin(pi * x)).^{\wedge 2};$$
   $$>>plot(x, y)$$



(c) By inspection, $\langle x \rangle = 0$, because the wavefunction is distributed symmetrically around the origin. Or you can compute

$$\langle x \rangle = \int_{-\infty}^{\infty} dx\ x|\psi(x)|^2 = \int_{-1}^{1} dx\ x \sin^2 \pi x = 0.$$

From the plot, the most likely positions to find the particle are $x = \pm\frac{1}{2}$.

(d) The uncertainty is formally equal to a standard deviation. Looking at the graph, we might intuit $\Delta x \sim \pm.5$, the distance to either peak from the mean value $\langle x \rangle = 0$. Or perhaps it's a little more than .5. Certainly it's less than one, since *all* possible values fall within ± 1 of the mean. Actually computing,

$$\langle x^2 \rangle = \int_{-1}^{1} dx\ x^2 \sin^2 \pi x \approx .283,$$

and so

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \approx .53.$$

One reason I asked you to estimate (besides it being a good expression of comprehension) was so you could avoid integrating multiple times by parts on the exam.

(e) You could compute

$$\langle p_x \rangle = \int dp\ p\ \psi^*(p)\psi(p),$$

but to do so you would first need to determine the momentum space wavefunction,

$$\psi(p) = \langle p|\psi \rangle = \int dx \langle p|x \rangle \langle x|\psi \rangle = \int dx \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}\psi(x).$$

Expand $\psi(x) = \sin \pi x$ interms of complex exponential and integrate the exponentials. It's doable enough. However, the hint was to use the position space representation and this is easier in this case:

$$\langle p_x \rangle = \int dx\ \psi^*(x)(-i\hbar)\frac{\partial \psi(x)}{\partial x} = -i\hbar \int_{-1}^{1} dx \sin \pi x(\pi \cos \pi x) = 0.$$

This is a standing wave, an equally-weighted superposition of left- and right-moving travelling waves, so we should expect $\langle p_x \rangle = 0$. Similarly,

$$\langle p_x^2 \rangle = \int dx\ \psi^*(x)(-\hbar^2)\frac{\partial^2 \psi(x)}{\partial x^2} = -\hbar^2 \int_{-1}^{1} dx \sin \pi x(-\pi^2) \sin \pi x = \hbar^2\pi^2.$$

You've already computed $\int dx\ \sin^2 \pi x = 1$, right?

(f) First,

$$\Delta p_x = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2} = \pi\hbar.$$

Then,

$$\Delta x \Delta p_x \sim .5 \cdot \pi\hbar \geq \hbar/2.$$

2. More particle in the (same) box.

(a) I had hoped you would recognize the wavefunction here as one of the energy eigenfunctions. You can check this by applying the x-representation of the Hamiltonian to $\psi(x)$,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}(\sin \pi x) = +\frac{\hbar^2\pi^2}{2m}\sin \pi x.$$

(Where the wavefunction is non-zero the potential $V(x) = 0$.) The energy is the eigenvalue, $E_2 = \hbar^2\pi^2/(2m)$. (I call it E_2 because this is the second energy eigenstate, as you can see by comparing to the eigenstates given in the problem.) This is, of course, also the expectation value of the energy since the energy is known precisely. More mechanistically,

$$\langle \frac{p_x^2}{2m} \rangle = \frac{1}{2m}\int dx\, \psi^*(x)(-\frac{\hbar^2}{2m})\frac{\partial^2\psi(x)}{\partial x^2} = -\frac{\hbar^2}{2m}\int_{-1}^{1} dx \sin \pi x(-\pi^2)\sin \pi x = \frac{\hbar^2\pi^2}{2m}.$$

(b) Being an energy eigenstate, this is a stationary state:

$$\psi(x,t) = e^{-iE_2 t/\hbar}\psi(x) = e^{-iE_2 t/\hbar}\sin \pi x.$$

It remains in the second energy eigenstate for all time and there is no probability of finding the particle in the ground energy state. You can also compute this directly. Calling $|\psi_1\rangle$, $|\psi_2\rangle$ the first and second energy eigentates,

$$\langle \psi_1 | e^{-i\hat{H}t/\hbar} | \psi_2 \rangle = \int dx\, \psi_1^*(x) e^{-iE_2 t/\hbar}\psi_2(x) = e^{-iE_2 t/\hbar}\int_{-1}^{1} dx \cos\frac{\pi x}{2}\sin \pi x = 0.$$

That this integral is zero expresses the orthogonality of the eigenstates.

3. This problem is adapted from the Feynman Lectures, Volume III, and I encourage you to read through his always joyfully lucid and physical reasoning. The relevant section is available online, http://www.feynmanlectures.caltech.edu/III_10.html.

Formally, this problem is identical to that of the ammonia molecule as explained on pp. 128-131 of Townsend. The only difference is that we started in state $|2\rangle$ and asked when the electron would be found in $|1\rangle$, the other way around from Townsend (cf. eqns. 4.54-55). Calling the ground state $|I\rangle$ (with energy $E_I = E_0 - A$) and excited state $|II\rangle$ ($E_{II} = E_0 + A$), you should have found

$$\psi(t) = e^{-i\hat{H}t/\hbar}\psi(0) = e^{-i\hat{H}t/\hbar}\left(\frac{1}{\sqrt{2}}|I\rangle - \frac{1}{\sqrt{2}}|II\rangle\right) = \frac{1}{\sqrt{2}}e^{-i(E_0-A)t/\hbar}|I\rangle - \frac{1}{\sqrt{2}}e^{-i(E_0+A)t/\hbar}|II\rangle.$$

Given that $|1\rangle = \frac{1}{\sqrt{2}}|I\rangle + \frac{1}{\sqrt{2}}|II\rangle$,

$$\begin{aligned}
\langle 1|\psi(t)\rangle &= \frac{1}{\sqrt{2}}\left(\langle I| + \langle II|\right)\frac{1}{\sqrt{2}}\left(e^{-i(E_0-A)t/\hbar}|I\rangle - e^{-i(E_0+A)t/\hbar}|II\rangle\right) \\
&= \frac{1}{2}e^{-i(E_0-A)t/\hbar} - \frac{1}{2}e^{-i(E_0+A)t/\hbar} \\
&= ie^{-iE_0t/\hbar}\sin\frac{At}{\hbar}.
\end{aligned}$$

Squaring to get the probability,

$$|\langle 1|\psi(t)\rangle|^2 = \sin^2\frac{At}{\hbar}.$$

This is one when $At/\hbar$ is $\pi/2$, $3\pi/2$, $5\pi/2$, $\ldots$.

When A decreases, the ground state energy decreases, indicating an attractive interaction between the electron and two protons. The one piece missing is that if the protons get too close, the electron can no longer shield the positive charges, and they repel. In between, there is a potential well and a possible stable bound state for H_2^+. For more details I refer you to Feynman.