Name_____ Student Number_____

Mid-Term #1

Show your work clearly. I will give partial credit in some cases, but *only* to the extent that I can clearly understand your work. The exam is marked out of 100 points.

You may use any non-internet-enabled calculator for the exam. You may not use any internet-enabled device (including e-readers, tablets, laptops, cellular phones, ...). You may not use any notes, books, or other materials.

10 questions @ 10 points each.

1 Bonus questions worth 10 points (see the last page).

Key integrals and identities:

$$\left(\frac{a}{2}\right)\delta_{mn} = \int_{0}^{a} \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) dx$$

$$\left(\frac{a}{2}\right)\delta_{mn} = \int_{0}^{a} \cos\left(\frac{n\pi x}{a}\right) \cos\left(\frac{m\pi x}{a}\right) dx$$

$$0 = \int_{0}^{a} \cos\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) dx$$

$$\frac{a^{2}}{4} = \int_{0}^{a} \left(\sin\left(\frac{n\pi x}{a}\right)\right)^{2} x dx$$

$$\left(\frac{a}{2\pi n}\right)^{3} \left(\frac{4\pi^{3}n^{3}}{3} - 2\pi n\right) = \int_{0}^{a} \left(\sin\left(\frac{n\pi x}{a}\right)\right)^{2} x^{2} dx$$

$$\frac{1}{2}\sqrt{\frac{\pi}{\alpha}} = \int_{0}^{\infty} e^{-ax^{2}} dx$$

$$\left(\frac{1}{2}\sqrt{\frac{\pi}{\alpha}}\right) \left(\frac{(2n-1)(2n-3)\cdots(3)(1)}{(2\alpha)^{n}}\right) = \int_{0}^{\infty} x^{2n} e^{-ax^{2}} dx$$

$$n = 1, 2, 3, \dots$$

$$\left(\frac{1}{2}\right) \left(\frac{n!}{\alpha^{n+1}}\right) = \int_{0}^{\infty} x^{2n+1} e^{-ax^{2}} dx$$

$$n = 0, 1, 2, \dots$$

$$\int x \sin(bx) dx = \frac{\sin(bx)}{b^{2}} - \frac{x \cos(bx)}{b} + \text{constant}$$

$$\int x^{2} \sin(bx) dx = -\left(\frac{x^{2} \cos(bx)}{b} + \frac{2x \cos(bx + \frac{1}{2}\pi)}{b^{2}} + \frac{2\cos(bx + \pi)}{b^{3}}\right) + \text{constant}$$

$$2 \sin(x) \sin(y) = \cos(x - y) - \cos(x + y) \rightarrow 2 \sin^{2} x = 1 - \cos(2x)$$

$$2 \cos(x) \cos(y) = \cos(x - y) + \cos(x + y) \rightarrow 2 \cos^{2} x = 1 + \cos(2x)$$

$$2 \sin(x) \cos(y) = \sin(\alpha + \beta) + \sin(\alpha - \beta) \rightarrow 2 \sin x \cos x = \sin(2x)$$

$$\sin(x + y) = \sin x \cos y + \cos x \sin y \rightarrow \sin(2x) = 2 \sin x \cos x$$

$$\cos(x + y) = \cos x \cos y - \sin x \sin y \rightarrow \cos(2x) = \cos^{2} x - \sin^{2} x$$

1 eV = 1.602 × 10 ⁻¹⁹ 96.48 = 1.602 × 10 ⁻¹⁸ 96.48 = 4.359 × 10 ⁻¹⁸ 2625	.602 × 10 ⁻¹⁹	lev	=1.661×10 ⁻²¹ 1	1 Jour 6.022×10 ²⁰	Joure Ky mor		CONVERSION FACTORS FOR ENERGY UNITS			Stefan-Boltzmann constant	Bohr magneton	First Bohr radius	Rydberg constant (infinite nuclear mass)	Permittivity of a vacuum	Molar gas constant	Boltzmann constant	Proton rest mass	Electron rest mass	Atomic mass unit	Speed of light in vacuum	Planck's constant	Proton charge	Avogadro's number	Constant	VALUES OF SOME PHYSICAL CONSTANTS		
	27.21	1	1.036×10^{-2}	6.242×10^{18}	4.9	A.V	OR ENERGY			q	μ_B	a_0	R_{ω}	$\frac{\varepsilon_0}{4\pi\varepsilon_0}$	R	k_B	m_p	m_e	amu	c	* *	e	N_{0}	Symbol	CAL CONSTA		
4.556 × 10 ⁻⁶	1 2.195×10 ⁵	3.675×10^{-2} 8065	3.089×10^{-4} 83.60	$2.2939 \times 10^{17} 5.035 \times 10^{22}$	uu cm		UNITS			$5.67032 \times 10^{-8} \mathrm{J \cdot m^{-2} \cdot K^{-4} \cdot s^{-1}}$	$9.27409 \times 10^{-24} \text{ J} \cdot \text{T}^{-1}$	$5.29177 \times 10^{-11} \mathrm{m}$	$2.179914 \times 10^{-23} \text{ J}$ 1.097373 cm^{-1}	$\begin{array}{l} 8.854188 \times 10^{-12} \ \mathrm{C^2 \cdot s^2 \cdot kg^{-1} \cdot m^{-3}} \\ 1.112650 \times 10^{-10} \ \mathrm{C^2 \cdot s^2 \cdot kg^{-1} \cdot m^{-3}} \end{array}$	8.31441 J·K ⁻¹ ·mol ⁻¹	$1.38066 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$ 0.69509 cm^{-1}	$1.67265 \times 10^{-27} \mathrm{kg}$	$9.10953 \times 10^{-31} \mathrm{kg}$	$1.66056 \times 10^{-27} \mathrm{kg}$	$2.997925 \times 10^8 \mathrm{m \cdot s^{-1}}$	$6.62618 \times 10^{-34} \text{ J} \cdot \text{s}$ $1.05459 \times 10^{-34} \text{ J} \cdot \text{s}$	$1.60219 \times 10^{-19} \mathrm{C}$	$6.02205 \times 10^{23} \text{ mol}^{-1}$	Value	NTS		
2.998 × 1010	6.580×10^{15}	2.418×10^{14}	2.506×10^{12}	1.509×10^{33}	ZH					1				m-3													
			$\int_0^a \cos \frac{n\pi x}{a} \sin \frac{n\pi x}{a} dx =$	$\int_0^a \sin \frac{m\omega}{a} \sin \frac{m\omega}{a} dx =$	$\int_0^0 2a^{n+1}$	$x^{2n+1}e^{-ax^2}dx =$	$\int_0^\infty x^2 n e^{-ax^2} dx = \frac{1 \cdot 3}{}$	$\int_0^\infty e^{-ax^2} dx = \left(\frac{\pi}{4a}\right)^{1/2}$	$\int_0^\infty x^n e^{-\alpha x} dx = \frac{n!}{a^{n+1}}$		$(1+x)^n = 1 + nx + \frac{n(n-x)^n}{n(n-x)^n}$	$\frac{1-x}{1-x} = \frac{1+x+x^{2}+x^{2}+x^{2}}{1+x^{2}$	31 +	$\cos x = 1 - \frac{1}{2!} + \frac{1}{4!} - \frac{1}{4!}$	x ² x ⁴	$e^{x} = 1 + x + \frac{x^{2}}{2!} + \frac{x^{3}}{3!}$	f(x) = f(a) + f'(a)(x - a)		$\sin \theta = \frac{\varepsilon - \varepsilon}{2i}$	$\theta i = 0 - \theta i \phi$	$\cos\theta = \frac{e^{i\theta} + e^{-i\theta}}{2}$	$e^{\pm i\theta} = \cos\theta \pm i\sin\theta$	$\sin(\alpha \pm \beta) = \sin \alpha \cos \beta \pm \cos \alpha \sin \beta$ $\cos(\alpha \pm \beta) = \cos \alpha \cos \beta \mp \sin \alpha \sin \beta$	$\sin \alpha \cos \beta = \frac{1}{2} \sin (\alpha + \beta) + \frac{1}{2} \sin (\alpha - \beta)$	$\sin \alpha \sin \beta = \frac{1}{2} \cos (\alpha - \beta)$ $\cos \alpha \cos \beta = \frac{1}{2} \cos (\alpha - \beta)$	SOME MATHEMATICAL FORMULAS	

 $J(oule) = 1 \text{ kg} \cdot \text{m}^2/\text{s}^2 = 1 \text{ C}(oulomb) \cdot \text{V}(olt)$

(c) stay about the same.

2.	_	<u>=</u>		ex is 1 eV (1 electron-volt).
	The particle is then s	queezed, so that the nev	w box is half the length	of the old box, $a_{\text{new}} = \frac{1}{2} a_{\text{old}}$
	. What is the zero-p			
	(a) 1 eV	(c) 2eV	(e) 4 eV	(g) 8 eV (h) can't tell from the
	(b) 0.5 eV	(d) 0.25 eV	(f) 0.125 eV	(h) can't tell from the information given
3.	temperature 298.15	K, with kinetic energy		That is, for neutrons with e Broglie wavelength. The
	mass of the neutron	is $1.6749 \cdot 10^{-27}$ kg.		
4.	What is the momen	tum of a photon with	wavenumber 1.500.1	0^7 m^{-1} .
••		32 W P333 W-W	1.000 1	· · · ·

1. As the quantum number n increases, the energy levels of a particle in a one-dimensional

(b) further apart

box with infinitely high sides become

(a) closer together

5. Write a Slater determinant for the 1s²2s¹2p¹ triplet excited state of the Beryllium atom. Write out the Slater determinant in full, showing every element, including the normalization constant.

6. To a reasonable approximation, a quantum dot can be approximated as an electron in a 3-dimensional box with infinite sites. Consider eight electrons in a cubic quantum dot with length 1 nm. (1 nm = 10⁻⁹ m) What is the wavelength corresponding to the lowest-energy absorption of light for this system?

Consider a particle of mass m in a one-dimensional box with length 2ℓ centered at the origin, with potential

$$V_{\text{pib0}}(x) = \begin{cases} +\infty & x < -\ell \\ 0 & -\ell \le x \le \ell \\ +\infty & x > \ell \end{cases}$$

7. What is the expression for the energy eigenvalues of this system?

8. What is the expression for the eigenfunctions of the Hamiltonian for this system? You do not need to normalize the eigenfunctions.

Consider a system defined for $-\infty < x < \infty$. You may assume that all wavefunctions approach zero as $x \to \pm \infty$. (Otherwise the wavefunctions are not normalized.) It is not strictly necessary, but if you find it helpful, you may also assume that all the derivatives of the wavefunction go to zero at $x \to \pm \infty$ also. (This is for problems #9, #10, and the bonus on the next page.)

9. Give a mathematical proof that the momentum operator is Hermitian.

10. Show that the momentum-operator-squared, \hat{p}^2 , is Hermitian. You can use the result from problem 9. (I.e., you may assume that the momentum operator is Hermitian.)

BONUS: Show that \hat{p}^n is Hermitian for *any* positive integer *n*.

Name_____ Student Number_____

Mid-Term #1

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Part 1: 6 questions @ 10 points each.

Part 2: Pick 2 of 3 questions @ 20 points each.

Bonus: 10 points

Key integrals and identities:

$$\left(\frac{a}{2}\right)\delta_{mn} = \int_{0}^{a} \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) dx$$

$$\left(\frac{a}{2}\right)\delta_{mn} = \int_{0}^{a} \cos\left(\frac{n\pi x}{a}\right) \cos\left(\frac{m\pi x}{a}\right) dx$$

$$0 = \int_{0}^{a} \cos\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) dx$$

$$\frac{a^{2}}{4} = \int_{0}^{a} \left(\sin\left(\frac{n\pi x}{a}\right)\right)^{2} x dx$$

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$$\frac{1}{2}\sqrt{\frac{\pi}{\alpha}} = \int_{0}^{\infty} e^{-\alpha x^{2}} dx$$

$$\left(\frac{1}{2}\sqrt{\frac{\pi}{\alpha}}\right) \left(\frac{(2n-1)(2n-3)\cdots(3)(1)}{(2\alpha)^{n}}\right) = \int_{0}^{\infty} x^{2n} e^{-\alpha x^{2}} dx$$

$$n = 1, 2, 3, \dots$$

$$\left(\frac{1}{2}\right) \left(\frac{n!}{\alpha^{n+1}}\right) = \int_{0}^{\infty} x^{2n+1} e^{-\alpha x^{2}} dx$$

$$n = 0, 1, 2, \dots$$

$$\int x \sin(bx) dx = \frac{\sin(bx)}{b^{2}} - \frac{x \cos(bx)}{b} + \text{constant}$$

$$\int x^{2} \sin(bx) dx = -\left(\frac{x^{2} \cos(bx)}{b} + \frac{2x \cos(bx + \frac{1}{2}\pi)}{b^{2}} + \frac{2\cos(bx + \pi)}{b^{3}}\right) + \text{constant}$$

$$2\sin(x)\sin(y) = \cos(x-y) - \cos(x+y) \rightarrow 2\sin^2 x = 1 - \cos(2x)$$

$$2\cos(x)\cos(y) = \cos(x-y) + \cos(x+y) \rightarrow 2\cos^2 x = 1 + \cos(2x)$$

$$2\sin(x)\cos(y) = \sin(\alpha+\beta) + \sin(\alpha-\beta) \rightarrow 2\sin x \cos x = \sin(2x)$$

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VALUES OF SOME PHYSICAL CONSTANTS	SICAL CONSTA	NTS
Constant	Symbol	Value
Avogadro's number	N_0	$6.02205 \times 10^{23} \mathrm{mol^{-1}}$
Proton charge	e	$1.60219 \times 10^{-19} \mathrm{C}$
Planck's constant	7 7	$6.62618 \times 10^{-34} \text{ J} \cdot \text{s}$ $1.05459 \times 10^{-34} \text{ J} \cdot \text{s}$
Speed of light in vacuum	c	$2.997925 \times 10^8 \mathrm{m \cdot s^{-1}}$
Atomic mass unit	amu	$1.66056 \times 10^{-27} \mathrm{kg}$
Electron rest mass	m _e	$9.10953 \times 10^{-31} \text{ kg}$
Proton rest mass	m_p	$1.67265 \times 10^{-27} \mathrm{kg}$
Boltzmann constant	k_B	$1.38066 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$ 0.69509 cm^{-1}
Molar gas constant	R	8.31441 J·K ⁻¹ ·mol ⁻¹
Permittivity of a vacuum	$\frac{\varepsilon_0}{4\pi\varepsilon_0}$	$8.854188 \times 10^{-12} \text{ C}^2 \cdot \text{s}^2 \cdot \text{kg}^{-1} \cdot \text{m}^{-3}$ $1.112650 \times 10^{-10} \text{ C}^2 \cdot \text{s}^2 \cdot \text{kg}^{-1} \cdot \text{m}^{-3}$
Rydberg constant (infinite nuclear mass)	R_{∞}	$2.179914 \times 10^{-23} \text{ J}$ 1.097373 cm^{-1}
First Bohr radius	a_0	$5.29177 \times 10^{-11} \mathrm{m}$
Bohr magneton	μ_B	$9.27409 \times 10^{-24} \text{J} \cdot \text{T}^{-1}$
Steian-Boitzmann constant	9	3.6/032 × 10 ° J·m ~·K ~·s ·
CONVERSION FACTORS FOR ENERGY UNITS	S FOR ENERGY	SIIND
joule kJ⋅mol ⁻¹	-1 eV	au cm ⁻¹ Hz
1 joule 6.022 × 10 ²⁰) ²⁰ 6.242×10 ¹⁸	2.2939×10^{17} 5.035×10^{22} 1.509×10^{33}
$= 1.661 \times 10^{-21}$	1.036×10^{-2}	3.089×10^{-4} 83.60 2.506×10^{12}
$=1.602 \times 10^{-19}$ 96.48	-	3.675×10^{-2} 8065 2.418×10^{14}
1 au = 4.359 × 10 ⁻¹⁸ 2625	27.21	1 2.195×10^5 6.580×10^{15}
		4.556×10^{-6} 1 2.998×10^{10}
1.19	-2 1.240 × 10 ⁻⁴	

 $J(oule) = 1 \text{ kg} \cdot \text{m}^2/\text{s}^2 = 1 \text{ C}(oulomb) \cdot \text{V}(olt)$

- 1. As the quantum number n increases, the energy levels of a particle in a one-dimensional box with infinitely high sides become
 - (a) closer together
- (b) further apart
- (c) stay about the same.
- 2. You are given told that the zero-point energy of a particle in a box is 1 eV (1 electron-volt). The particle is then squeezed, so that the new box is half the length of the old box, $a_{\text{new}} = \frac{1}{2} a_{\text{old}}$
 - . What is the zero-point energy now?
 - (b) 1 eV
- (c) 2eV
- (e) 4 eV
- (g) 8 eV

- (b) 0.5 eV
- (d) 0.25 eV
- (f) 0.125 eV
- (h) can't tell from the

information given

I know it is $\underline{\mathbf{4}} \ \mathbf{eV}$ because the energy is proportional to a^{-2} . However, if I wanted to show it explicitly,

$$1 \text{ eV} = \frac{h^2 \left(1^2\right)}{8ma_{\text{old}}^2}$$
new energy =
$$\frac{h^2 \left(1^2\right)}{8ma_{\text{new}}^2} = \frac{h^2 \left(1^2\right)}{8m\left(\frac{1}{2}a_{\text{old}}\right)^2} = \frac{h^2 \left(1^2\right)}{\left(\frac{1}{2}\right)^2 8ma_{\text{old}}^2} = \frac{1 \text{ eV}}{\frac{1}{4}} = 4\text{eV}$$

3. What is the De Broglie wavelength for thermal neutrons? That is, for neutrons with temperature 298.15 K, with kinetic energy $\frac{3}{2}k_BT$, what is the De Broglie wavelength. The mass of the neutron is $1.6749 \cdot 10^{-27}$ kg.

From the kinetic energy, I can determine the momentum,

$$\frac{p^2}{2m} = \text{k.e.} = \frac{3}{2}k_BT$$
$$p = \sqrt{2m \cdot \frac{3}{2}k_BT}$$

The De Broglie wavelength is $\lambda = h/p$ so

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m \cdot \frac{3}{2} k_B T}} = \frac{6.626 \cdot 10^{-34} \text{ kg} \cdot \text{m}^2 \cdot \text{s}^{-1}}{\sqrt{2 \left(1.6749 \cdot 10^{-27} \text{ kg}\right) \frac{3}{2} \left(1.3806 \cdot 10^{-23} \frac{\text{kg} \cdot \text{m}^2}{\text{s}^2 \cdot \text{K}}\right) \left(298.15 \text{ K}\right)}}$$

 $=1.457 \cdot 10^{-10} \text{ m}$

4. What is the momentum of a photon with wavenumber $1.500 \cdot 10^7 \text{ m}^{-1}$.

$$p = \hbar k = (1.055 \cdot 10^{-34} \,\mathrm{kg} \cdot \mathrm{m}^2 \mathrm{s}^{-1}) \cdot (1.5 \cdot 10^7 \,\mathrm{m}^{-1}) = 1.583 \cdot 10^{-27} \,\frac{\mathrm{kg} \cdot \mathrm{m}}{\mathrm{s}}$$

5. Write a Slater determinant for the 1s²2s¹2p¹ triplet excited state of the Beryllium atom. Write out the Slater determinant in full, showing every element, including the normalization constant.

$$\frac{1}{\sqrt{4!}} \begin{vmatrix} \psi_{1s}(\mathbf{r}_{1})\alpha(1) & \psi_{1s}(\mathbf{r}_{1})\beta(1) & \psi_{2s}(\mathbf{r}_{1})\alpha(1) & \psi_{2p_{x}}(\mathbf{r}_{1})\alpha(1) \\ \psi_{1s}(\mathbf{r}_{2})\alpha(2) & \psi_{1s}(\mathbf{r}_{2})\beta(2) & \psi_{2s}(\mathbf{r}_{2})\alpha(2) & \psi_{2p_{x}}(\mathbf{r}_{2})\alpha(2) \\ \psi_{1s}(\mathbf{r}_{3})\alpha(3) & \psi_{1s}(\mathbf{r}_{3})\beta(3) & \psi_{2s}(\mathbf{r}_{3})\alpha(3) & \psi_{2p_{x}}(\mathbf{r}_{3})\alpha(3) \\ \psi_{1s}(\mathbf{r}_{4})\alpha(4) & \psi_{1s}(\mathbf{r}_{4})\beta(4) & \psi_{2s}(\mathbf{r}_{4})\alpha(4) & \psi_{2p_{x}}(\mathbf{r}_{4})\alpha(4) \end{vmatrix}$$

6. To a reasonable approximation, a quantum dot can be approximated as an electron in a 3-dimensional box with infinite sites. Consider eight electrons in a cubic quantum dot with length 1 nm. (1 nm = 10⁻⁹ m) What is the wavelength corresponding to the lowest-energy absorption of light for this system?

The lowest energy states are:

With 8 electrons, we fill the first two of these sets of orbitals, and the lowest-energy absorption is from the second line to the third line, e.g., $(1,1,2) \rightarrow (1,2,2)$. The energy of the transition is:

$$\Delta E = \frac{9h^2}{8ma^2} - \frac{6h^2}{8ma^2} = \frac{3h^2}{8ma^2} = h\nu = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc \cdot 8ma^2}{3h^2} = \frac{8ma^2c}{3h}$$

$$= \frac{8 \cdot (9.109 \cdot 10^{-31} \text{ kg}) (1 \cdot 10^{-9} \text{ m})^2 (2.998 \cdot 10^8 \frac{\text{m}}{\text{s}})}{3 \cdot 6.626 \cdot 10^{-34} \frac{\text{kg} \cdot \text{m}^2}{\text{s}}}$$

$$= 1.099 \cdot 10^{-6} \text{ m} = 1099 \text{ nm}$$

7-8. Consider a particle of mass m in a one-dimensional box with length 2ℓ centered at the origin, with potential

$$V_{\text{pib0}}(x) = \begin{cases} +\infty & x < -\ell \\ 0 & -\ell \le x \le \ell \\ +\infty & x > \ell \end{cases}$$

a. What is the expression for the energy eigenvalues of this system?

This is a box with length 2ℓ . So the energy eigenvalues are:

$$E_n = \frac{h^2 n^2}{8m(2\ell)^2} = \frac{h^2 n^2}{32m\ell^2}$$

b. What is the expression for the eigenfunctions of the Hamiltonian for this system?

There are several ways to do this. One way is to notice that if we define $y=x+\ell$, then this is a box with width 2ℓ starting at x=0, with eigenfunctions that are the (normal) particle-in-a-box functions, namely, $\psi_n\left(y\right)=\sqrt{\frac{2}{2\ell}}\sin\left(\frac{n\pi y}{2\ell}\right)$. Then, using $y=x+\ell$, we have

$$\psi_{n}(x) = \sqrt{\frac{1}{\ell}} \sin\left(\frac{n\pi x + n\pi \ell}{2\ell}\right) = \sqrt{\frac{1}{\ell}} \sin\left(\frac{n\pi x}{2\ell} + \frac{n\pi}{2}\right) = \sqrt{\frac{1}{\ell}} \left(\sin\left(\frac{n\pi x}{2\ell}\right)\cos\left(\frac{n\pi}{2}\right) + \cos\left(\frac{n\pi x}{2\ell}\right)\sin\left(\frac{n\pi}{2}\right)\right)$$
$$= \sqrt{\frac{1}{\ell}} \left(0 + \cos\left(\frac{n\pi x}{\ell}\right)(-1)^{n-1}\right)$$

and this (using the fact we can choose whichever choice we wish for the square root of unity) gives

$$\psi_n(x) = \sqrt{\frac{1}{\ell}} \cos\left(\frac{n\pi x}{\ell}\right)$$

The other way to do this is the way we did things in class, where we noticed that the Schrödinger equation,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi_n(x) = E_n\psi_n(x)$$

means that the second derivative of the wavefunction must equal a constant multiple of itself. This means that we have solutions like e^{-kx} , $\sin(ax)$, $\cos(kx)$, $\sinh(kx)$, $\cosh(kx)$. Since the wavefunction must be zero at the edges of the box, but need not be zero at the middle of the box, we need to choose $\cos(kx)$; since $\cos(kx) = 0$ when k is a half-integer multiple of π (i.e., $k = \frac{1}{2}n\pi$) we have that $\psi_n(x) = A\cos\left(\frac{n\pi x}{2\ell}\right)$.

Consider a system defined for $-\infty < x < \infty$. You may assume that all wavefunctions approach zero at $\pm \infty$. (Otherwise they would not be normalized.)

9. Give a mathematical proof that the momentum operator is Hermitian. We need to show that:

$$0 = \int_{-\infty}^{\infty} \psi^*(x) \hat{p} \psi(x) - \int_{-\infty}^{\infty} (\hat{p} \psi(x))^* \psi(x) dx$$

Inserting the definition of the momentum operator,

$$0 = \int_{-\infty}^{\infty} \psi_1^*(x) - i\hbar \frac{d\psi_2(x)}{dx} - \int_{-\infty}^{\infty} i\hbar \frac{d\psi_1^*(x)}{dx} \psi_2(x) dx$$

$$= -i\hbar \int_{-\infty}^{\infty} \psi_1^*(x) \frac{d\psi_2(x)}{dx} + \psi_2(x) \frac{d\psi_1^*(x)}{dx} dx$$

$$= -i\hbar \int_{-\infty}^{\infty} \frac{d(\psi_2(x)\psi_1^*(x))}{dx} dx$$

$$= -i\hbar \left(\lim_{x \to \infty} (\psi_2(x)\psi_1^*(x)) - \lim_{x \to -\infty} (\psi_2(x)\psi_1^*(x)) \right)$$

$$= 0$$

10. Show that the momentum-operator-squared, \hat{p}^2 , is Hermitian. You can use the result from problem 9. (I.e., you may assume that the momentum operator is Hermitian.) You can do this problem by doing integration of parts (twice) but it is easier to use the result from the earlier problem. Let's write,

$$\int_{-\infty}^{\infty} \psi_{2}^{*}(x) \hat{p}^{2} \psi_{1}(x) dx = \int_{-\infty}^{\infty} \psi_{2}^{*}(x) \hat{p} \cdot \hat{p} \psi_{1}(x) dx$$

Defining $\tilde{\psi}_1(x) \equiv \hat{p}\psi_1(x)$ and using the fact that the momentum operator is Hermitian, we have,

$$\int_{-\infty}^{\infty} \psi_{2}^{*}(x) \hat{p}^{2} \psi_{1}(x) dx = \int_{-\infty}^{\infty} \psi_{2}^{*}(x) \hat{p} \cdot \hat{p} \psi_{1}(x) dx = \int_{-\infty}^{\infty} \psi_{2}^{*}(x) \hat{p} \cdot \tilde{\psi}_{1}(x) dx$$
$$= \int_{-\infty}^{\infty} (\hat{p} \psi_{2}(x))^{*} \tilde{\psi}_{1}(x) dx = \int_{-\infty}^{\infty} (\hat{p} \psi_{2}(x))^{*} \hat{p} \psi_{1}(x) dx$$

Now we'll do the same trick, defining $\tilde{\psi}_2^*(x) = (\hat{p}\psi_2(x))^*$ and using the Hermitian property of the momentum,

$$\int_{-\infty}^{\infty} \psi_{2}^{*}(x) \hat{p}^{2} \psi_{1}(x) dx = \int_{-\infty}^{\infty} (\hat{p} \psi_{2}(x))^{*} \hat{p} \psi_{1}(x) dx = \int_{-\infty}^{\infty} \tilde{\psi}_{2}^{*}(x) \hat{p} \psi_{1}(x) dx$$

$$= \int_{-\infty}^{\infty} (\hat{p} \tilde{\psi}_{2}(x))^{*} \psi_{1}(x) dx = \int_{-\infty}^{\infty} (\hat{p} \cdot \hat{p} \psi_{2}(x))^{*} \psi_{1}(x) dx$$

$$= \int_{-\infty}^{\infty} (\hat{p}^{2} \psi_{2}(x))^{*} \psi_{1}(x) dx$$

But this means that \hat{p}^2 is Hermitian because

$$\int_{-\infty}^{\infty} \psi_2^*(x) \, \hat{p}^2 \psi_1(x) \, dx = \int_{-\infty}^{\infty} \left(\hat{p}^2 \psi_2(x) \right)^* \psi_1(x) \, dx$$

BONUS: Show that \hat{p}^n is Hermitian for *any* positive integer *n*.

There are a couple different ways to do this. If you know that \hat{p}^m is Hermitan for any $m \ge \frac{1}{2}n$, then you can write $\hat{p}^n = \hat{p}^m.\hat{p}^{m-n}$ and using the same argument as in problem #10, you can prove this result. That is the "most elegant" way, perhaps.

However, as a very explicit form of this result, suppose that we know that \hat{p}^{n-1} is Hermitian. Then:

$$\int_{-\infty}^{\infty} \psi_{2}^{*}(x) \hat{p}^{n} \psi_{1}(x) dx = \int_{-\infty}^{\infty} \psi_{2}^{*}(x) \hat{p}^{n-1} \cdot \hat{p} \psi_{1}(x) dx$$

Defining $\tilde{\psi}_1(x) \equiv \hat{p}\psi_1(x)$ and using the fact that \hat{p}^{n-1} is Hermitian, we have,

$$\int_{-\infty}^{\infty} \psi_{2}^{*}(x) \hat{p}^{n} \psi_{1}(x) dx = \int_{-\infty}^{\infty} \psi_{2}^{*}(x) \hat{p}^{n-1} \cdot \hat{p} \psi_{1}(x) dx = \int_{-\infty}^{\infty} \psi_{2}^{*}(x) \hat{p}^{n-1} \cdot \tilde{\psi}_{1}(x) dx$$
$$= \int_{-\infty}^{\infty} (\hat{p}^{n-1} \psi_{2}(x))^{*} \tilde{\psi}_{1}(x) dx = \int_{-\infty}^{\infty} (\hat{p}^{n-1} \psi_{2}(x))^{*} \hat{p} \psi_{1}(x) dx$$

Now we'll do the same trick, defining $\tilde{\psi}_{2}^{*}(x) = (\hat{p}^{n-1}\psi_{2}(x))^{*}$ and using the Hermitian property of the momentum,

$$\int_{-\infty}^{\infty} \psi_{2}^{*}(x) \hat{p}^{n} \psi_{1}(x) dx = \int_{-\infty}^{\infty} (\hat{p}^{n-1} \psi_{2}(x))^{*} \hat{p} \psi_{1}(x) dx = \int_{-\infty}^{\infty} \tilde{\psi}_{2}^{*}(x) \hat{p} \psi_{1}(x) dx$$

$$= \int_{-\infty}^{\infty} (\hat{p} \tilde{\psi}_{2}(x))^{*} \psi_{1}(x) dx = \int_{-\infty}^{\infty} (\hat{p} \cdot \hat{p}^{n-1} \psi_{2}(x))^{*} \psi_{1}(x) dx$$

$$= \int_{-\infty}^{\infty} (\hat{p}^{n} \psi_{2}(x))^{*} \psi_{1}(x) dx$$

But this means that \hat{p}^n is Hermitian if \hat{p}^{n-1} is Hermitian because

$$\int_{-\infty}^{\infty} \psi_{2}^{*}(x) \hat{p}^{n} \psi_{1}(x) dx = \int_{-\infty}^{\infty} (\hat{p}^{n} \psi_{2}(x))^{*} \psi_{1}(x) dx$$

But we know that \hat{p} is Hermitian (problem 9) and \hat{p}^2 is Hermitian (problem 10). Which implies that $\hat{p}^{2+1} = \hat{p}^3$ is Hermitian, which implies that \hat{p}^4 is Hermitian, ... By this argument \hat{p}^n is Hermitian for any positive integer n. (This is called a "proof by induction.)