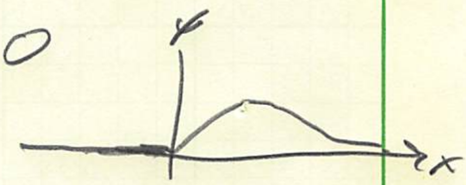
Wave Fcn Push-Ups

$$\psi(x) = \begin{cases} N x e^{-\alpha x}, & x \geq 0 \\ 0, & x < 0 \end{cases}$$



1) Normalization

$$1 = \int dx\, |\psi|^2$$

$$= |N|^2 \int_0^\infty dx\, x^2 e^{-2\alpha x}$$

Tabular integration

x^2	(+)	$e^{-2\alpha x}$
$2x$	(−)	$-\frac{1}{2\alpha} e^{-2\alpha x}$
2	(+)	$\frac{1}{4\alpha^2} e^{-2\alpha x}$
0		$-\frac{1}{8\alpha^3} e^{-2\alpha x}$

$\rightarrow -\frac{1}{2\alpha} e^{-2\alpha x} x^2$

$\rightarrow -\frac{1}{2\alpha^2} e^{-2\alpha x} x$

$\rightarrow -\frac{1}{4\alpha^3} e^{-2\alpha x}$

These two terms are zero at both bounds

$$1 = |N|^2 \left[-\frac{1}{4\alpha^3} e^{-2\alpha x} \right]_0^\infty$$

$$= |N|^2 \left(\frac{1}{4\alpha^3} \right) \Rightarrow |N| = 2\alpha^{3/2}$$

Since the problem says N is real $\boxed{N = \pm 2\alpha^{3/2}}$

b) Looking for maximum of $|\psi|^2$

$$\frac{d}{dx}|\psi|^2 = 0$$

$$|N|^2 \frac{d}{dx}\left(x^2 e^{-2\alpha x}\right) = \cancel{|N|^2}\left(2x\cancel{e^{-2\alpha x}} + x^2(-2\alpha)\cancel{e^{-2\alpha x}}\right) = 0$$

$$\cancel{2}\cancel{x} - \cancel{2}\alpha x^{\cancel{2}} = 0$$

$$1 - \alpha x = 0$$

$$\boxed{x_{max} = 1/\alpha}$$

c)

$$\langle x\rangle = \langle\psi|\hat{x}|\psi\rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x)\, x\, \psi(x)$$

$$= |N|^2 \int_0^{\infty} dx\; xe^{-\alpha x} \; x \; xe^{-\alpha x}$$

$$= |N|^2 \int_0^{\infty} dx\; x^3 e^{-2\alpha x}$$

The procedure here is the same as a), or we can re-arrange to make it look like the Γ-fcn.

$u = 2\alpha x$
$du = 2\alpha dx$

$$\Rightarrow \langle x\rangle = \left(\frac{1}{2\alpha}\right)^4 |N|^2 \underbrace{\int_0^{\infty} du\, u^{4-1} e^{-u}}_{\Gamma(4) = 3! = 6}$$

Wave fcn
pushups

$$\langle x \rangle = \left(\frac{1}{2\alpha}\right)^{\cancel{4}\,2} \frac{\cancel{(2\alpha)^3}}{\underset{\substack{\uparrow \\ |N|^2}}{2}} \; 6$$

$$\boxed{\langle x \rangle = \frac{3}{2}\frac{1}{\alpha}} \qquad (1)$$

d) Similarly

$$\langle x^2 \rangle = \left(\frac{1}{2\alpha}\right)^{\cancel{5}\,2} \left(\frac{\cancel{(2\alpha)^3}}{2}\right) \Gamma(5)$$

$$= \left(\frac{1}{2\alpha}\right)^2 \frac{24}{2} = \frac{12}{4\alpha^2} = \boxed{\frac{3}{\alpha^2} = \langle x^2 \rangle}$$

e)

$$\sigma_x^{\,2} = \langle x^2 \rangle - \langle x \rangle^2 = \frac{3}{\alpha^2} - \frac{9}{4}\frac{1}{\alpha^2}$$

$$\boxed{\sigma_x^{\,2} = \frac{3}{4}\frac{1}{\alpha^2}}$$

f) For $\hat{p}$:

$$\langle \psi | \hat{p} | \psi \rangle = \langle \hat{p} \rangle = |N|^2 \int_0^\infty dx \; x e^{-\alpha x} \left(-i\hbar \frac{\partial}{\partial x}\right) x e^{-\alpha x}$$

$$= -i\hbar |N|^2 \int_0^\infty dx \; x e^{-\alpha x} \left(e^{-\alpha x} + x e^{-\alpha x}(-\alpha) \right)$$

$$= -i\hbar |N|^2 \int_0^\infty dx \, (x - \alpha x^2) e^{-2\alpha x}$$

$u = 2\alpha x$

$du = 2\alpha\, dx$

$$\langle \hat{p} \rangle = -i\hbar |N|^2 \left(\frac{1}{2\alpha}\right) \int_0^\infty du \left(\frac{u}{2\alpha} - \frac{u}{4\alpha^2}\alpha\right) e^{-u}$$

$$= -\frac{i\hbar |N|^2}{2\alpha} \left(\cancel{\frac{1}{2\alpha}\Gamma(2) - \frac{1}{2\cdot 2\alpha}\Gamma(3)} \right)$$

$$\boxed{\langle \hat{p} \rangle = 0}$$

g)

$$\langle \hat{p}^2 \rangle = \int_{-\infty}^{\infty} dx\ \psi^*(x) \left(-i\hbar \frac{d}{dx}\right)^2 \psi(x)$$

$$= -\hbar^2 |N|^2 \int_0^\infty dx\ x e^{-\alpha x} \frac{d^2}{dx^2}\left(x e^{-\alpha x}\right)$$

$$= -\hbar^2 |N|^2 \int_0^\infty dx\ x e^{-\alpha x} \frac{d}{dx}\left(e^{-\alpha x} - \alpha x e^{-\alpha x}\right)$$

$$= -\hbar^2 |N|^2 \int_0^\infty dx\ x e^{-\alpha x} \left(-\alpha e^{-\alpha x} - \alpha e^{-\alpha x} - \alpha x e^{-\alpha x}(-\alpha)\right)$$

$$= -\hbar^2 |N|^2 \int_0^\infty dx \left(\alpha^2 x^2 - 2\alpha x\right) e^{-2\alpha x}$$

$$= -\hbar^2 |N|^2 \left(\alpha^2 \underbrace{\int_0^\infty dx\ x^2 e^{-2\alpha x}}_{1/|N|^2 = \frac{1}{4\alpha^3}} - 2\alpha \underbrace{\int_0^\infty dx\ x e^{-2\alpha x}}_{\frac{1}{(2\alpha)^2}\Gamma(2)} \right)$$

$$= -\hbar^2\, 4\alpha^3 \left(\frac{1}{4\alpha} - \frac{1}{2\alpha} \right)$$

$$= \boxed{\hbar^2 \alpha^2 = \langle \hat{p}^2 \rangle}$$

h)

$$\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2$$

$$= \hbar^2 \alpha^2 - 0$$

$$\boxed{\sigma_p^2 = \hbar^2 \alpha^2}$$

i)

$$\sigma_x \sigma_p = \sqrt{\frac{3}{4}} \frac{1}{\cancel{\alpha}} \times \hbar \cancel{\alpha}$$

$$= \frac{\sqrt{3}}{2} \hbar > \frac{\hbar}{2}$$

Heisenberg!

✓

a)

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_0^\infty dx \, e^{-ipx/\hbar} \, N x e^{-\alpha x}$$

let $k = p/\hbar$

$$\phi(k) = \frac{N}{\sqrt{2\pi\hbar}} \int_0^\infty dx \, e^{-(\alpha+ik)x} \, x$$

Tabular method

$$\begin{array}{ccc}
x & & e^{-(\alpha+ik)x} \\
 & (+) & \\
1 & & -\frac{1}{(\alpha+ik)} e^{-(\alpha+ik)x} \\
 & (-) & \\
0 & & \frac{1}{(\alpha+ik)^2} e^{-(\alpha+ik)x}
\end{array} \rightarrow 0 \text{ at both band}$$

$$\Rightarrow \boxed{\phi(k) = \frac{2\alpha^{3/2}}{\sqrt{2\pi\hbar}} \frac{1}{(\alpha+ik)^2}}$$

b) Normalization

$$\int_{-\infty}^{\infty} dp \, |\phi(p)|^2 = \hbar \int_{-\infty}^{\infty} dk \, |\phi(k)|^2$$

$$= \frac{4\alpha^3}{2\pi\cancel{\hbar}} \cancel{\hbar} \underbrace{\int_{-\infty}^{\infty} dk \, \frac{1}{(\alpha-ik)^2} \frac{1}{(\alpha+ik)^2}}_{I_1}$$

This integral can be done in many ways. The fastest way is to rewrite it as a contour integral on the complex plane and use the residue thm. Rewriting the integrand

$$W = \frac{1}{(\alpha - ik)^2}\,\frac{1}{(\alpha + ik)^2}$$

$$= \frac{1}{(k - i\alpha)^2}\,\frac{1}{(k + i\alpha)^2}$$

and closing in the upper half plane around $z = i\alpha$ (second order pole), the residue is given by

$$C_{-1} = \lim_{k \to i\alpha} \frac{d}{dk}\left(\frac{1}{k + i\alpha}\right)^2$$

$$= \lim_{k \to i\alpha} \frac{-2}{(k + i\alpha)^3} = \frac{-2}{-8i\alpha^3} = \frac{1}{4i\alpha^3}$$

$$\Rightarrow I_1 \to 2\pi i C_{-1} = 2\pi \cancel{i}\left(\frac{1}{4\cancel{i}\alpha^3}\right)$$

$$= \frac{2\pi}{4\alpha^3}$$

$$\Rightarrow \boxed{\int_{-\infty}^{\infty} dp\, |\phi(p)|^3 = \frac{\cancel{4\alpha^3}}{\cancel{2\pi}}\,\frac{\cancel{2\pi}}{\cancel{4\alpha^3}} = 1} \checkmark$$

$\phi(p)$ is normalized

c) Again using the residue thm.

$$\langle p \rangle = \frac{4\alpha^3}{2\pi \cancel{\hbar}} \hbar \int_{-\infty}^{\infty} dk \, \frac{1}{(k-i\alpha)^2} \, \hbar k \, \frac{1}{(k+i\alpha)^2}$$

Use 2nd order pole at $k = i\alpha$

$$\lim_{k \to i\alpha} \frac{d}{dk} \frac{\hbar k}{(k+i\alpha)^2} = \lim_{k \to i\alpha} \hbar\left(\frac{1}{(k+i\alpha)^2} - \frac{2k}{(k+i\alpha)^3} \right)$$

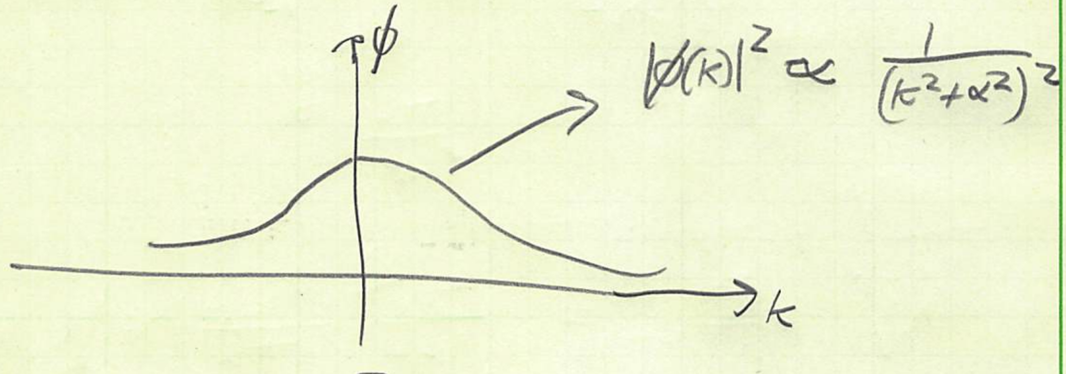
$$= \hbar\left(\frac{-1}{4\alpha^2} - \frac{2i\alpha}{(2i\alpha)^3} \right)$$

$$= \hbar\left(\frac{-1}{4\alpha^2} - \frac{\cancel{2i\alpha}}{\underset{4}{-\cancel{8i\alpha^3}}} \right)$$

$$= \hbar\left(\frac{-1}{4\alpha^2} + \frac{1}{4\alpha^2} \right)$$

$$\boxed{\langle p \rangle = 0}$$

Which could also be deduced from a symmetry argument b/c $|\phi(p)|^2$ is even



so that $\int dk \, \underset{\text{odd}}{k} \, \underset{\text{even}}{|\phi(k)|^2} = 0$

Complex Absorbing Potentials

a) From the TDSE

$$\frac{\partial}{\partial t}|\Psi(x,t)|^2 = \Psi^*\frac{\partial \Psi}{\partial t} + \Psi\frac{\partial \Psi^*}{\partial t}$$

$$= \Psi^*\left(\frac{1}{i\hbar}\left(\frac{\hat{p}^2}{2m}\Psi + V\Psi\right)\right) + \Psi\left(\frac{-1}{i\hbar}\left(\frac{\hat{p}^2}{2m}\Psi^* + V^*\Psi^*\right)\right)$$

Note $\hat{p}^2$ is Hermitian so $(\hat{p}^2)^\dagger = \hat{p}^2$.

$$= \underbrace{\frac{i}{\hbar}\left(\Psi\hat{p}^2\Psi^* - \Psi^*\hat{p}^2\Psi\right)}_{} + \frac{i}{\hbar}|\Psi|^2(V^* - V)$$

This term will integrate to zero b/c $\hat{p}^2$ is Hermitian, as shown in Griffiths

$$V^* - V = 2i\Gamma$$

so $$\frac{\partial}{\partial t}|\Psi|^2 = -\frac{2\Gamma}{\hbar}|\Psi|^2$$

$$\Rightarrow \boxed{\frac{dP}{dt} = -\frac{2\Gamma}{\hbar}P}$$

b) $\boxed{P(t) = P_0 e^{-t/\tau}}$ w/ $\boxed{\tau = \frac{\hbar}{2\Gamma}}$

$1/e$ lifetime

a)
$$|\phi\rangle = a|f\rangle + b|g\rangle$$

We seek a normalized $N|\phi\rangle$ such that
$$|N|^2 \langle\phi|\phi\rangle = 1$$
$$|N|^2\left[\left(\langle f|a^* + \langle g|b^*\right)\left(a|f\rangle + b|g\rangle\right)\right] = 1$$
$$1 = |N|^2\left[|a|^2\underbrace{\langle f|f\rangle}_{1} + a^*b\cancelto{0}{\langle f|g\rangle} + b^*a\cancelto{0}{\langle g|f\rangle} + |b|^2\underbrace{\langle g|g\rangle}_{1}\right] \quad (1)$$
$$|N|^2\left[|a|^2 + |b|^2\right] = 1$$
$$\boxed{|N| = \frac{1}{\sqrt{|a|^2+|b|^2}}}$$
Any complex number that satisfies this will work

b) Now equation (1) becomes
$$1 = |N|^2\left[|a|^2 + a^*bS + ab^*S^* + |b|^2\right]$$
$$\Rightarrow \boxed{|N| = \frac{1}{\sqrt{|a|^2 + |b|^2 + 2\mathrm{Re}(a^*bS)}}}$$
Any complex number that satisfies this will work.

a) Particle in a box energies are (width a)

$$E = \frac{n^2 h^2}{8 m^* a^2} \qquad m^* = 0.07\, m_e$$

effective mass

Energy of photon is energy difference between two levels

$$\hbar \omega_{photon} = E_{n+1} - E_n$$

$$= \frac{h^2}{8 m^* a^2}\left((n+1)^2 - n^2\right)$$

$$\boxed{\hbar \omega_{photon} = \frac{h^2}{8 m^* a^2}(2n+1)}$$

n refers to lower level quantum number

b) $\lambda = 10\,\mu m$ has energy of

$$E = \frac{hc}{\lambda}$$

$$\Rightarrow \quad \frac{hc}{\lambda} = \frac{h^{\cancel{2}}}{8 m^* a^2}(3)$$

$$a^2 = \frac{3 h \lambda}{8 m^* c}$$

$$a = \sqrt{\frac{3 h \lambda}{8 m^* c}} = \sqrt{\frac{3 \cdot 6.626\times 10^{-34}\,J\text{-}s \cdot 10^{-5}\,m}{8 \cdot 0.07 \cdot 9.109\times 10^{-31}\,kg \cdot 3\times 10^{8}\,m/s}}$$

$$\boxed{a = 11.4\,nm}$$

a)
$$\Psi(x,t) = \frac{1}{\sqrt{2}}\psi_1(x)e^{-i\frac{E_1 t}{\hbar}} + \frac{1}{\sqrt{2}}\psi_2(x)e^{-i\frac{E_2 t}{\hbar}}$$

b) See Matlab code and plots

c)
$$\langle\hat{H}\rangle = \langle\Psi|\hat{H}|\Psi\rangle$$

$$= \frac{1}{2}\left(\langle\psi_1|e^{+i\frac{E_1 t}{\hbar}} + \langle\psi_2|e^{+i\frac{E_2 t}{\hbar}}\right)\left(E_1 e^{-iE_1 t/\hbar}|\psi_1\rangle + E_2 e^{-iE_2 t/\hbar}|\psi_2\rangle\right)$$

$$\boxed{\langle\hat{H}\rangle = \frac{1}{2}(E_1 + E_2)}$$ independent of time. (1)

We have made use of the facts that the $|\psi_n\rangle$ are orthognol and normalized.

d)
$$\langle x\rangle(t) = \langle\Psi(x,t)|\hat{x}|\Psi(x,t)\rangle$$

Now the key thing to realize here is to use the symmetry of the wavefunctions about $x = L/2$, the center of the box.

Let's recognize that

$$x = x - L/2 + L/2$$

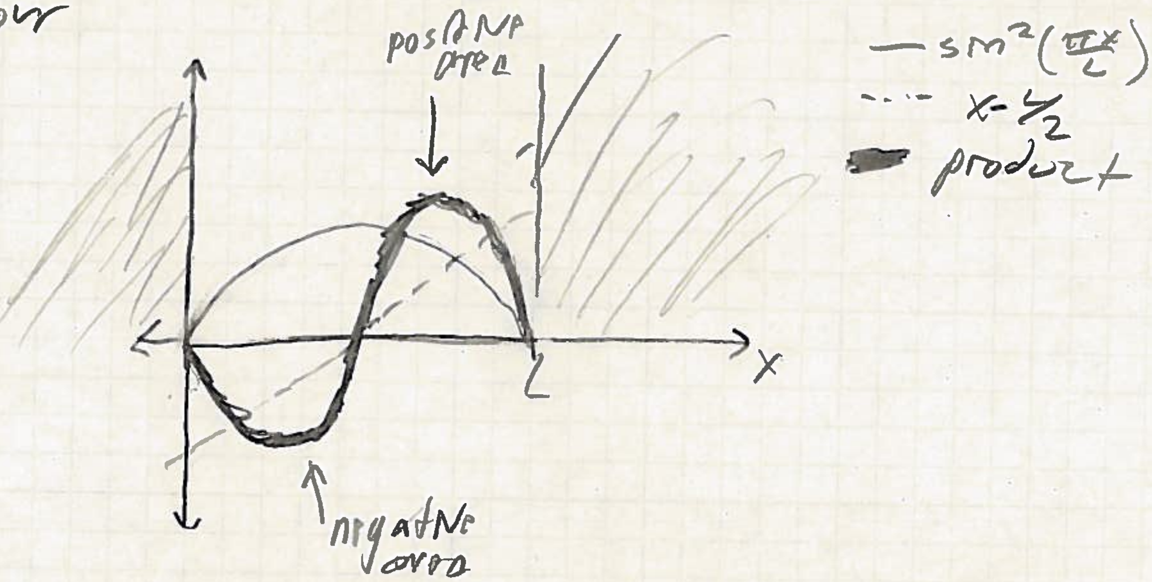
and
$$\langle L/2\rangle = L/2 \quad \text{b/c } \psi \text{ is normalized}$$

Now $x - L/2$ is odd about $L/2$, so examining the integrals

$$\langle \psi_1 | (x - L/2) | \psi_1 \rangle = \left(\frac{2}{L}\right)\int_0^L dx \, \sin\left(\frac{\pi x}{L}\right)(x - L/2)\sin\left(\frac{\pi x}{L}\right)$$

even about $L/2$ odd about $L/2$ even about $L/2$

since even x even x odd = odd
The integrand is odd about $L/2$ and the area will be zero. This is illustrated below



similarly for

$$\langle \psi_2 | (x - L/2) | \psi_2 \rangle = \int \text{odd} \times \text{odd} \times \text{odd}$$

odd odd odd

$$= \int \text{odd} = \emptyset$$

Now for the cross terms

$$\langle \psi_1 | (x - L/2) | \psi_2 \rangle \neq 0$$

even odd odd

So we need to evaluate the integral

$$\langle \psi_1 | (x - L/2) | \psi_2 \rangle = \frac{2}{L}\int_0^L dx \sin\left(\frac{\pi x}{L}\right)(x - L/2)\sin\left(\frac{2\pi x}{L}\right)$$

Using the orthogonality of $\langle \psi_1 | \psi_2 \rangle = 0$ we can throw away the $-L/2$ term.

$$\frac{2}{L}\int_0^L dx \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) x$$

$$= \frac{2}{L}\int_0^L dx \sin\left(\frac{\pi x}{L}\right)\left(2\sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)\right) x$$

$$= \frac{4}{L}\int_0^L dx \sin^2\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right) x$$

Use integration by parts

$$\int_a^b u\,dv = uv\Big|_a^b - \int_a^b v\,du$$

$u = x$ $\quad dv = dx \sin^2\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)$

$du = dx$

$$v = \int dv = \int dx \sin^2\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)$$

$z = \sin\left(\frac{\pi x}{L}\right)$

$dz = \cos\left(\frac{\pi x}{L}\right)\frac{\pi}{L}dx$

$$= \frac{L}{\pi}\int dz\, z^2$$

$$= \frac{L}{\pi}\frac{z^3}{3} = \frac{L}{3\pi}\sin^3\left(\frac{\pi x}{L}\right)$$

So we have

0 at both bounds

$$\int u\,dv = \cancel{\frac{L}{3\pi} x \sin^3\left(\frac{\pi x}{L}\right)\Big|_0^L} - \int_0^L dx \frac{L}{3\pi} \sin^3\left(\frac{\pi x}{L}\right)$$

$$\sin^3\left(\frac{\pi x}{L}\right) = \sin\left(\frac{\pi x}{L}\right)\left(1 - \cos^2\left(\frac{\pi x}{L}\right)\right)$$

so now using $z = \cos\left(\frac{\pi x}{L}\right)$ $dz = -\sin\left(\frac{\pi x}{L}\right)\frac{\pi}{L}dx$

$$-\int_a^b dx \frac{L}{3\pi}\sin^3\left(\frac{\pi x}{L}\right) = +\frac{L}{3\pi}\frac{L}{\pi}\int_1^{-1} dz\,(1-z^2)$$

$$= \frac{-L^2}{3\pi^2}\int_{-1}^{1} dz\,(1-z^2)$$

$$= \frac{-L^2}{3\pi^2}\left(2 - \frac{2}{3}\right)$$

$$= \frac{-L^2}{3\pi^2}\frac{4}{3} = \frac{-4L^2}{9\pi^2}$$

so putting it all together, we will have

$$\langle x - L/2 \rangle = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\langle \psi_1 | x - L/2 | \psi_2 \rangle e^{-i(E_2 - E_1)t/\hbar}$$

$$+ \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\langle \psi_2 | (x - L/2) | \psi_1 \rangle e^{+i(E_2 - E_1)t/\hbar}$$

$$= \frac{1}{2}\frac{-4}{\cancel{L}}\left(\frac{4L^{\cancel{2}}}{9\pi^2}\right)\left(\underbrace{e^{-i\omega t} + e^{i\omega t}}_{2\cos(\omega t)}\right) \quad \text{w/ } \omega \equiv \frac{E_2 - E_1}{\hbar}$$

$$= \frac{-16}{9\pi^2} L \cos(\omega t)$$

So

$$\langle \hat{x} \rangle(t) = \frac{L}{2} + \langle x - L/2 \rangle$$

$$= \frac{L}{2} - \frac{16}{9\pi^2} L \cos(\omega t)$$

This is also confirmed numerically in the MATLAB code.

Table of Contents


```
%ParticleMovingInBox
%
%This script makes plots of a superposition of two states in a box.
%
%Tom Allison 8/8/2013

set(0,'DefaultLineLineWidth',2);
```

Preliminaries

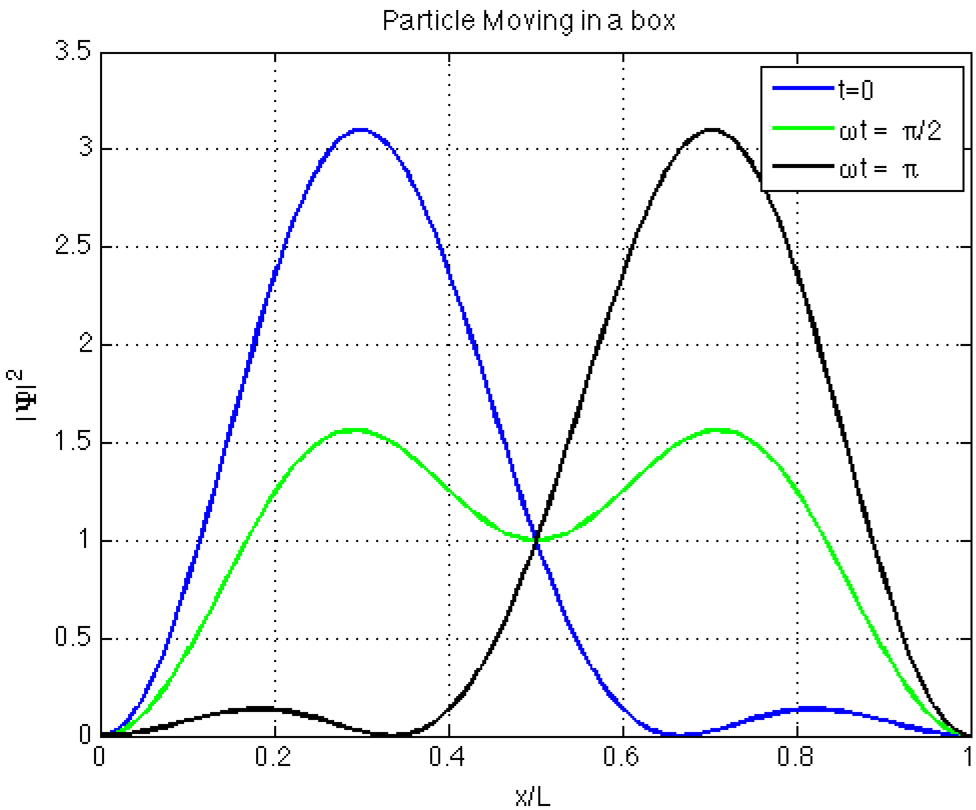
```
L = 1; %Define length of box
x = linspace(0,L); % make linearly spaced array for x-axis
psi1 = sqrt(2/L)*sin(pi*x/L); %first stationary state.
psi2 = sqrt(2/L)*sin(2*pi*x/L); %second stationary state.
```

Add stationary states with appropriate relative phase.

The thing to realize here is that all that matters is the relative phase between the stationary states, because an overal phase of the wavefunction does not matter in quantum mechanics.

```
psi_t0 = 1/sqrt(2)*psi1 + 1/sqrt(2)*psi2; % no phase factors at t=0;
psi_t1 = 1/sqrt(2)*psi1 + 1/sqrt(2)*psi2*exp(-i*pi/2); % DeltaE*t/hbar = pi/2
psi_t2 = 1/sqrt(2)*psi1 + 1/sqrt(2)*psi2*exp(-i*pi); % % DeltaE*t/hbar = pi

figure(1);
h0 = plot(x,psi_t0.*conj(psi_t0),'b');
hold on
h1 = plot(x,psi_t1.*conj(psi_t1),'g');
h2 = plot(x,psi_t2.*conj(psi_t2),'k');
hold off
xlabel('x/L');
ylabel('|\Psi|^2');
grid on
legend([h0,h1,h2],'t=0','\omegat = \pi/2','\omegat = \pi');
title('Particle Moving in a box');
setfigfont(1,14);
```



Check integral from part d)

```
dx = x(2)-x(1); % construct dx from difference of first two points.
xbar0 = dx*trapz(conj(psi_t0).*x.*psi_t0) %perform trapezoidal integration.

%compare to the analytical result
xbar0_analytical = L/2 - 16/(9*pi^2)*L*cos(0)
```

```
xbar0 =

    0.3199


xbar0_analytical =

    0.3199
```

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a) $\Psi(x,t) = Ae^{i(k_0 x - \omega t)}$

Insert into 1D TDSE

LHS: $i\hbar \frac{\partial \Psi}{\partial t} = i\hbar(-i\omega)\Psi = \hbar\omega\Psi$

RHS: $\frac{-\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = \frac{-\hbar^2}{2m}(ik_0)^2 = \frac{\hbar^2 k_0^2}{2m}$

Equating LHS and RHS, we get

$$\cancel{\hbar}\omega = \frac{\hbar^{\cancel{2}} k_0^2}{2m}$$

$$\boxed{\omega = \frac{\hbar k_0^2}{2m}} \qquad (1)$$

To get the wave speed, we recognize that

$$\Psi(x,t) = Ae^{ik_0(x - \frac{\omega}{k_0}t)}$$

So the whole pattern moves in the +x direction w/ phase velocity

$$\boxed{v_p = \frac{\omega}{k_0} = \frac{\hbar k_0}{2m}} \qquad (2)$$

b) For the wave eqn.

LHS: $\frac{\partial^2\Psi}{\partial t^2} = (-i\omega)^2\Psi = -\omega^2\Psi$

RHS: $c^2\frac{d^2\Psi}{dt^2} = c^2(ik_0)^2\Psi = -k_0^2c^2\Psi$

Equating LHS and RHS, we get

$$\boxed{\omega = ck_0} \qquad (3)$$

c) Now for the diffusion eqn. and

$$\Psi = \sqrt{\frac{t_0}{t}}\exp\left(\frac{-x^2}{4Dt}\right)$$

LHS: $$\frac{\partial\Psi}{\partial t} = -\frac{1}{2}\frac{t_0^{1/2}}{t^{3/2}}\exp\left(\frac{-x^2}{4Dt}\right) + \sqrt{\frac{t_0}{t}}\exp\left(\frac{-x^2}{4Dt}\right)\left(\frac{+x^2}{4Dt^2}\right)$$

$$= \sqrt{\frac{t_0}{t}}\exp\left(\frac{-x^2}{4Dt}\right)\left[\frac{x^2}{4Dt^2} - \frac{1}{2t}\right]$$

RHS: $$D\frac{\partial^2\Psi}{\partial x^2} = D\frac{\partial}{\partial x}\left[\sqrt{\frac{t_0}{t}}\exp\left(\frac{-x^2}{4Dt}\right)\left(\frac{-2x}{4Dt}\right)\right]$$

$$= \cancel{D}\sqrt{\frac{t_0}{t}}\left(\frac{-2}{4\cancel{D}t}\right)\exp\left(\frac{-x^2}{4Dt}\right)\left[1 + x\left(\frac{-2x}{4Dt}\right)\right]$$

$$= \sqrt{\frac{t_0}{t}}\exp\left(\frac{-x^2}{4Dt}\right)\left[\frac{x^2}{4Dt^2} - \frac{1}{2t}\right]$$

The LHS agrees w/ the RHS, so Ψ satisfies the diffusion equation.

The width of Ψ is proportional to the $\sqrt{t}$. You can see this by, for example, looking at the time dependence of the $1/e$ half width x_e, which would be when

$$\frac{x_e^2}{4Dt} = 1$$

$$\Rightarrow \boxed{x_e = \sqrt{4Dt}}$$

(4)

d) Now for 1D TDSE

$$\Psi = \sqrt{\frac{\pi}{\alpha + i\beta t}}\, e^{i(k_0 x - \omega_0 t)} \exp\left(-\frac{(x - V_g t)^2}{4(\alpha + i\beta t)}\right) \qquad (5)$$

We need to use the chain rule a lot here, lets make some definitions to save writing

$$f \equiv \sqrt{\frac{\pi}{\alpha + i\beta t}}$$

$$g \equiv e^{i(k_0 x - \omega_0 t)}$$

$$h \equiv \exp\left(\frac{-(x - V_g t)^2}{4(\alpha + i\beta t)}\right)$$

So $\Psi = fgh$

Now

$$\frac{\partial f}{\partial t} = \frac{\left(\frac{-1}{2}\right)\sqrt{\pi}}{(\alpha + i\beta t)^{3/2}}(i\beta)$$

$$= -\frac{1}{2}\frac{i\beta}{\alpha + i\beta t} f$$

$$\frac{\partial f}{\partial x} = 0$$

$$\frac{\partial g}{\partial t} = -i\omega_0 g \qquad \frac{\partial h}{\partial x} = \frac{-2(x - V_g t)}{4(\alpha + i\beta t)} h$$

$$\frac{\partial g}{\partial x} = +ik_0 g$$

$$\frac{\partial h}{\partial t} = \left(\frac{-2(x - V_g t)(-V_g)}{4(\alpha + i\beta t)} + \frac{(x - V_g t)^2}{(4(\alpha + i\beta t))^2} 4i\beta\right) h$$

$$\frac{\partial h}{\partial t} = \frac{x - v_g t}{4(\alpha + i\beta t)}\left(2v_g + i\beta\frac{(x - v_g t)}{4(\alpha + i\beta t)}\right) h$$

So the LHS of the TDSE reads

$$i\hbar\frac{\partial \Psi}{\partial t} = i\hbar\left(\frac{\partial f}{\partial t} gh + f\frac{\partial g}{\partial t} h + fg\frac{\partial h}{\partial t}\right)$$

$$= i\hbar fgh\left(\underbrace{-\frac{1}{2}\frac{i\beta}{\alpha + i\beta t}}_{LHS1} \underbrace{- i\omega_0}_{LHS2} + \underbrace{\frac{2v_g(x - v_g t)}{4(\alpha + i\beta t)}}_{LHS3} \underbrace{+ 4i\beta\frac{(x - v_g t)^2}{(4(\alpha + i\beta t))^2}}_{LHS4}\right)$$

The RHS reads

$$-\frac{\hbar^2}{2m} f \frac{\partial}{\partial x}\left(ik_0 gh - \frac{2(x - v_g t)}{4(\alpha + i\beta t)} gh\right)$$

$$= -\frac{\hbar^2}{2m} f\left(ik_0\left(h\frac{\partial g}{\partial x} + g\frac{\partial h}{\partial x}\right) - \frac{2}{4(\alpha + i\beta t)} gh - \frac{2(x - v_g t)}{4(\alpha + i\beta t)}\left(h\frac{\partial g}{\partial x} + g\frac{\partial h}{\partial x}\right)\right)$$

$$= -\frac{\hbar^2}{2m} fgh\left(\underbrace{(ik_0)^2}_{RHS1} \underbrace{- ik_0\frac{2(x - v_g t)}{4(\alpha + i\beta t)}}_{RHS2} \underbrace{- \frac{2}{4(\alpha + i\beta t)}}_{RHS3} \right.$$

$$\left. \underbrace{- \frac{2(x - v_g t)}{4(\alpha + i\beta t)}\left(ik_0\right.}_{RHS4} \underbrace{\left. - \frac{2(x - v_g t)}{4(\alpha + i\beta t)}\right)}_{RHS5}\right)$$

If we take $\boxed{\omega_0 = \frac{\hbar k_0^2}{2m}}$ as in a) then

RHS1 = LHS2 and if we take

$\boxed{v_g = \frac{\hbar k_0}{m}}$, then RHS4 + RHS2 = LHS3

and we are left with an equation for β

$$\frac{1}{2}\frac{\hbar\beta}{\alpha+i\beta t} - \hbar\beta\frac{4(x-v_g t)^2}{(4(\alpha+i\beta t))^2} = \frac{\hbar^2}{2m}\left(\frac{2}{4(\alpha+i\beta t)} - 4\frac{(x-v_g t)^2}{[4(\alpha+i\beta t)]^2}\right)$$

$$\hbar\beta\left(\cancel{\frac{1}{2}\frac{1}{\alpha+i\beta t} - 4\frac{(x-v_g t)^2}{[4(\alpha+i\beta t)]^2}}\right) = \frac{\hbar^2}{2m}\left(\cancel{\frac{1}{2}\frac{1}{\alpha+i\beta t} - 4\frac{(x-v_g t)^2}{[4(\alpha+i\beta t)]^2}}\right)$$

$$\Rightarrow \boxed{\beta = \frac{\hbar}{2m}}$$

(e) The center moves at $\boxed{v_g = \frac{\hbar k_0}{m}}$

(f) $|\Psi|^2 \propto \exp\left[-(x-v_g t)^2\left(\frac{1}{4(\alpha+i\beta t)} + \frac{1}{4(\alpha-i\beta t)}\right)\right]$

$$= \exp\left[\frac{-(x-v_g t)^2}{4}\left(\frac{2\alpha}{\alpha^2+\beta^2 t^2}\right)\right]$$

As in part c), the width of the Gaussian is determined by the denominator of the exponent. For $\beta t \gg \alpha$, the width of $|\Psi|^2$ will grow as

width $\propto t$

This is faster than for the diffusion equation result, for which the width was proportional to $\sqrt{t}$.

(g) The plane wave sol^n is not normalizable and does not represent a real particle. Only through a superposition of waves that make up a wavepacket can we accurately describe a free particle. The wavepacket moves at the group velocity which is $\hbar k_0/m$. This result is actually independent of the precise functional form of the wavepacket (see Griffiths' Book).

The result of $\hbar k_0/m = v_g$ makes sense b/c classically, we would expect

$$p = mv \quad \text{and} \quad v = \frac{mv}{m} = \frac{p}{m}$$

The plane wave result give $v = \frac{p}{2m}$ which does not correspond to classical mechanics in the appropriate limit ($\hbar \to 0$)

It is also interesting to note that quantum diffusion coefficient $\beta = \frac{\hbar}{2m}$ goes to zero in the classical limit while the group velocity remains finite at p/m b/c for a particle of energy E

$$E = \frac{\hbar^2 k^2}{2m}$$

as $\hbar \to 0$ $k \to \infty$ in the classical limit so $\hbar k/m = v_g \to p_{classical}/m = v$.

$\beta \to 0$ in the classical limit makes sense b/c baseballs retain their size.

Image Potential States

a) Since $V=\infty$ for $x<0$, must have $\psi=0$ there.

Must also have $\psi(x=\infty)\to 0$ s.t. $|\psi|^2$ can be normalized.

b) $\psi = 2\alpha^{3/2} x e^{-\alpha x}$ ← try this

The TISE reads, for $x>0$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(\cancel{2\alpha^{3/2}} x e^{-\alpha x}\right) - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{4\cancel{x}}\left(\cancel{2\alpha^{3/2}}\cancel{x} e^{-\alpha x}\right)$$

$$= E\left(\cancel{2\alpha^{3/2}} x e^{-\alpha x}\right)$$

$$-\frac{\hbar^2}{2m}\frac{d}{dx}\left(e^{-\alpha x} - \alpha x e^{-\alpha x}\right) - \frac{e^2}{16\pi\varepsilon_0}e^{-\alpha x} = E x e^{-\alpha x}$$

$$-\frac{\hbar^2}{2m}\left(-\alpha \cancel{e^{-\alpha x}} - \alpha\left(\cancel{e^{-\alpha x}} - \alpha x \cancel{e^{-\alpha x}}\right)\right) - \frac{e^2}{16\pi\varepsilon_0}\cancel{e^{-\alpha x}} = E x \cancel{e^{-\alpha x}}$$

$$\frac{\hbar^2}{2m}\left(2\alpha - \alpha^2 x\right) - \frac{e^2}{16\pi\varepsilon_0} = E x$$

$$\left(E + \frac{\hbar^2\alpha^2}{2m}\right)x - \left(\frac{e^2}{16\pi\varepsilon_0} - \frac{\hbar^2\alpha}{m}\right) = 0$$

This eqn. can only be solved for <u>all</u> x if both terms in ( ) are zero.

Image Potential States

2

$$\Rightarrow \boxed{\alpha = \frac{m}{\hbar^2}\frac{e^2}{16\pi\varepsilon_0} = \frac{1}{4a_0}}$$

where a_0 is the Bohr radius

$$E = -\frac{\hbar^2\alpha^2}{2m} = \frac{-1}{16}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\left(\frac{m}{\hbar^2}\right)^{\cancel{2}}\left(\frac{\cancel{\hbar^2}}{m}\right)\frac{1}{2}$$

$$= -\frac{1}{16}\underbrace{\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2}_{Ry = 13.6\,eV}$$

$$\boxed{E = \frac{-Ry}{16} = -0.85\,eV}$$

c) At $x=0$ $\quad \psi \propto 0\,e^0 = 0$

$x=\infty$ $\quad \psi \propto \infty e^{-\infty} \to 0$

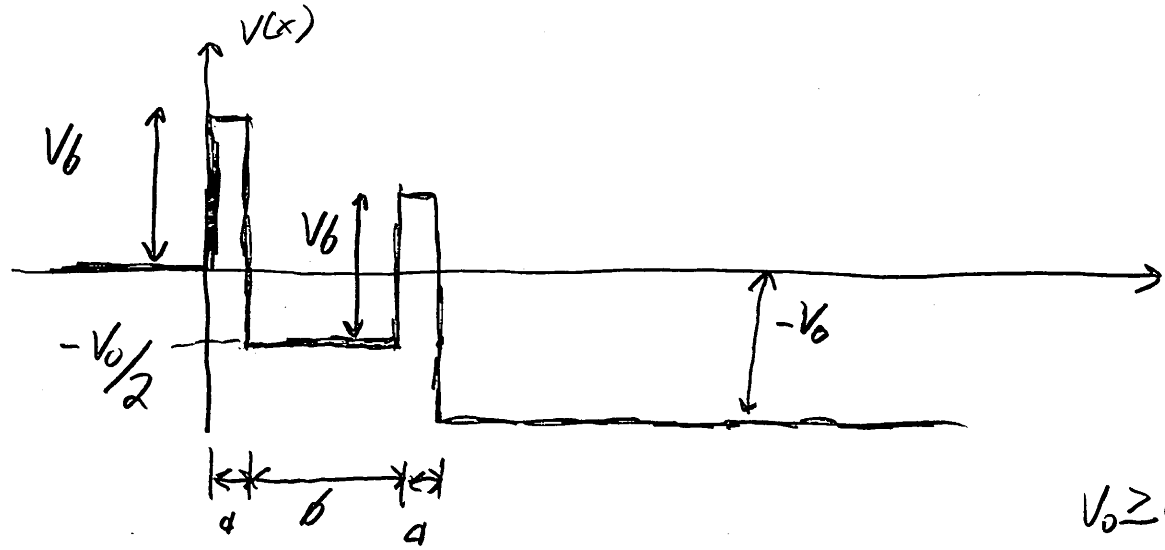
Nothing wins against an exp.

d) From problem "Wavefcn pushups"

$$\langle x\rangle = \frac{3}{2}\frac{1}{\alpha} = \frac{3}{2}4a_0 = 6a_0$$

$$= 6\times 0.529\,\text{Å}$$

$$\boxed{\langle x\rangle = 3.174\,\text{Å}}$$



$V_0 \geq 0$

I II III IV V

a)
In region I $E > V$ so

$$\psi_{I}(x) = Ae^{ik_1x} + Be^{-ik_1x} \qquad k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

II $E < V_b$

$$\psi_{II}(x) = Ce^{-K_2x} + De^{+K_2x} \qquad K_2 = \sqrt{\frac{2m(V_b - E)}{\hbar^2}}$$

III $E > -V_0/2$

$$\psi_{III}(x) = Fe^{+ik_3x} + Ge^{-ik_3x} \qquad k_3 = \sqrt{\frac{2m(E + V_0/2)}{\hbar^2}}$$

IV

$$\psi_{IV}(x) = He^{-K_4x} + Ie^{+K_4x} \qquad K_4 = \sqrt{\frac{2m(V_b - E - V_0/2)}{\hbar^2}}$$

V

$$\psi_{V}(x) = Je^{ik_5x} \qquad k_5 = \sqrt{\frac{2m(E + V_0)}{\hbar^2}}$$

For transmission calc., will set $A = 1$, but leave it for now.

b) At $x=0$, must have $\psi_I(0) = \psi_{II}(0)$

$$\psi_I'(0) = \psi_{II}(0)$$

set $A=1$

$$\Rightarrow \quad 1 + B = C + D \longrightarrow \boxed{-B + C + D = 1} \quad (1)$$

$$ik_1 - ik_1 B = -CK_2 + DK_2 \longrightarrow \boxed{ik_1 B - CK_2 + DK_2 = ik_1} \quad (2)$$

At $x=a$, must have $\psi_{II}(a) = \psi_{III}(a)$

$$\psi_{II}'(a) = \psi_{III}'(a)$$

$$Ce^{-K_2 a} + De^{+K_2 a} = Fe^{ik_3 a} + Ge^{-ik_3 a}$$

$$\boxed{Ce^{-K_2 a} + De^{+K_2 a} - Fe^{ik_3 a} - Ge^{-ik_3 a} = 0} \quad (3)$$

$$-K_2 Ce^{-K_2 a} + K_2 De^{K_2 a} = ik_3 Fe^{ik_3 a} - ik_3 Ge^{-ik_3 a}$$

$$\boxed{\left(-K_2 e^{-K_2 a}\right)C + \left(K_2 e^{K_2 a}\right)D - ik_3 e^{ik_3 a} F + ik_3 e^{-ik_3 a} G = 0} \quad (4)$$

At $x = a+b$, must have $\psi_{III}(a+b) = \psi_{IV}(a+b)$

$$\psi_{III}'(a+b) = \psi_{IV}'(a+b)$$

$$Fe^{ik_3(a+b)} + Ge^{-ik_3(a+b)} = He^{-K_4(a+b)} + Ie^{+K_4(a+b)} \quad (5)$$

$$(5) \Rightarrow \boxed{Fe^{ik_3(a+b)} + Ge^{-ik_3(a+b)} - He^{-K_4(a+b)} - Ie^{K_4(a+b)} = 0}$$

$$ik_3 Fe^{ik_3(a+b)} - ik_3 Ge^{-ik_3(a+b)} = -K_4 He^{-K_4(a+b)} + K_4 Ie^{+K_4(a+b)}$$

$$(6) \quad \boxed{ik_3 e^{ik_3(a+b)} F - ik_3 e^{-ik_3(a+b)} G + K_4 e^{-K_4(a+b)} H - K_4 e^{K_4(a+b)} I = 0}$$

At $x = a+b+a = 2a+b$ $\qquad \psi_{IV}(2a+b) = \psi_{V}(2a+b)$

$$\psi'_{IV}(2a+b) = \psi'_{V}(2a+b)$$

$$He^{-K_4(2a+b)} + Ie^{K_4(2a+b)} = Je^{ik_5(2a+b)}$$

$$\boxed{He^{-K_4(2a+b)} + Ie^{K_4(2a+b)} - Je^{ik_5(2a+b)} = 0}$$

$$-K_4 He^{-K_4(2a+b)} + K_4 Ie^{K_4(2a+b)} = ik_5 Je^{ik_5(2a+b)}$$

$$\boxed{-K_4 e^{-K_4(2a+b)}H + K_4 e^{K_4(2a+b)}I - ik_5 e^{ik_5(2a+b)}J = 0}$$

Turning it into a Matrix equation → See Next Page

x

$$\begin{bmatrix} -1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ iK_1 & -K_2 & +K_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & e^{-K_2 a} & e^{K_2 a} & e^{ik_3 a} & e^{-K_3 a} & 0 & 0 & 0 \\ 0 & -K_2 e^{-K_2 a} & K_2 e^{K_2 a} & -ik_3 e^{ik_3 a} & ik_3 e^{-ik_3 a} & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{ik_3(a+b)} & e^{-ik_3(a+b)} & -e^{-K_4(a+b)} & -e^{K_4(a+b)} & 0 \\ 0 & 0 & 0 & ik_3 e^{ik_3(a+b)} & -ik_3 e^{-ik_3(a+b)} & +K_4 e^{-K_4(a+b)} & -K_4 e^{K_4(a+b)} & 0 \\ 0 & 0 & 0 & 0 & 0 & e^{-K_4(2a+b)} & e^{K_4(2a+b)} & e^{ik_5(2a+b)} \\ 0 & 0 & 0 & 0 & & -K_4 e^{-K_4(2a+b)} & K_4 e^{K_4(2a+b)} & -ik_5 e^{ik_5(2a+b)} \end{bmatrix} \begin{bmatrix} B \\ C \\ D \\ F \\ G \\ H \\ I \\ J \end{bmatrix} = \begin{bmatrix} 1 \\ iK_1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

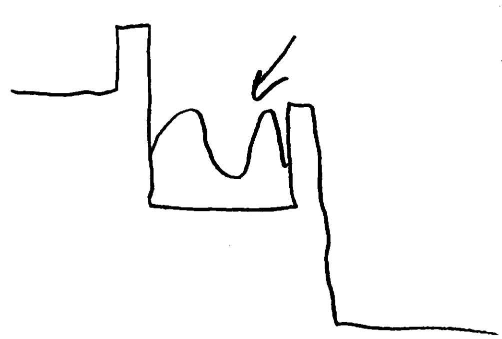
c) The transmission is not just $|J|^2$ because the potential is different in region V than region I. One must use the probability current

$$\text{Prob. Current} = \frac{i\hbar}{2m}\left[\psi \frac{d\psi^*}{dx} - \psi^* \frac{d\psi}{dx}\right]$$

For plane waves this is $\propto k|\psi|^2$, such that you will have

$$T = \frac{k_5}{k_1}|J|^2$$

d) You observe resonace when an integer # of half waves fit between the barriers! At these 'bias' pot., the incident energy coincides with a quasi-bound state of the well, analogous to a shape resonance.



e) There are no truly bound states because they would eventually leak out via tunneling to the lowest potential of $-V_0$.

f) They get sharper as the barriers get higher because the barriers are more reflective and the particle can be trapped in the well longer. This is similar to increasing the reflectivity of the mirrors in a Fabry-Pérot interferometer.

Contents


```
%ResonantTunnelingDiode.m
%
%This script calculates the transmission of a model resonant tunneling
%diode potential. Solution to "Resonant Tunneling Diode" PHY308 problem.
%
%Tom Allison 1/11/2017
```

Preliminaries

```
set(0,'DefaultLineLineWidth',2);
i = sqrt(-1);

% Work in units where length is measured in Angstrom and Energy in eV.
E = 0.1; %Incident electron energy in eV.
a = 10;
b = 50;
hb2ov2m = 3.81; % hbar^2/2m_e in units of eV-Angstrom^2

Vb = 0.2;
V0 = linspace(0,2,1000); % bias potential in 30 steps between 0 and 2 eV.

k1 = sqrt(E/hb2ov2m);
kap2 = sqrt((Vb-E)/hb2ov2m);
k3 = sqrt((E+V0/2)/hb2ov2m);  % this one and the ones below will be an array because V0 is an
array.
kap4 = sqrt((Vb-E-V0/2)/hb2ov2m);
k5 = sqrt( (E+V0)/hb2ov2m );

VOUT = zeros(8,length(E));
T = zeros(1,length(E));
R = zeros(1,length(E));
detM = zeros(1,length(E));
```

Calculate coefficients at each bias potential.

```
for j = 1:length(V0);
    M = [-1             1                           1                        0
       0                               0                               0
      0;
        i*k1            -kap2                       kap2                   0
      0                               0                               0
     0;
        0               exp(-kap2*a)                exp(kap2*a)            -exp(i*k3(j)*a)
       -exp(-i*k3(j)*a)                 0                               0
       0;
        0               -kap2*exp(-kap2*a)          kap2*exp(kap2*a)       -
i*k3(j)*exp(i*k3(j)*a)     i*k3(j)*exp(-i*k3(j)*a)         0                               0
                         0;
        0               0                           0                        exp(i*k3(j)*(a+b))
       exp(-i*k3(j)*(a+b))              -exp(-kap4(j)*(a+b))            -exp(kap4(j)*(a+b))
       0;
        0               0                           0                        i*k3(j)*exp(i*k3(j)*
```

```
(a+b))   -i*k3(j)*exp(-i*k3(j)*(a+b))     kap4(j)*exp(-kap4(j)*(a+b))     -kap4(j)*exp(kap4(j)*
(a+b))        0;
         0                0                              0                         0
        0                              exp(-kap4(j)*(2*a+b))            exp(kap4(j)*(2*a+b))
       -exp(i*k5(j)*(2*a+b));
         0                0                              0                         0
        0                              -kap4(j)*exp(-kap4(j)*(2*a+b))   kap4(j)*exp(kap4(j)*
(2*a+b))     -i*k5(j)*exp(i*k5(j)*(2*a+b))];

    VRHS = [1;
            i*k1;
            0;
            0;
            0;
            0;
            0;
            0];

VOUT(:,j) = inv(M)*VRHS; % assign the jth row to be the solution for energy E(j);

R(j) = VOUT(1,j)*conj(VOUT(1,j));
T(j) = 1-R(j);
detM(j) = det(M);

end

% plot the wavefunction for a selected point.
Iplot = 71;
Vplot = VOUT(:,Iplot);
x = linspace(-100,2*a+b+100,1E4);
psi = zeros(1,length(x));
V = zeros(1,length(x));
```

Construct psi

```
I = find(x<0);
psi(I) = exp(i*k1*x(I)) + Vplot(1)*exp(-i*k1*x(I));
V(I) = 0;
I = find(x >= 0 & x < a);
psi(I) = Vplot(2)*exp(-kap2*x(I)) + Vplot(3)*exp(kap2*x(I));
V(I) = Vb;
I = find(x >= a & x < a+b);
psi(I) = Vplot(4)*exp(i*k3(Iplot)*x(I)) + Vplot(5)*exp(-i*k3(Iplot)*x(I));
V(I) = -V0(Iplot)/2;
I = find(x >= a+b & x < 2*a+b);
psi(I) = Vplot(6)*exp(-kap4(Iplot)*x(I)) + Vplot(7)*exp(kap4(Iplot)*x(I));
V(I) = -V0(Iplot)/2 + Vb;
I = find(x >= 2*a+b);
psi(I) = Vplot(8)*exp(i*k5(Iplot)*x(I));
V(I) = -V0(Iplot);
```

Plot Results

```
figure(1);
hV = plot(x,V,'k','LineWidth',3);
hold on
hr = plot(x,real(psi)/3); % divide by 3 just for scale.
him = plot(x,imag(psi)/3);
hold off
xlabel('x');
grid on
title(['Wave Function with V_0 = ',num2str(V0(Iplot)), ' eV']);
```

```
ylabel('V(x)');
xlabel('x [angstrom]');
%setfigfont(gcf,14);


figure(2);
%TfromJ = (k5/k1).*VOUT(8,:).*conj(VOUT(8,:)); Can also calculate transmission from wave function
 in amplitude in region V, but mind the prob. current!!!

hT = plot(V0,T);
hold on
hR = plot(V0,R);
%hT = plot(V0,TfromJ,'r--');
hold off
legend([hT,hR],'Transmission','Reflection');
grid on
xlabel('V_0 [eV]');
ylabel('R and T');
%setfigfont(gcf,14)

% %% Extra stuff to plot if desired.
% % plot the potential V0 = 1 eV.
% [crap,I1] = min(abs(V0-0.3));
% V1 = VOUT(:,I1);
% x = linspace(-100,2*a+b+100,1E4);
% V1 = zeros(1,length(x));
%
% %% Construct psi
%
% I = find(x<0);
% V1(I) = 0;
% I = find(x >= 0 & x < a);
% V1(I) = Vb;
% I = find(x >= a & x < a+b);
% V1(I) = -V0(I1)/2;
% I = find(x >= a+b & x < 2*a+b);
% V1(I) = -V0(I1)/2 + Vb;
% I = find(x >= 2*a+b);
% V1(I) = -V0(I1);
%
% figure(10);
% plot(x,V1,'k','LineWidth',3);
% xlabel('x [angstrom]');
% ylabel('V [eV]');
% grid on
% setfigfont(gcf,14);
% axis([-25,100,-0.4,0.3]);
%


% figure(3);
% plot(V0,real(detM));
% hold on
% plot(V0,imag(detM));
% hold off
% xlabel('V_0 [eV]');
% ylabel('Determinant');
% grid on

% %% Does it solve the Schrodinger equation?
% psi1 = diff(psi)./diff(x)
% x1 = (x(1:end-1) + x(2:end))/2;
% psi2 = diff(psi1)./diff(x1);
% x2 = (x1(1:end-1) + x1(2:end))/2;
%
```

```
% LHS = -hb2ov2m*psi2 + V(2:end-1).*psi(2:end-1);
% RHS = E*psi(2:end-1);
% figure(4);
% subplot(3,1,1);
% plot(x2,real(LHS-RHS));
% hold on
% plot(x2,imag(LHS-RHS));
% hold off
% grid on
% xlabel('x [angstrom]');
% ylabel('RHS-LHS of TISE');
%
% subplot(3,1,2);
% plot(x2,real(RHS));
% xlabel('x [angstrom]');
% ylabel('RHS');

% subplot(3,1,3);
% plot(x2,real(LHS));
% xlabel('x [angstrom]');
% ylabel('RHS');
%
% is first derivative continuous.
% figure(5);
% plot(x1,psi1);
```

Projection onto Basis Sol^n

$$\psi(x) = \left(\frac{1}{L}\right)^{1/2}\left[\frac{1}{4} - \left(\frac{x}{L} - \frac{1}{2}\right)^2\right]$$

$$f_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right)$$

a) Convert to Dirac notation

$$|\psi\rangle = \sum_{n=1}^{\infty} c_n |f_n\rangle$$

$$c_n = \langle f_n|\psi\rangle$$

b)

$$c_1 = \frac{\sqrt{2}}{L}\int_0^L dx \sin\left(\pi \frac{x}{L}\right)\left[\frac{1}{4} - \left(\frac{x}{L} - \frac{1}{2}\right)^2\right]$$

let $u = x/L - \frac{1}{2}$

$$du = \frac{dx}{L}$$

$$c_1 = \frac{\sqrt{2}}{\cancel{L}} \cancel{L} \int_{-1/2}^{+1/2} du \sin\left(\pi u + \pi/2\right)\left[\frac{1}{4} - u^2\right]$$

$$\sin(t + \pi/2) = \cos t$$

$$= \sqrt{2}\left\{\frac{1}{4}\int_{-1/2}^{+1/2} du \cos(\pi u) - \int_{-1/2}^{1/2} du\, u^2 \cos(\pi u)\right\}$$

The first integral is trivial

$$\frac{1}{4}\int_{-1/2}^{1/2} du \cos(\pi u) = \frac{1}{4\pi}\left[\sin\left(\pi/2\right) - \sin\left(-\pi/2\right)\right] \quad (1)$$

$$= \frac{1}{2\pi}$$

The second integral can be done quickly w/ the tabular method

$$\begin{array}{ccc} u^2 & & \cos \pi u \\ & (+) & \\ 2u & & \frac{1}{\pi} \sin \pi u \\ & (-) & \\ 2 & & -\frac{1}{\pi^2} \cos \pi u \\ & (+) & \\ 0 & & -\frac{1}{\pi^3} \sin(\pi u) \end{array}$$

$$\int_{-1/2}^{1/2} du\, u^2 \cos(\pi u) =$$

0 at both bounds

$$\left[\frac{u^2}{\pi} \sin \pi u + \frac{2u}{\pi^2} \cos \pi u - \frac{2}{\pi^3} \sin \pi u\right]_{-1/2}^{1/2} \quad (2)$$

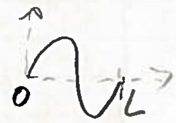
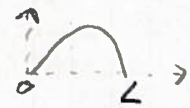
$$\frac{1}{4\pi} \cdot 2 + 0 - \frac{2}{\pi^3} \cdot 2$$

$$\frac{1}{2\pi} - \frac{4}{\pi^3}$$

$$\Rightarrow C_1 = \sqrt{2}\left[\cancel{\frac{1}{2\pi}} - \left(\cancel{\frac{1}{2\pi}} - \frac{4}{\pi^3}\right)\right]$$

$$\boxed{C_1 = \frac{4\sqrt{2}}{\pi^3}}$$

Now C_2 and C_4 are zero by symmetry b/c

$C_2 = \int$  $\times$ 

odd even

$$\int \text{odd} = 0$$

and likewise for C_4. So we are left w/ C_3. Using same u-sub as ~~before~~

$$C_3 = \sqrt{2} \int_{-1/2}^{1/2} du \, \sin\left(3\pi u + \tfrac{3\pi}{2}\right) \left[\tfrac{1}{4} - u^2\right]$$

$\vdots$

similar algebra to that done for C_1 gives

$$C_3 = \frac{4\sqrt{2}}{27\pi^3}$$

See MATLAB for plot.

```
%ProjectOnBasis.m
%
%This script shows a parabola represented in a basis of sine waves.
%
%Tom Allison 8/24/2014

set(0,'DefaultLineLineWidth',2);

L = 1;
x = linspace(0,1);
dx = x(2)-x(1);

psi = (1/L)^0.5 * (1/4 - (x/L-1/2).^2);
f1 = sqrt(2/L)*sin(pi*x/L);
f3 = sqrt(2/L)*sin(3*pi*x/L);

c1 = 4*sqrt(2)/pi^3;
c3 = 4*sqrt(2)/(27*pi^3);

% sanity check with numerical integrals.
c1num = dx*trapz(f1.*psi);
c3num = dx*trapz(f3.*psi);

figure(1);
hpsi = plot(x,psi,'k','LineWidth',3);
hold on
hf1 = plot(x,c1*f1,'r--');
hfsum = plot(x,c1*f1 + c3num*f3,'g--');
hold off
grid on
xlabel('x/L');
ylabel('\psi');
legend([hpsi,hf1,hfsum],'\psi','c_1 f_1','c_1 f_1 + c_3 f_3');
setfigfont(1,14)
```

a)
$$\left[\frac{1}{x}, \hat{p}_x\right] = -i\hbar\left[\frac{1}{x}, \frac{\partial}{\partial x}\right]$$

It is often helpful to use a test function to not get mixed up

$$\left[\frac{1}{x}, \frac{\partial}{\partial x}\right] f = \frac{1}{x}\frac{\partial f}{\partial x} - \frac{\partial}{\partial x}\left(\frac{1}{x} f\right)$$

$$= \cancel{\frac{1}{x}\frac{\partial f}{\partial x}} - \left(-\frac{1}{x^2} f + \cancel{\frac{1}{x}\frac{\partial f}{\partial x}}\right)$$

$$= \frac{1}{x^2} f$$

$$\Rightarrow \boxed{\left[\frac{1}{x}, \hat{p}_x\right] = \frac{-i\hbar}{x^2}} \qquad (1)$$

b)
$$[V, \hat{p}] f = V\left(-i\hbar\frac{\partial f}{\partial x}\right) - \left(-i\hbar\frac{\partial}{\partial x}\right)(Vf)$$

$$= \cancel{-i\hbar V\frac{\partial f}{\partial x}} + i\hbar f\frac{\partial V}{\partial x} + \cancel{i\hbar V\frac{\partial f}{\partial x}}$$

$$= i\hbar f\frac{\partial V}{\partial x}$$

$$\Rightarrow [V, \hat{p}] = i\hbar\frac{\partial V}{\partial x}$$

c)
$$[x\hat{p}_y - y\hat{p}_x, y\hat{p}_z - z\hat{p}_y] = [x\hat{p}_y, y\hat{p}_z - z\hat{p}_y] - [y\hat{p}_x, y\hat{p}_z - z\hat{p}_y]$$

$$= [x\hat{p}_y, y\hat{p}_z] - [x\hat{p}_y, z\hat{p}_y] - [y\hat{p}_x, y\hat{p}_z] + [y\hat{p}_x, z\hat{p}_y] \qquad (2)$$

Now the 2^{nd} and 3^{rd} commutators here are obviously zero because the derivatives do not involve the coordinates.

The remaining commutators can be rearranged using the identities

$$[AB, C] = A[B, C] + [A, C]B$$

$$[A, BC] = B[A, C] + [A, B]C$$

so $$[x\hat{p}_y, y\hat{p}_z] = x[\hat{p}_y, y\hat{p}_z] + \cancelto{0}{[x, y\hat{p}_z]}\hat{p}_y$$

$$= x\left(y\cancelto{0}{[\hat{p}_y, \hat{p}_z]} + [\hat{p}_y, y]\hat{p}_z\right)$$

$$= -i\hbar\, x\hat{p}_z$$

And $$[y\hat{p}_x, z\hat{p}_y] = \cancelto{0}{x[\hat{p}_x, z\hat{p}_y]} + [y, z\hat{p}_y]\hat{p}_x$$

$$= \left(z[y, \hat{p}_y] + \cancelto{0}{[y, z]}\hat{p}_y\right)\hat{p}_x$$

$$= z\hat{p}_x(i\hbar)$$

So the final result is

$$\boxed{[x\hat{p}_y - y\hat{p}_x, y\hat{p}_z - z\hat{p}_y] = i\hbar(zp_x - xp_z)}$$

If you already know about angular momentum, you can identify this as a commutator relation for orbital angular momentum

$$\boxed{[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y}$$

(d) $\left[x^2\frac{\partial^2}{\partial y^2}, y\frac{\partial}{\partial x}\right] = x^2\left[\frac{\partial^2}{\partial y^2}, y\frac{\partial}{\partial x}\right]$

$+\left[x^2, y\frac{\partial}{\partial x}\right]\frac{\partial^2}{\partial y^2}$

$= -x^2\left(y\cancel{\left[\frac{\partial}{\partial x}, \frac{\partial^2}{\partial y^2}\right]}^{0} + \left[y, \frac{\partial^2}{\partial y^2}\right]\frac{\partial}{\partial x}\right)$

$-\left(y\left[\frac{\partial}{\partial x}, x^2\right] + \cancel{\left[y, x^2\right]}^{0}\frac{\partial}{\partial x}\right)\frac{\partial^2}{\partial y^2}$

$= +x^2\left[\frac{\partial^2}{\partial y^2}, y\right]\frac{\partial}{\partial x} + y\left[x^2, \frac{\partial}{\partial x}\right]\frac{\partial^2}{\partial y^2}$

$= x^2\left(\frac{\partial}{\partial y}\left[\frac{\partial}{\partial y}, y\right] + \left[\frac{\partial}{\partial y}, y\right]\frac{\partial}{\partial y}\right)\frac{\partial}{\partial x}$

$+ y\left(x\left[x, \frac{\partial}{\partial x}\right] + \left[x, \frac{\partial}{\partial x}\right]x\right)\frac{\partial^2}{\partial y^2}$

Now this is broken down into the elementary commutator

$$\left[q, \frac{\partial}{\partial q}\right]f = q\frac{\partial f}{\partial q} - \frac{\partial}{\partial q}(qf)$$

$$= -f$$

$$\left[q, \frac{\partial}{\partial q}\right] = -1$$

So we have

$$\left[x^2\frac{\partial^2}{\partial y^2}, y\frac{\partial}{\partial x}\right] = x^2\left(\cancel{2}\,1 + 1\frac{\partial}{\partial y}\right)\frac{\partial}{\partial x} + y\left(-x - x\right)\frac{\partial^2}{\partial y^2}$$

$$= \boxed{2x^2\frac{\partial^2}{\partial x\partial y} - 2xy\frac{\partial^2}{\partial y^2}}$$

a) To constitute a vector space, the elements of a set must satisfy

$$\alpha f_1 + \beta f_2 = f_3 \in \text{vector space} \quad (1)$$

If we take any two polynomials $f_1(x)$ and $f_2(x)$ with degree less than N, e.g. of the form

$$f_1(x) = a_0 + a_1 x + \ldots + a_N x^N$$
$$f_2(x) = b_0 + b_1 x + \ldots + b_N x^N \quad (2)$$

Their sum (1) will be

$$\alpha f_1 + \beta f_2 = (\alpha a_0 + \beta b_0) + (\alpha a_1 + \beta b_1) x + \ldots + (\alpha a_N + \beta b_N) x^N \quad (3)$$

which is a polynomial with degree $\leq N$. Also, addition is commutative, e.g.

$$f_1 + f_2 = f_2 + f_1 \quad (4)$$

So the polynomials form a vector space.

b) This is easily seen by evaluating the trace. For a vector space of dimension N

$$\text{trace}(I) = N \quad (5)$$

where I is the identity operator

But finite dimensional vector spaces also satisfy the trace rule

$$\mathrm{trace}(AB) = \mathrm{trace}(BA) \tag{6}$$

so if

$$[A, B] = I \tag{7}$$

we would have

$$\mathrm{trace}(AB - BA) = \mathrm{trace}(AB) - \mathrm{trace}(BA) = N$$

$$0 = N \tag{8}$$

which cannot be satisfied for finite N. The trace of an operator in an infinite dimensional vector/Hilbert space is more subtle, and there it is possible to have $[\hat{A}, \hat{B}] = \hat{I}$

a) Take $|\psi\rangle = c_1|\beta\rangle + c_2|\gamma\rangle$ w/ c_1 and c_2 arbitrary

$$\hat{H}|\psi\rangle = c_1 E_2|\beta\rangle + c_2 E_2|\gamma\rangle$$

$$= E_2(c_1|\beta\rangle + c_2|\gamma\rangle)$$

$$\Rightarrow \boxed{\hat{H}|\psi\rangle = E_2|\psi\rangle} \qquad (1)$$

b) The matrix elements are $\langle\psi_1|H|\psi_2\rangle$. Since $|\alpha\rangle$, $|\beta\rangle$, and $|\gamma\rangle$ are orthogonal and eigenkets of A, ~~the~~ off diagonal terms such as $\langle\alpha|\hat{H}|\gamma\rangle$ will vanish, and we have

$$\boxed{H = \begin{bmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_2 \end{bmatrix}} \qquad (2)$$

c) The matrix for A is found in similar fashion

$$\langle\alpha|\hat{A}|\alpha\rangle = a$$

$$\langle\alpha|\hat{A}|\beta\rangle = \langle\beta|\hat{A}|\alpha\rangle = 0$$

$$\langle\alpha|\hat{A}|\gamma\rangle = \langle\gamma|\hat{A}|\alpha\rangle = 0$$

$$\langle\beta|\hat{A}|\beta\rangle = \langle\beta|\left(b|\beta\rangle + c|\gamma\rangle\right) = b$$

$$\langle\beta|\hat{A}|\gamma\rangle = \langle\beta| -ic|\beta\rangle + b|\gamma\rangle) = -c$$

$$\langle\gamma|\hat{A}|\gamma\rangle = \langle\gamma|\left(-ic|\beta\rangle + b|\gamma\rangle\right) = b$$

$$\langle\gamma|\hat{A}|\beta\rangle = \langle\gamma|\left(ic|\beta\rangle + ic|\gamma\rangle\right) = c$$

Putting it all together

$$\boxed{A = \begin{bmatrix} a & 0 & 0 \\ 0 & b & -ic \\ 0 & ic & b \end{bmatrix}} \qquad (3)$$

We can verify that this is correct by doing $A|\beta\rangle$ in matrix/coloumn vector notation

$$A|\beta\rangle \rightarrow \begin{bmatrix} a & 0 & 0 \\ 0 & b & -ic \\ 0 & ic & b \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ b \\ c \end{bmatrix} \rightarrow b|\beta\rangle + c|\gamma\rangle \qquad (4)$$

✓

Does $\hat{A}$ commute with $\hat{H}$?

$$AH = \begin{bmatrix} a & 0 & 0 \\ 0 & b & -ic \\ 0 & ic & b \end{bmatrix} \begin{bmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_2 \end{bmatrix} = \begin{bmatrix} aE_1 & 0 & 0 \\ 0 & E_2 b & -icE_2 \\ 0 & iE_2 c & E_2 b \end{bmatrix} \leftarrow AH$$

$$HA = \begin{bmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_2 \end{bmatrix} \begin{bmatrix} a & 0 & 0 \\ 0 & b & -ic \\ 0 & ic & b \end{bmatrix} = \begin{bmatrix} aE_1 & 0 & 0 \\ 0 & bE_2 & -icE_2 \\ 0 & icE_2 & bE_2 \end{bmatrix} \qquad (5)$$

$\leftarrow$ HA is the same as AH

so $[A, H] = 0$

d) Now we can use the fact that commuting observables can have simultaneous eigenkets, so if we diagonalize A and find its eigenvectors, they will be eigenvectors of H.

To find the eigenvalues of A

$$\begin{vmatrix} a-\lambda & 0 & 0 \\ 0 & b-\lambda & -ic \\ 0 & ic & b-\lambda \end{vmatrix} = (a-\lambda)\left((b-\lambda)^2 - c\right) = 0$$

$$\Rightarrow \lambda = a \quad \text{or} \quad \lambda_\pm = b \pm c$$

$|\alpha\rangle \leftrightarrow \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ is one obvious eigenvector w/ eigenvalue a. The other eigenvectors are found from solving

$$\lambda_+ \Rightarrow \begin{bmatrix} b & -ic \\ ic & b \end{bmatrix}\begin{bmatrix} V_1 \\ V_2 \end{bmatrix} = (b+c)\begin{bmatrix} V_1 \\ V_2 \end{bmatrix}$$

$$bV_1 - icV_2 = (b+c)V_1$$

$$icV_1 + bV_2 = (b+c)V_2$$

$$\Rightarrow \boxed{V_1 = -iV_2} \Rightarrow \chi_+ = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ -i \\ 1 \end{bmatrix} \qquad (6)$$

Similarly

$$\text{for } \lambda_- \Rightarrow \boxed{V_1 = +iV_2} \Rightarrow \chi_- = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 \\ +i \\ 1 \end{bmatrix} \qquad (7)$$

Or in terms of ket notation, we have new simultaneous eigenkets

$$\boxed{\begin{aligned} |E_1, a\rangle &= |\alpha\rangle \\ |E_2, b+c\rangle &= \frac{1}{\sqrt{2}}\left(-i|\beta\rangle + |\gamma\rangle\right) \\ |E_2, b-c\rangle &= \frac{1}{\sqrt{2}}\left(+i|\beta\rangle + |\gamma\rangle\right) \end{aligned}} \tag{8}$$

This problem can be solved by considering the derivative of $\int dx\, \Psi^* \hat{p} \Psi$, but it is much easier to use the hint.

Recognize

$$[\hat{H}, \hat{p}] = [\hat{p}^2/2m + \hat{V}, \hat{p}]$$

$$= [\hat{V}, \hat{p}] = i\hbar \frac{dV}{dx}$$

so

$$\langle \Psi | [\hat{H}, \hat{p}] | \Psi \rangle = i\hbar \left\langle \frac{dV}{dx} \right\rangle \tag{1}$$

$$= \langle \Psi | [\hat{H}\hat{p} - \hat{p}\hat{H}] | \Psi \rangle$$

$$= \langle \Psi | \hat{H}\hat{p} | \Psi \rangle - \langle \Psi | \hat{p}\hat{H} | \Psi \rangle$$

since $\hat{H}$ is Hermitian, it can go left or right. The TDSE says

$$\hat{H} | \Psi \rangle = i\hbar \frac{\partial}{\partial t} | \Psi \rangle$$

$$\langle \Psi | \hat{H} = (\hat{H} | \Psi \rangle)^*$$

$$= -i\hbar \frac{\partial}{\partial t} | \Psi \rangle$$

so

$$\langle \Psi | \hat{H}\hat{p} | \Psi \rangle = \left(-i\hbar \frac{\partial}{\partial t} \langle \Psi | \right) \hat{p} | \Psi \rangle$$

$$- i\hbar \langle \Psi | \hat{p} \left(\frac{\partial}{\partial t} | \Psi \rangle \right) \Big)$$

Since $\hat{p}$ doesn't depend on time, this is the same thing you get from

$$\langle [\hat{H}, \hat{p}] \rangle = -i\hbar \frac{\partial}{\partial t} \left(\langle \Psi | \hat{p} | \Psi \rangle \right) \qquad (2)$$

when you use the product rule.

So combining (1) and (2)

$$\cancel{i\hbar} \left\langle \frac{dV}{dx} \right\rangle = -\cancel{i\hbar} \frac{\partial}{\partial t} \langle \hat{p} \rangle$$

$$\boxed{\frac{\partial \langle \hat{p} \rangle}{\partial t} = \left\langle -\frac{dV}{dx} \right\rangle}$$

Contents


```
%ClassicallyForbiddenRegion.m
%
%This script calculates the probability of finding a harmonic oscillator in
%its classically forbidden region and also makes some nice plots.
%
%Tom Allison 8/26/2013
```

Initialize and Calculate

```
set(0,'DefaultLineLineWidth',2);
N = 10; % number of wavefunctions to plot
xi = linspace(-2*sqrt(N),2*sqrt(N),1E4); %xi axis

%initialize arrays to calculate in for loop.
psi_n = zeros(N,length(xi));
psi_nplot = zeros(N,length(xi));
psi_nsq = zeros(N,length(xi));
Pforb = zeros(N,1);
xiforb = zeros(N,1);
Pclass = zeros(N,length(xi));

for n = 1:N
    psi_n(n,:) = pi^(-1/4)*1/(sqrt(2^(n-1)*factorial(n-1)))...
        *polyval(HermitePoly(n-1),xi).*exp(-xi.^2/2);
    psi_nsq(n,:) = psi_n(n,:).*conj(psi_n(n,:)); %square modulus of wavefunction
    psi_nplot(n,:) = psi_n(n,:) + 1 + 2*(n-1);
    xiforb(n) = sqrt(2*(n-1+1/2));        %boundary of the classically forbidden region in xi
    [crap,I] = min(abs(xi-xiforb(n))); % find index closest to forbidden region
    Pforb(n) = 2*(xi(2)-xi(1))*trapz(psi_nsq(n,I:end)); %integrate to \psi^2 to find probability
of particle being in forbidden region
                                                        %multiply by 2 to
                                                        %account for +x and
                                                        %-x.

    % construct classical probability distribution
    Pclass(n,:) = 2*1./(2*pi*xiforb(n))*1./sqrt(1-(xi/xiforb(n)).^2); % analytic expression from
SHO equations.
    I = find(abs(xi)>=xiforb(n));
    Pclass(n,I) = 0;
end
```

plot wavefunctions

```
figure(1);
plot(xi,psi_nplot,'r');
hold on
plot(xi,xi.^2,'k');;
for n= 1:N;
    hline(gcf,1+2*(n-1),'k--');
end
```

```
hold off
xlabel('\xi');
ylabel('\psi_n');
set(gca,'YTickLabel',[]);
set(gca,'Xgrid','on');
axis([xlim,0,2.2*N]);
```

Plot probability of being found in classicaly forbidden region

The probability of being in the forbidden region decreases rapidly as the quantum number and energy increases and the system behaves "more classically".

```
figure(2);
plot((1:N)-1,Pforb,'o-');
xlabel('n');
ylabel('Probability of finding particle in forbidden region');
grid on
```

Plot quantum vs. classical probability for n=0 and n=N

```
figure(3);
numplot = 9
hquant = plot(xi,psi_nsq(numplot+1,:),'k');
hold on
hclass = plot(xi,smooth(Pclass(10,:),4),'g');
hold off
grid on
xlabel('x');
ylabel('Probability Density');
legend([hclass,hquant],'Classical','Quantum');
title(['Results for n = ',num2str(numplot)])
```

```
numplot =

     9
```

Part b)

Wave function has no nodes in the forbidden region because the local wavevector is approximately

and for (allowed region) k is real and is oscillatory and wavelike. But for , k is imaginary and is an exponential decay with no oscillations.

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The key to this problem is to write the Hamiltonian in the form

$$\hat{H} = \hat{a}^{+}\hat{a} + \hbar\omega/2 \tag{1}$$

and use $[\hat{a},\hat{a}^{+}] = \hbar\omega$

$$[\hat{H},\hat{a}] = [\hat{a}^{+}\hat{a},\hat{a}] = \hat{a}^{+}\cancel{[\hat{a},\hat{a}]}^{0} + [\hat{a}^{+},\hat{a}]\hat{a}$$

$$= -\hbar\omega\hat{a}$$

similarly

$$[\hat{H},\hat{a}^{+}] = [\hat{a}^{+}a, a^{+}] = a^{+}[a,a^{+}] + \cancel{[a^{+},a^{+}]}^{0}a$$

$$= \hbar\omega a$$

so we have for the Heisenberg equations of motion

$$\frac{d\hat{a}}{dt} = \frac{i}{\hbar}(-\hbar\omega)\hat{a}$$

$$\frac{d\hat{a}}{dt} = -i\omega\hat{a} \Rightarrow \boxed{\hat{a}(t) = \hat{a}(t=0)\,e^{-i\omega t}} \tag{2}$$

similarly

$$\frac{d\hat{a}^{+}}{dt} = i\omega a^{+} \Rightarrow \boxed{a^{+}(t) = a^{+}(t=0)\,e^{i\omega t}} \tag{3}$$

Quantum or Classical Wave perspective

d) $R \approx 384 \times 10^3$ km

$\approx 3.8 \times 10^8$ m

$x = 2\pi R = 2.4 \times 10^9$ m

What is momentum?

Orbit is ~ 27 days $= T$

$$V = \frac{2\pi R}{T} = \omega R$$

$$= \frac{2.4 \times 10^9 \text{ m}}{27 \cancel{\text{days}} \times 24 \cancel{h}/\cancel{\text{day}} \times 60 \cancel{\text{min}}/\cancel{\text{hour}} \times 60 s/\cancel{\text{min}}}$$

$= 1029 \text{ m/s}$

$M_{moon} = 7.34 \times 10^{22}$ kg

$$\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34} \text{ J-s}}{7.3 \times 10^{22} \text{ kg} \cdot 10^3 \text{ m/s}}$$

$= 10^{-59}$ m

$\boxed{\frac{x}{\lambda} \approx 10^{69}}$ Very classical b)

$$\frac{1}{2}mv^2 = 13.6\,eV = \frac{p^2}{2m}$$

$$p = \sqrt{2mE}$$

$$p = \sqrt{2 \times 0.511 \times 10^6\,eV/c^2 \times 13.6\,eV}$$

$$= 3700\,eV/c^2$$

$$\lambda = \frac{h}{p} = \frac{2\pi \times 6.58 \times 10^{-16}\,\cancel{eV}\text{-}s}{3700\,\cancel{eV}/c}$$

$$= 1 \times 10^{-18}\ c\text{-}s$$

$$= 3 \times 10^{-10}\,m$$

$$\lambda = 3\,Å$$

$$X = 2\pi \times a_0 \approx 3\,Å \Rightarrow \boxed{\frac{X}{\lambda} \sim 1}$$

Definitely Quantum

c) The de Broglie wavelength is about the same as the hydrogen case above since KE is nearly the same and X is also close.

$$\boxed{\frac{X}{\lambda} \sim 1}$$ Quantum.

d) Now the particle is relativistic

$$p \approx \frac{E}{c} = 1\ \frac{GeV}{c}$$

$$\lambda = \frac{h}{p} = \frac{2\pi \times 6.58\times10^{-16}\ eV\text{-}s}{10^9\ eV/c}$$

$$= 4\times10^{-24}\ \cancel{s} \times 3\times10^{8}\ m/\cancel{s}$$

$$= 1.24\times10^{-15}\ m$$

$$\boxed{\frac{X}{\lambda} \approx 10^5} \rightarrow \text{classical}$$

e) $M_{neutron} = 940\ MeV/c^2$

$$p = \sqrt{2\times 940\ MeV/c^2 \times 4\ MeV}$$

$$= 87\ \frac{MeV}{c}$$

$$\lambda = \frac{2\pi \times 6.58\times10^{-16}\ eV\text{-}s}{87\times10^6\ eV/c}$$

$$= 14\ fm$$

$$\Rightarrow \boxed{\frac{X}{\lambda} \sim \frac{1}{2} \Rightarrow \text{Quantum.}}$$

f) $v \approx \sqrt{\frac{kT}{m}} \approx \sqrt{\frac{0.025\,eV}{938\ MeV/c^2}} = 5\times10^{-6}\,c$

Room Temp

$$= 1500\ m/s$$

$$p = mv = 1.7\times10^{-27}\,kg \times 1500\,m/s$$

$$= 2.6\times10^{-24}\ kg\text{-}m/s$$

$$\lambda = \frac{h}{p} = \frac{6\times10^{-34}\ J\text{-}s}{2.6\times10^{-24}\ kg\text{-}m/s} \approx 2\times10^{-10}\ m$$

$$= 2\ \text{Å}$$

$$\boxed{\frac{x}{\lambda} \sim 1}$$ $\Rightarrow$ Quantum effects are important, although in practice classical molecular dynamics or semiclassical methods (e.g. path-integral MD) can approach this problem!

g) Harmonic oscillator $x = 0.1\text{Å}\cos(2\pi\times100\,THz\times t)$

$$\dot{x}_{max} = (0.1\text{Å})(2\pi\times100\ THz)$$

$$= 6300\ m/s$$

This is a similar speed as f) (and the particle will go slower sometimes). So we again expect $\boxed{\frac{x}{\lambda} \sim 1}$ Quantum

Note: mass of proton and mass of H-atom are almost the same since (e^-)'s are light!

h) Simple pendulum

$$\omega = \sqrt{\frac{g}{L}} = \sqrt{\frac{9.8\,m/s^2}{50\,cm}}$$

$$\omega = 4.43\ rad/s$$

$$V_{max} = \omega X_{max}$$
$$= 4.4\,rad/s \times 10^{-19}\,m = 4.4 \times 10^{-19}\ m/s$$

$$p = 40\,kg \times V_{max} = 1.8 \times 10^{-17}\ m/s \cdot kg$$

$$\lambda = \frac{h}{p} = \frac{6 \times 10^{-34}\ J\text{-}s}{1.8 \times 10^{-17}\ kg\text{-}m/s}$$

$$\boxed{\lambda \approx 3 \times 10^{-17}\,m} \qquad \frac{\overset{10^{-19}\,m}{x}}{\lambda} < 1$$

Interesting that this comes out less than one... The real resonant frequency could be higher due to radiation pressure. I think the motion of the test masses in LIGO is still considered to be classical. Certainly the (frequency integrated) excursions are much larger than 10^{-19} m.

Q/C waves

i) Agarm

$$V_{max} = \omega x_{max}$$

$$= 2\pi \times 10^{5}\,Hz \times 10^{-9}\,m$$

$$\approx 10^{-3}\,m/s$$

$$\lambda = \frac{h}{m V_{max}} = \frac{6\times10^{-34}\,J\text{-}s}{5\times10^{-12}\,kg \times 10^{-3}\,m/s}$$

$$\approx 10^{-19}\,m \ll 10\,nm$$

$$\frac{x}{\lambda} \approx 10^{11} \qquad \frac{x}{\lambda} \gg 1 \qquad \text{classical}$$

j) $M_{Homework} \approx 2\,oz. \approx 0.05\,kg$

$$\lambda = \frac{6\times10^{-34}\,J\text{-}s}{0.05\,kg \times 1\,m/s} \approx 1\times10^{-32}\,m$$

$$\boxed{\frac{x}{\lambda} \approx 3\times10^{31}} \qquad \underline{\text{Very}} \quad \text{classical}$$

a) For particle on a ring

$$E = \frac{\hbar^2 k^2}{2m} \qquad k \cdot \cancel{2\pi} R = n \cancel{2\pi}$$

integer

$$k = \frac{n}{R}$$

For moon, $\lambda \approx 10^{-59}$ m (see last problem)

$$R \approx 4\times10^{8}\,m$$

$$\Rightarrow n = \frac{2\pi}{10^{-59}\,\cancel{m}} \times 4\times10^{8}\,\cancel{m}$$

$$= 2.5\times10^{68}$$

$$E = \frac{\hbar^2}{2m}\frac{n^2}{R^2}$$

$$\Delta E = \frac{\cancel{2}\hbar^2}{\cancel{2}mR^2}\,\Delta n\, n \qquad \Delta n = 1 \text{ for adjacent states}$$

$$\Delta E = \frac{\hbar^2 n}{MR^2}$$

$$= \frac{(1\times10^{-34}\,J\text{-}s)^2 \times 2.5\times10^{68}}{7.3\times10^{22}\,kg \times (3.8\times10^{8}\,m)^2}$$

$$= 2.4\times10^{-40}\,J$$

$$k_BT = 1.38\times10^{-23}\,J/K \times 1700\,K$$

$$= 2.34\times10^{-20}\,J$$

$$\boxed{\frac{k_BT}{\Delta E} \sim 10^{20}}$$

Very Classical

Q/C w/ DOS

2

b) $\Delta E = \left(-\frac{1}{2^2} - \frac{1}{1^2}\right) 13.6\,eV$

$= \frac{3}{4} 13.6\,eV = 10.2\,eV$

$k_B T = 0.025\,eV$ at Room Tem

$$\boxed{\frac{k_B T}{\Delta E} \simeq \frac{0.025\,eV}{10.2\,eV} = 2 \times 10^{-3}}$$ quantum

Only $e^{-\Delta E / k_B T} = e^{-500}$ prob. of finding excited H atom at room temp.

c) From Ashcroft and Mermin, the DOS at the Fermi level is

$$\left.\frac{dN}{dE}\right|_{\varepsilon_F} = \frac{3}{2}\frac{n}{\varepsilon_F}$$

For Al $n \simeq 18 \times 10^{22}\ cm^3$ $\varepsilon_F = 11.7\,eV$

$$\left.\frac{dN}{dE}\right|_{\varepsilon_F} = \frac{3}{2}\frac{2 \times 10^{23}\,cm^{-3}}{11.7\,eV}$$

$$= 2.6 \times 10^{22}\ \text{states}/cm^3\text{-}eV$$

So for $1\,cm^3$ and $kT = 25\,meV$

we have $\sim 2.6 \times 10^{22} \frac{\text{states}}{\cancel{cm^3}\text{-}\cancel{eV}} \times 0.025\,\cancel{eV} \times \cancel{1\,cm^3}$

$= \boxed{7 \times 10^{20}\ \text{states}}$

$\Rightarrow$ Huge. $\Rightarrow$ Classical

From this perspective the electrons near the Fermi energy behave classically. Indeed many transport properties of metals can be deduced w/ reasonable accuracy treating the e^- classically $\rightarrow$ the "Drude model", but other properties, such as the heat capacity and bulk modulus, require the (quantum) Sommerfeld model.

d) Now we must consider a <u>relativistic</u> particle on a ring.

$$p = \frac{E}{c} = \hbar k$$

Boundary conditions

$$k(792\text{m}) = 2\pi n$$

$$\frac{2\pi n}{792\text{m}} = \frac{E}{\hbar c}$$

$$\Rightarrow n = \frac{3\text{ GeV} \cdot 792\text{m}}{2\pi \cdot 6.582\times10^{-16}\text{eV-s} \cdot 3\times10^{8}\text{ m/s}}$$

$$n = 2\times10^{19}$$

for $\Delta n = 1$

$$\Delta E = \frac{2\pi\hbar c}{792\text{m}} = 10^{-9}\text{ eV}$$

0.1% energy bandwidth is 3 MeV

$$\Rightarrow \frac{3\text{ MeV}}{10^{-9}\text{ eV}} = 3\times10^{15}\text{ states}$$

$\uparrow$ ΔE

<u>Very</u> Classical

e) PIB $E = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$

$\Delta E = \frac{\hbar^2 \pi^2}{2ma^2} n \, \Delta n$ take n, $\Delta n = 1$ diff. between $n=1$ and $n=2$

$\Delta E = \frac{\hbar^2 \pi^2}{2ma^2}$

$= \frac{(6\times10^{-34}\,J\text{-}s)^2 (\pi)^2}{(2 \times 1.7\times10^{-27}\,kg)\times(7.5\times10^{-15}\,m)^2}$

$= 2\times10^{-11}\,J \approx 100\,MeV$

$\boxed{\frac{K_B T}{100\,MeV} \approx 10^{-9} \rightarrow \text{Quantum}}$

f) Harmonic Oscillator State spacing is $\hbar\omega$

$\hbar\omega = 6.58\times10^{-16}\,eV\text{-}\cancel{s} \times 80\times10^{12}\,\cancel{s}^{-1} \times 2\pi$

$= 0.33\,eV$

$K_B T = 0.025\,eV$ at R.T.

$\Rightarrow$ Somewhat Quantum

$\boxed{\frac{K_B T}{\hbar\omega} \sim 10}$

g) Same as f)

$$\boxed{\frac{k_B T}{\hbar\omega} \approx 10}$$

h) The natural frequency is still $\omega \approx 4.4$ rad/s

$$\hbar\omega = (4.4 \text{ rad/s})(6.58\times10^{-16} \text{ eV-s})$$

$$\approx 2\times10^{-15} \text{ eV}$$

$k_B T = 2.5\times10^{-2}$ eV at R.T.

$\Rightarrow \frac{k_B T}{\hbar\omega} \approx 10^{13} \rightarrow$ Very Classical!

i) Now $\hbar\omega = 2\pi \times 10^5 \text{ Hz} \times 6.582\times10^{-16} \text{ eV-s}$

$$= 4\times10^{-10} \text{ eV}$$

$\Rightarrow \frac{k_B T}{\hbar\omega} \approx 6\times10^{7}$ still Classical, although small

j) Box is 30 cm now

$M = 0.05$ kg

$$\Delta E = \frac{\hbar^2\pi^2}{2ma^2} = \frac{(6\times10^{-34} \text{ J-s})^2\pi^2}{2\times 0.05\text{kg} \times (0.3\text{m})^2}$$

Very Classical!

$= 4\times10^{-64}$ eV $\Rightarrow$ $\boxed{10^{62} \text{ states}}$

$k_B T \sim 10^{-2}$ eV

a) $\langle \hat{L}_z \rangle = \langle \Psi | \hat{L}_z | \Psi \rangle = \langle \Psi | \hbar l | \Psi \rangle$
$= \hbar l \langle \Psi | \Psi \rangle$

$$\boxed{\langle \hat{L}_z \rangle = \hbar l}$$

b) The raising and lowering operators
$\hat{L}_\pm = \hat{L}_x \pm i \hat{L}_y$
can be used to show this. Since $\hat{L}^2 |\Psi\rangle = l(l+1)\hbar^2 |\Psi\rangle$, we are on the top rung and

$$\hat{L}_+ |\Psi\rangle = 0$$

so $\langle \Psi | \hat{L}_+ | \Psi \rangle$

$$= \langle \Psi | \hat{L}_x | \Psi \rangle + i \langle \Psi | \hat{L}_y | \Psi \rangle \qquad (1)$$

Now, since $\hat{L}_x$, $\hat{L}_y$ are Hermitian, they must have <u>real</u> expectation values. This means that both terms in (1) must be zero independently, or

$$\boxed{\langle \hat{L}_x \rangle = \langle \hat{L}_y \rangle = 0}$$

c) $\langle \hat{L}^2 \rangle - \langle \hat{L}_z^2 \rangle = \langle \hat{L}_x^2 \rangle + \langle \hat{L}_y^2 \rangle$

$\hbar^2 l(l+1) - \hbar^2 l^2 = 2 \langle \hat{L}_x^2 \rangle$

$$\Rightarrow \boxed{\langle \hat{L}_x^2 \rangle = \langle \hat{L}_y^2 \rangle = \frac{\hbar^2 l}{2}}$$

d) $\sigma_{L_x}^{2} = \langle \hat{L}_x^{2} \rangle - \cancel{\langle \hat{L}_x \rangle^2}^{\,0}$

$= \frac{\hbar^2 \ell}{2}$

$\sigma_{L_y}^{2} = \frac{\hbar^2 \ell}{2}$ by same reasoning

Generalized uncertainty princ:

$\sigma_{L_x} \sigma_{L_y} \overset{?}{\geq} \frac{1}{2} \left| \langle [\hat{L}_x, \hat{L}_y] \rangle \right|$ $[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$

$\frac{\hbar^2 \ell}{2} \overset{?}{\geq} \frac{1}{2} \left| i\hbar \langle \hat{L}_z \rangle \right|$

$\frac{\hbar^2 \ell}{2} \overset{?}{\geq} \frac{1}{2} \left| i\hbar \, \hbar \ell \right|$

$\frac{\hbar^2 \ell}{2} \geq \frac{\hbar^2 \ell}{2}$ ✓ satisfies gen. unc. princ.

a)

$$\frac{d\sigma}{d\Omega} = \frac{\sigma}{4\pi}\left(1+\beta P_2(\cos\theta)\right)$$

Collecting at all angles amounts to integrating over all angles

$$\int d\Omega \frac{d\sigma}{d\Omega} = \sigma + \frac{\beta\sigma}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta\, P_2(\cos\theta) \qquad (1)$$

$$P_2(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$$

Substituting $u = \cos\theta$, $du = -\sin\theta d\theta$

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta = -2\pi \int_1^{-1} du\, \frac{1}{2}(3u^2-1)$$

$$= \pi \int_{-1}^{1} du\, (3u^2-1)$$

$$= \pi\left[u^3\Big|_{-1}^{1} - 2\right] = 0$$

So the second term of (1) vanishes and you have

$$\boxed{\int \frac{d\sigma}{d\Omega} d\Omega = \sigma \quad \text{independant of } \beta}$$

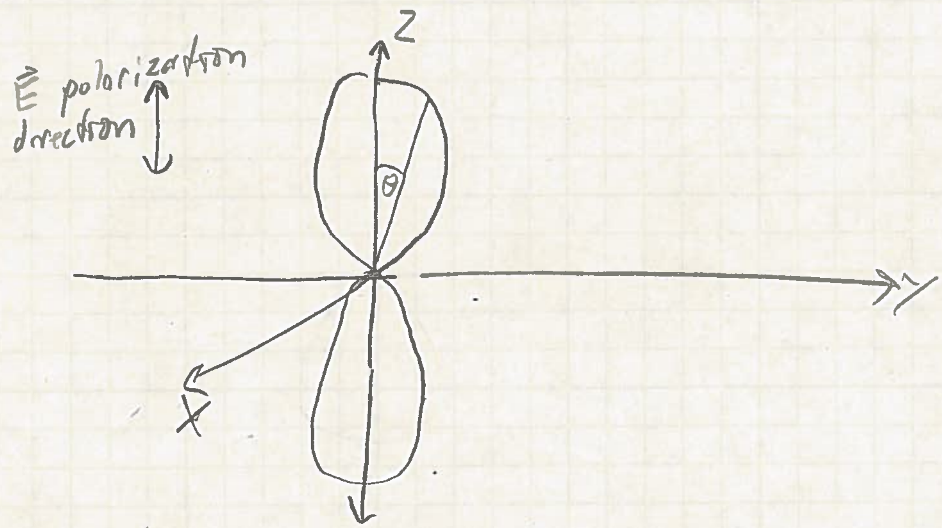
b) The second term vanishes when

$$P_2(\cos\theta) = 0 = \frac{1}{2}(3\cos^2\theta - 1)$$

or $\cos^2\theta = \frac{1}{3}$ $\quad \boxed{\theta = \cos^{-1}\left(\frac{1}{\sqrt{3}}\right) = 54.736}$

The magic angle

c) For $\beta = 2$, the intensity is maximal for $\theta = 0$ (along the light polarization) and zero for $\theta = 90°$. The distribution looks like this on a radial plot



Assuming the dissociation is much faster than molecular rotation (and judging from the potential curves in the quoted paper, it definitely is), the molecular dipole must be ∥ to the molecular axis, so that the molecules that absorbed light and dissociated were the ones that were ∥ to $\vec{E}$.

Contents


```
%FieldFreeAlignment.m
%
%This script calculates expectation values of cos^2(theta) for a rotational
%wavepacket. Uses function Ylm.m
%
%Tom Allison 8/10/2013
```

Preliminatries

```
set(0,'DefaultLineLineWidth',2);

i = sqrt(-1);

c = 3E10; %speed of light in cm/s
Bcm = 1.9896; % rotational constant in wavenumbers
BHz = c*Bcm; % rotational constant in Hz.
Binvps = BHz*1E-12; % Rotational constant in 1/10 Hz.

theta = linspace(0,pi); %linear array in theta
t = linspace(0,10,500); %linear array in time, spanning one to 10 ps. Units of ps
psi = zeros(length(t),length(theta));

J = (0:1:10)'; % needs to be a column vector so fancy matrix multiplication works out later.

psi_J = zeros(length(J),length(theta)); % initialize psi_J, a matrix containing all the
wavefunctions
psi_t = zeros(length(t),length(theta)); %initialize psi_t, a matrix where each row is the wave
function at a different time
psi2 = zeros(length(t),length(theta)); %initialize psi2, the square modulus of psi_t
cos2th = zeros(length(t),1); % initialize array for recording <cos^2(th)> at each time step.
```

Construct initially phased rotational states

```
for k = 1:length(J)
    psi_J(k,:) = Ylm(J(k),0,theta,0)*exp(i*pi/4*J(k)); %phi is irrelevant because everything is
azimuthally symmetric for m=0
end
```

Calculate time dependent superposition and expectation value of cos^2(theta)

```
for k = 1:length(t)
    if length(J) > 1 % handle the exception of only one rotational state
        % do sneaky matrix multiplications to multiply each row by its appropriate phase factor
        phasemat = exp(-i*2*pi*Binvps*(J.*(J+1))*ones(1,length(theta))*t(k));
        psi_t(k,:) = 1/sqrt(length(J))*sum(phasemat.*psi_J);
    else
        psi_t(k,:) = psi_J; %if only one rotational state, there will be no time dependence
    end
    psi2(k,:) = psi_t(k,:).*conj(psi_t(k,:)); %\psi^2
```

```
    cos2th(k) = 2*pi*(theta(2)-theta(1))*trapz(sin(theta).*psi2(k,:).*cos(theta).^2);
end
```

Plot Results

```
figure(1);
plot(t,cos2th,'k');
grid on
xlabel('t [ps]');
ylabel('<cos^2(\theta)>');
```

Part c) Discussion

The molecule experiences a full "revival", where the wavefunction repeats itself at h/(2B) ~ 8.4 ps. "Fractional revivals" at fractions of the revival time also show transient alignment. The width of the alignment peaks is only about 0.3 ps, so any experiment that is be done on these aligned molecules must be done very quickly!!!

The results of the simple superposition wave function compare nicely to the real experimental data of Litvinyuk et al. The real wavefunction will be somewhat more complicated because of the selection rules of Raman excitation and the initial thermal ensemble.

Scaling in Hydrogenic Atoms

a) The 1s binding energy (and all the other energy scales) of the $+Ze, e^-$ system scales as Z^2, so for C^{5+}, we expect

$$IP\ C^{5+} = Z^2 \cdot 13.6\,eV$$
$$= \boxed{489.6\ eV} \qquad (1)$$

Carbon K-edge is only at 284.2 eV, substantially lower. The electron is less tightly bound in a real neutral carbon atom than C^{5+} because the other 5 electrons 1 screen the nuclear charge and 2 have repulsive interactions w/ the electron "in" the 1s orbital

b) For Uranium, $Z = 92$ and we expect

$$IP\ U^{91+} = Z^2 \cdot 13.6\,eV$$
$$= (92)^2 \cdot 13.6\,eV$$
$$= \boxed{115\ keV} \qquad (2)$$

c) The NIST database lists the binding energies

	U XCII	131.821	keV
and	C VI	489.9	eV

(3)

The Hydrogenic result for carbon is off by

$$\frac{0.3\,eV}{489.9\,eV} = 6\times10^{-4} = 0.06\%$$

For Uranium

$$\frac{17\,keV}{132\,keV} = 13\% \quad \text{much worse}$$

The Uranium result is quite a bit off because we are using a result from nonrelativistic quantum mechanics on this very heavy system. The Virial theorem tells us that $\langle T \rangle = -\frac{1}{2}\langle V \rangle$ so

$$\langle T \rangle \approx 66\ keV \approx 0.13\ m_e c^2 \tag{4}$$

and we see error on this level. A relativistic treatment is required either via perturbation theory (see for example Griffiths) or via Dirac and/or Dirac-Fock equations.

d) First convert the proton radius to atomic units

$$r_p = 8.78 \times 10^{-16}\ m = 1.66 \times 10^{-5}\ a.u.$$

So from this we can see this will be a small effect. In atomic units, the 1s orbital is

$$\psi_{100} = \frac{1}{\sqrt{\pi}} e^{-r}$$

The probability that we are inside the proton is

$$P_r = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta \int_0^{r_p} r^2 dr\, |\psi_{100}|^2 \tag{5}$$

since ψ_{100} does not depend on θ or ϕ $\int d\Omega \to 4\pi$

so we have $P_e = 4\int_0^{r_p} r^2 dr e^{-2r}$

Now since $r_p \ll 1$, we can to a good approximation neglect the exponential in the integrand and set $e^{-2r} \approx 1$, so then we get the intuitive result

$$P_e \approx \frac{4}{3} r_p^3 = 6\times10^{-15} \qquad (6)$$

e) Now for Muonic hydrogen we need to look at the mass dependence of the Bohr radius

$$a_0^{(e^-)} = \frac{4\pi\varepsilon_0 \hbar^2}{m_e e^2}$$

so now the orbital will be rescaled by the factor

$$\mathfrak{z} = \frac{a_0^{(\mu)}}{a_0^{(e^-)}} = \frac{m_e}{m_\mu} = \frac{1}{207}$$

so since the proton size is the same there will be $(207)^3$ more muon wave function inside of r_p.

More formally, in atomic units, the muonium 1s wavefunction is

$$\psi_{100}^{(\mu)} = \frac{1}{\sqrt{\pi \mathfrak{z}^3}} e^{-r/\mathfrak{z}}$$

and

$$P^{\mu} = \frac{1}{\pi\, 7^3} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_0^{r_p} dr\, r^2 e^{-2r/7}$$

$$= \frac{4\cancel{\pi}}{\cancel{\pi}\, 7^3} \int_0^{r_p} dr\, r^2 e^{-2r/m}$$

$$\simeq \frac{4}{3} r_p^3 \left(\frac{1}{7}\right)^3 = \boxed{(207)^3 P_e}$$

a) Take $\lambda = 550\,nm$ for visible light

$$\phi \approx \frac{2\pi}{\lambda} a_0 = \frac{2\pi}{5500\,Å} \cdot 0.5\,Å = 0.6\,mrad \qquad (1)$$

Yes neglecting this phase is customary. This is called the electric dipole approximation.

b) For a plane wave

$$I = \frac{1}{2} c \varepsilon_0 E_0^2$$

$$E_0 = \sqrt{\frac{2I}{\varepsilon_0 c}} = \sqrt{\frac{2 \times 1000\,W/m^2}{8.85 \times 10^{-12}\,C^2/Nm^2 \times 3 \times 10^8\,m/s}}$$

$$\boxed{E_0 = 868\,V/m} \qquad (2)$$

The atomic unit of electric field is

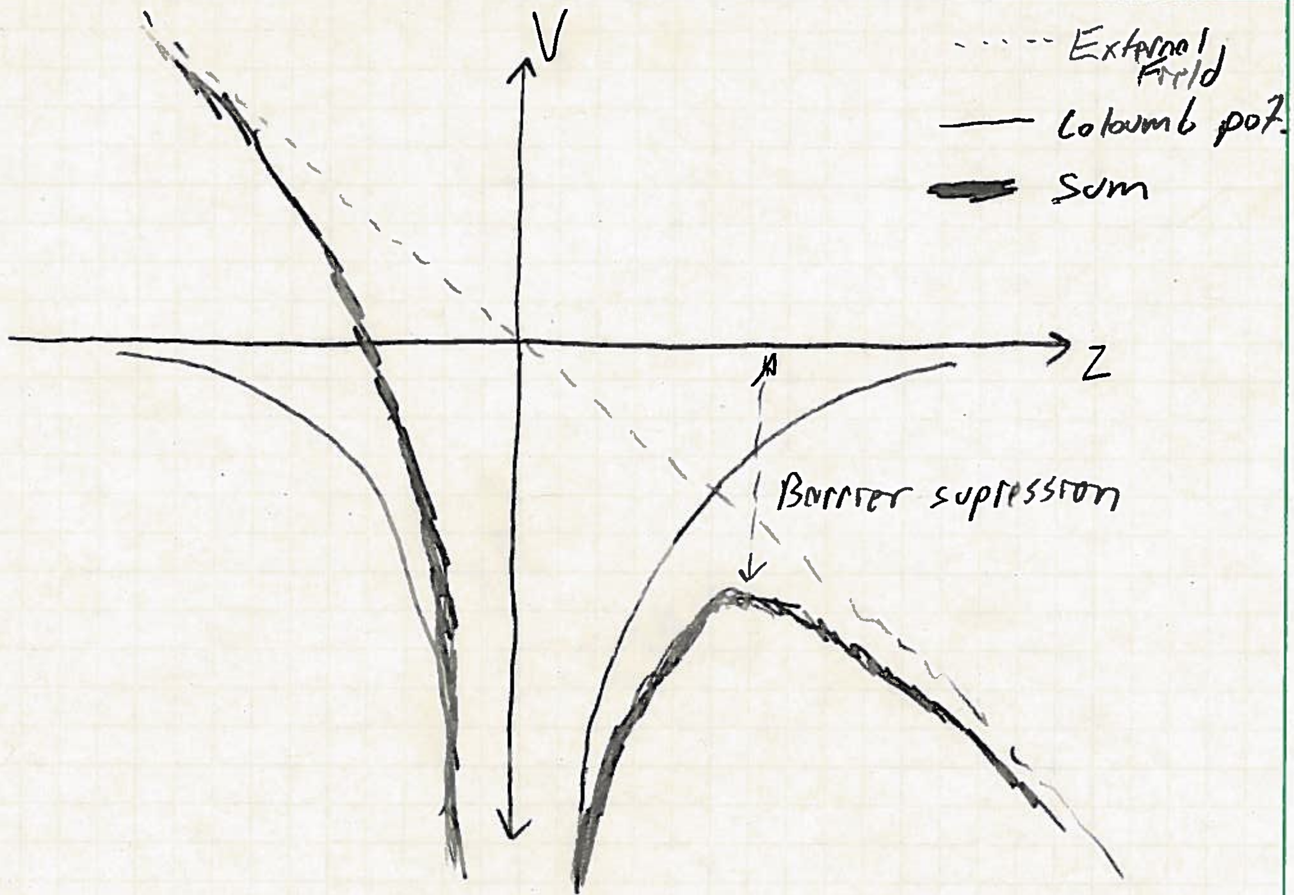
$$E_a = \frac{1\ \text{Hartree}}{e a_0} = \frac{e}{4\pi\varepsilon_0 a_0^2} = 5.14 \times 10^{11}\,V/m$$
$$= 51.4\,V/Å$$

So the field of the solar light wave is 1.7×10^{-9} a.u.

c) In atomic units, the potential is

$$V = -\frac{1}{r} - zE_0$$

This is sketched on the next page for a slice along the z-direction



(3)

To find the saddle point, we can look at $\frac{\partial V}{\partial z} = 0$ w/ $x=0, y=0$ (z-axis)

$$V(0,0,z) = \frac{-1}{z} - zE_0$$

$$\frac{\partial V}{\partial z} = +\frac{1}{z^2} - E_0 = 0 \Rightarrow z_{max} = \frac{1}{\sqrt{E_0}}$$

So we want the barrier height $= -1\,Ry = -\frac{1}{2}$ a.u.

$$V(z_{max}) = -\sqrt{E_0} - \sqrt{E_0} = -\frac{1}{2} \text{ a.u.}$$

$$= -2\sqrt{E_0} = -\frac{1}{2} \text{ a.u.}$$

$$\Rightarrow \boxed{E_0 = \frac{1}{16} \text{ a.u.} = 3.25\ V/Å = 3.25 \times 10^{10}\ V/m} \quad (4)$$

The corresponding intensity is

$$I = \frac{1}{2} c \varepsilon_0 E_0^2$$

$$= \frac{1}{2}(3\times10^8\ m/s)(8.85\times10^{-12}\ C^2/Nm^2)(3.25\times10^{10}\ V/m)^2$$

$$\boxed{I = 1.4\times10^{18}\ W/m^2} \quad (5)$$

This sounds like a lot, but consider a 1mJ, 100fs laser pulse focused to an area of $(10\mu m)^2$

$$I \approx \frac{1\times10^{-3}\ J}{1\times10^{-13}s \times (10^{-5}m)^2} = 10^{20}\ W/m^2 \quad (6)$$

Well in excess of the requirement.

Atomic Dipoles

a) Both the 1s and 2s states are parity even, whereas the dipole is parity odd, so

$$\boxed{\langle 2s | e\hat{z} | 1s \rangle = 0} \qquad (1)$$

$$\underset{\text{even} \times \text{odd} \times \text{even} = \text{odd}}{} \qquad \int \text{odd} = 0$$

b) In atomic units

$$\psi_{2p_z} = \frac{1}{4\sqrt{2\pi}} r e^{-r/2} \cos\theta$$

$$\psi_{2p_\pm} = \pm \frac{1}{8\sqrt{\pi}} r e^{-r/2} \sin\theta \, e^{\pm i\phi}$$

Now since neither ψ_{1s} or $ez = er\cos\theta$ have any ϕ dependance, we must have

$$\boxed{\langle 2p_\pm | \hat{z} | 1s \rangle = 0} \quad \left(\text{atomic units } e = 1\right) \qquad (2)$$

because

$$\int_0^{2\pi} d\phi \, e^{\pm i\phi} = \mp i \left[e^{\pm i 2\pi} - e^{\pm i 0} \right]$$

$$= \mp i \left[1 - 1 \right] = 0$$

So we are left with

$$\langle 2p_z | \hat{z} | 1s \rangle =$$

$$\frac{1}{\sqrt{\pi}} \frac{1}{4\sqrt{2\pi}} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_0^{\infty} dr \, r^2 \, r e^{-r/2} \cos\theta \, (r\cos\theta) e^{-r}$$

$$= \frac{1}{\cancel{4}\sqrt{2}\,\cancel{\pi}} \cancel{2\pi} \int_0^{\pi} d\theta \cos^2\theta \sin\theta \int_0^{\infty} dr\, r^4 e^{-\frac{3}{2}r} \qquad z = \frac{3}{2}r,\quad dz = \frac{3}{2}dr$$

(with 2 written under the crossed 4; $u = \cos\theta$, $du = -\sin\theta$)

$$= \frac{1}{2\sqrt{2}} \int_{-1}^{1} du\, u^2 \left(\frac{2}{3}\right)^5 \underbrace{\int_0^{\infty} dz\, z^4 e^{-z}}_{\Gamma(5) = 4!}$$

$$= \frac{1}{2\sqrt{2}} \left(\frac{2}{3}\right)\left(\frac{2}{3}\right)^5 4!$$

$$= \boxed{0.745 \text{ a.u.}} \qquad (3)$$

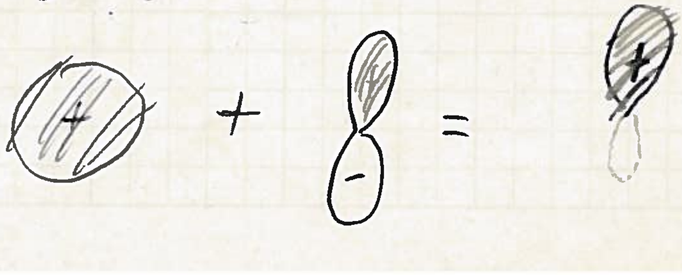
Since we are already in atomic units and the atomic unit of dipole is ea_0, the dipole is

$$\boxed{\langle 2p_z | e\hat{z} | 1s \rangle = 0.745\, ea_0} \qquad (4)$$

c) Drawing the orbitals

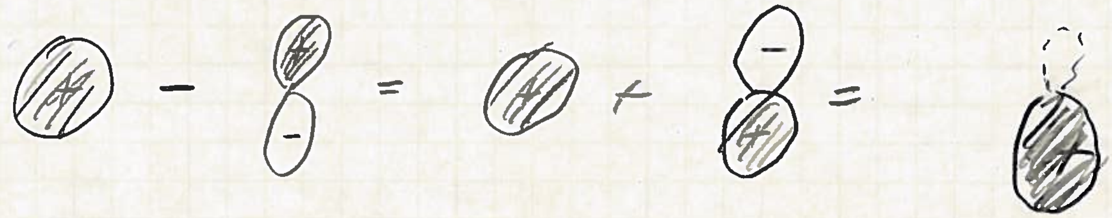
$|1s\rangle =$  $|2p_z\rangle =$  (5)

So now the phase difference between them will oscillate at frequency $\omega = (E_2 - E_1)/\hbar$, so adding the two at $\omega t = 0$, we get



Top lobe adds, bottom lobes destructively interfere. (6)

But a half cycle later $\omega t = \pi$, we have



since the charge density is $\propto |\psi|^2$, the charge density is oscillating along the z-axis and the atom is behaving like a small broadcast antenna, radiating EM waves.

A deeper question is why an atom in only $|2p_z\rangle$ will decay to $|1s\rangle$ by radiating, as there no superposition here at $t=0$, and thus no radiation in this picture.

Understanding "Spontaneous Emission" requires quantization of the electromagnetic field.

a) $\hat{H} = -\vec{\mu} \cdot \vec{B}$

$$\boxed{\hat{H} = -\gamma B_0 \hat{I}_z}$$

b) $E_\uparrow = \langle \uparrow | \hat{H} | \uparrow \rangle = -\frac{\gamma B_0 \hbar}{2}$

$E_\downarrow = \langle \downarrow | \hat{H} | \downarrow \rangle = +\frac{\gamma B_0 \hbar}{2}$

$\boxed{\Delta E = \hbar \gamma B_0}$ $\boxed{\omega \equiv \gamma B_0}$

$$\boxed{|\Psi(t)\rangle = \frac{1}{\sqrt{2}} |\uparrow\rangle + \frac{1}{\sqrt{2}} e^{-i\Delta E t/\hbar} |\downarrow\rangle}$$

Note, we do not need to keep track of any overall phase factor b/c it has no impact on observables.

c) Easiest to work w/ Pauli matrices

$$I_x = \frac{\hbar}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\langle \hat{I}_x \rangle = \frac{\hbar}{2}\left(\frac{1}{\sqrt{2}}, \frac{e^{i\omega t}}{\sqrt{2}}\right) \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{pmatrix} 1/\sqrt{2} \\ e^{-i\omega t}/\sqrt{2} \end{pmatrix}$$

$$= \frac{\hbar}{2}\left(\frac{1}{\sqrt{2}}, \frac{e^{i\omega t}}{\sqrt{2}}\right) \begin{pmatrix} e^{-i\omega t}/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

$$\langle I_x \rangle = \frac{\hbar}{2}\left(\frac{e^{-i\omega t}}{2} + \frac{e^{i\omega t}}{2} \right)$$

$$= \frac{\hbar}{2} \cos(\omega t)$$

$$\langle \hat{I}_y \rangle = \frac{\hbar}{2}\left(\frac{1}{\sqrt{2}}, \frac{e^{i\omega t}}{\sqrt{2}} \right) \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{pmatrix} 1/\sqrt{2} \\ e^{-i\omega t}/\sqrt{2} \end{pmatrix}$$

$$= \frac{\hbar}{2}\left(\frac{1}{\sqrt{2}}, \frac{e^{i\omega t}}{\sqrt{2}} \right) \begin{bmatrix} -i\frac{e^{-i\omega t}}{\sqrt{2}} \\ i/\sqrt{2} \end{bmatrix}$$

$$= -\frac{\hbar}{2} \; \frac{e^{i\omega t} - e^{-i\omega t}}{2i}$$

$$\boxed{\langle \hat{I}_y \rangle = -\frac{\hbar}{2} \sin(\omega t)}$$

$$\langle I_z \rangle = \frac{\hbar}{2}\left(\frac{1}{\sqrt{2}}, \frac{e^{i\omega t}}{\sqrt{2}} \right) \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{pmatrix} 1/\sqrt{2} \\ \frac{e^{-i\omega t}}{\sqrt{2}} \end{pmatrix}$$

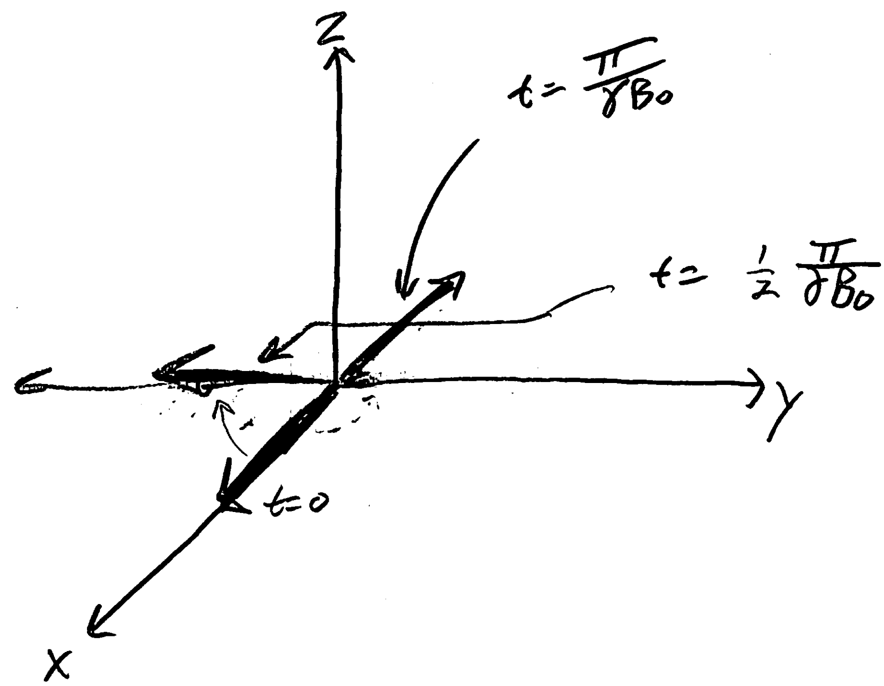
$$= \frac{\hbar}{2}\left(\frac{1}{2} - \frac{1}{2} \right) = \boxed{0 = \langle I_z \rangle}$$

Spin Precession

$$\omega t = 0 \quad \langle \vec{I} \rangle = \frac{\hbar}{2}\,\hat{e}_x$$

$$\omega t = \frac{\pi}{2} \quad \langle \vec{I} \rangle = \frac{\hbar}{2}\,\hat{e}_y$$

$$\omega t = \pi \quad \langle \vec{I} \rangle = -\frac{\hbar}{2}\,\hat{e}_x$$



spin precesses around magnetic field in x, y plane.

a) Integer Spin $\Rightarrow$ boson

b) $I_{min} = |I_1 - I_2| = |1-1| = 0$

$I_{max} = |I_1 + I_2| = |1+1| = 2$

$I = 2, 1, 0$ are the allowed values.

Degeneracy is $2I+1$, so

$I = 2$ is 5-fold degenerate

$I = 1$ is 3-fold degenerate

$I = 0$ is nondegenerate (1 state)

So there are 9 possible states. Does this make sense? Each individual spin has 3 possible states, and there are 2 spins.

$\boxed{3^2 = 9}$ states.

c)

$I = 2 \Rightarrow m_I = 2, 1, 0, -1, -2$

$I = 1 \Rightarrow m_I = 1, 0, -1$

$I = 0 \Rightarrow m_I = 0$

d)

All even under interchange

$|2\,2\rangle = |1\,1\rangle|1\,1\rangle$

$|2\,1\rangle = \frac{1}{\sqrt{2}}|1\,1\rangle|1\,0\rangle + \frac{1}{\sqrt{2}}|1\,0\rangle|1\,1\rangle$

$I=2$ $|2\,0\rangle = \frac{1}{\sqrt{6}}|1\,1\rangle|1\,{-1}\rangle + \sqrt{\frac{2}{3}}|1\,0\rangle|1\,0\rangle + \frac{1}{\sqrt{6}}|1\,{-1}\rangle|1\,1\rangle$

$|2\,{-1}\rangle = \frac{1}{\sqrt{2}}|1\,0\rangle|1\,{-1}\rangle + \frac{1}{\sqrt{2}}|1\,{-1}\rangle|1\,0\rangle$

$|2\,{-2}\rangle = |1\,{-1}\rangle|1\,{-1}\rangle$

$I=1 \rightarrow$ odd under interchange

$$|1\,1\rangle = \frac{1}{\sqrt{2}}|1\,1\rangle|1\,0\rangle - \frac{1}{\sqrt{2}}|1\,0\rangle|1\,1\rangle$$

$$|1\,0\rangle = \frac{1}{\sqrt{2}}|1\,{-1}\rangle|1\,1\rangle - \frac{1}{\sqrt{2}}|1\,1\rangle|1\,{-1}\rangle$$

$$|1\,{-1}\rangle = \frac{1}{\sqrt{2}}|1\,0\rangle|1\,{-1}\rangle - \frac{1}{\sqrt{2}}|1\,{-1}\rangle|1\,0\rangle$$

$I=0$ symmetric (even) under interchange

$$|0\,0\rangle = \frac{1}{\sqrt{3}}|1\,{+1}\rangle|1\,{-1}\rangle - \frac{1}{\sqrt{3}}|1\,0\rangle|1\,0\rangle + \frac{1}{\sqrt{2}}|1\,{-1}\rangle|1\,1\rangle$$

e) $I=2$ even
$I=1$ odd
$I=0$ even

f) Must have total wavefcn symmetric under C_2. $\psi_{\substack{nuc\\vib.}}\,\psi_{el}$ is <u>even</u>

must have
$$\psi^{(rot)}\,\psi^{(nuc.\ spin)} = \text{even}$$

$\Rightarrow$ even J must have $I=0$ or $I=2$

odd J must have $I=1$

g) Total degeneracy is a combination of m_J degeneracy and I, m_I degeneracy.

For even J, have $2J+1$ m_J states and each of these has $\underbrace{2\cdot 2+1}_{I=2} + \underbrace{2\cdot 0+1}_{I=0} = 6$

Nuclear spin states. So for even J, have

$$6(2J+1) \quad \text{even } J$$

For odd J, have only $I=1$, w 3 states, so degeneracy is

$$3(2J+1) \quad \text{odd } J.$$

h) since $e^{-\Delta E/k_BT} \to 1$, it is the ratio of the degeneracies that matters.

$$J=0 \Rightarrow 6\cdot(2\cdot 0+1) = 6 \text{ states}$$

$$J=1 \Rightarrow 3\cdot(2\cdot 1+1) = 9 \text{ states}$$

$$P(J=1) = \frac{9}{6+9} = \frac{9}{15} = \frac{3}{5} = 60\%$$

$$P(J=0) = \frac{6}{6+9} = \frac{6}{15} = \frac{2}{5} = 40\%$$

$\Rightarrow$ only 50% more likely.

Pauli Exclusion Principle

For part b), see MATLAB

a) show that wavefunction satisfies the TISE

set $L=1$

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx_1^2} - \frac{\hbar^2}{2m}\frac{d^2}{dx_2^2} + V(x_1, x_2)$$

$$V(x_1, x_2) = \begin{cases} 0, & 0<x_1<1 \text{ and } 0<x_2<1 \\ \infty, & \text{otherwise} \end{cases}$$

$$\psi_e = \left[\phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1)\right]\alpha(1)\alpha(2)$$

ϕ_1 and ϕ_2 are separately eigenstates of the Hamiltonian

$\hat{H}\phi_1 = E_1\phi_1$

e.g.

$$\frac{-\hbar^2}{2m}\frac{d^2}{dx_1^2}\phi_1 = \sqrt{2}\left(\frac{+\hbar^2}{2m}\right)\sin(\pi x_1)\pi^2 \qquad \frac{-\hbar^2}{2m}\frac{d^2}{dx_2^2}\phi_1(x_1) = 0$$

$$= \frac{\hbar^2\pi^2\overbrace{(1)^2}^{n^2}}{2m\underbrace{(1)^2}_{L^2}} = E_1\phi_1(x_1)$$

Write $\hat{H} = \hat{h}(x_1) + \hat{h}(x_2)$ $\quad \hat{h}(x_1) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2}$

$$\hat{h}(x_2) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2}$$

$\hat{h}(x_1)\phi_1(x_1) = E_1\phi_1(x_1)$ $\qquad \hat{h}(x_2)\phi_2(x_2) = E_2\phi_2(x_2)$

$\hat{h}(x_1)\phi_1(x_2) = 0$

$\hat{h}(x_2)\phi_1(x_2) = E_2\phi_2(x_2)$ $\qquad$ etc...

$$\hat{H} = \hat{h}(x_1) + \hat{h}(x_2)$$

$$\hat{H}\psi_e = \left(\hat{h}(x_1) + \hat{h}_2(x_2)\right)\left(\phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1)\right)$$

$$= E_1\phi_1(x_1)\phi_2(x_2) - E_2\phi_1(x_2)\phi_2(x_1)$$

$$+ E_2\phi_1(x_1)\phi_2(x_2) - E_1\phi_1(x_2)\phi_2(x_1)$$

$$= (E_1 + E_2)\left(\phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1)\right)$$

$$= (E_1 + E_2)\psi_e$$

Contents


```
%PauliExclusion.m
%
%This script makes plots of an excited configuration of the two electron in
%a box problem. Illustrates the Pauli Exclusion principle.
%
%Tom Allison 11/10/2013
```

Part a)

See pdf scan

Part b)

```
x1 = linspace(0,1);
x2 = linspace(0,1);

[X1,X2] = meshgrid(x1,x2);

PSI = 2*(sin(pi*X1).*sin(2*pi*X2) - sin(pi*X2).*sin(2*pi*X1));

figure(1)
surf(X1,X2,PSI.^2);
xlabel('x_1/L');
ylabel('x_2/L');
view([0 0 1]);
setfigfont(1,14);
```

Interpretation

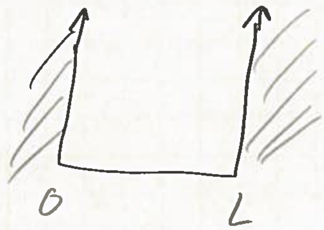
The wavefunction has a node when x1 = x2 because the two particles have the same spin. When they have the same spin, the Pauli exclusion principle prevents them from being at the same place. This problem shows that the antisymeterization requirement takes care of the particles not being at the same place with the same spin because the probability of that happening is Psi(x,x) with x1 = x2, and this is identicaly zero.

Published with MATLAB® R2012b

Particle w/ Speed Bump

a)

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} +$$



$$\hat{H}' =$$

$$\psi_n^{(0)} = \begin{cases} \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) & 0<x<L \\ 0 & \text{otherwise} \end{cases} \qquad n=1,2,\ldots$$

$$E_1^{(1)} = \langle \psi_1^{(0)} | \hat{H}' | \psi_1^{(0)} \rangle$$

$$= \int_{\frac{3}{8}L}^{\frac{5}{8}L} dx \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right) V_0 \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)$$

$$= \frac{2V_0}{L}\int_{3/8L}^{5/8L} dx \sin^2\left(\frac{\pi x}{L}\right) = \frac{2V_0}{L}\int_{3/8L}^{5/8L} dx \left(\frac{1-\cos(2\pi x/L)}{2}\right)$$

$$= \frac{V_0}{L}\int_{3/8L}^{5/8L} dx - \frac{V_0}{L}\int_{3/8L}^{5/8L} dx \cos\left(\frac{2\pi x}{L}\right)$$

$$= \frac{V_0}{4} - \frac{V_0}{L}\frac{L}{2\pi}\left[\sin\left(\frac{2\pi x}{L}\right)\right]_{3/8L}^{5/8L}$$

$$= \frac{V_0}{4} - \frac{V_0}{2\pi}\left[\underbrace{\sin\left(\frac{5\pi}{4}\right)}_{-\frac{\sqrt{2}}{2}} - \underbrace{\sin\left(\frac{3\pi}{4}\right)}_{\frac{\sqrt{2}}{2}}\right] \qquad (1)$$

$$E_1^{(1)} = \frac{V_0}{4} - \frac{V_0}{2\pi}\left(-\sqrt{2}\right)$$

$$\boxed{E_1^{(1)} = V_0\left(\frac{1}{4} + \frac{\sqrt{2}}{2\pi}\right)}$$

For $n=2$, everything is the same except $\pi \to 2\pi$ in eqn. 1

$$E_2^{(2)} = \frac{V_0}{4} - \frac{V_0}{2\cdot 2\pi}\left[\underbrace{\sin\left(\frac{10\pi}{4}\right)}_{+1} - \underbrace{\sin\left(\frac{6\pi}{4}\right)}_{-1}\right]$$

$+1 \; - \; -1 \; = 2$

$$\boxed{E_2^{(2)} = \frac{V_0}{4} - \frac{V_0}{2\pi}}$$

b)

$$|\psi_1^{(1)}\rangle = \sum_{m=2}^{\infty} \frac{\langle \psi_m^{(0)} | \hat{H}' | \psi_1^{(0)} \rangle}{E_1^{(0)} - E_m^{(0)}} |\psi_m^{(0)}\rangle$$

$$\psi_1^{(1)}(x) = \sum_{m=2}^{\infty} \frac{V}{(1^2 - m^2)\frac{m^2 h^2}{8mL^2}} \left[\int_{\frac{3}{8}L}^{\frac{5}{8}L} dx \sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{\pi x}{L}\right)\right] \psi_m^{(0)}(x)$$

$$\left[\frac{\sin\left(\frac{\pi x}{L}(m-1)\right)}{\frac{2\pi}{L}(m-1)} - \frac{\sin\left(\frac{\pi x}{L}(m+1)\right)}{\frac{2\pi}{L}(m+1)}\right]_{x=\frac{3}{8}L}^{x=\frac{5}{8}L}$$

Every other term is zero b/c since the perturbation is even around $x = 1/2$, the product $\psi_m^* \psi_1$ needs to be even as well, which means only even m will contribute.

a)

$$\hat{U}' = k\hat{Q}_1\hat{Q}_2^2$$

Use $\hat{a}$ and $\hat{a}^+$

$$\hat{a}_i^+ = \frac{1}{\sqrt{2\mu_i}}\left(\hat{p}_i + i\mu\omega\hat{Q}_i\right)$$

$$\hat{a}_i = \frac{1}{\sqrt{2\mu_i}}\left(\hat{p}_i - i\mu\omega\hat{Q}_i\right)$$

so

$$\hat{Q}_i = \frac{\sqrt{2\mu_i}}{2i\mu\omega}\left(\hat{a}_i^+ - \hat{a}_i\right)$$

so

$$\hat{U}' = k\hat{Q}_1\hat{Q}_2^2 \overset{\text{prop. to}}{\propto} \left(\hat{a}_1^+ - \hat{a}_1\right)\left(\hat{a}_2^+ - \hat{a}_2\right)^2$$

$$= (a_1^+ - a_1)\left(\hat{a}_2^+\hat{a}_2^+ - \hat{a}_2^+\hat{a}_2 - \hat{a}_2\hat{a}_2^+ + \hat{a}_2\hat{a}_2\right)$$

so this part says

$\Delta V_1 = \pm 1$

b/c $a_1^+|V_1, V_2, \ldots\rangle$

$\propto |V_1+1, V_2, \ldots\rangle$

and $a_1|V_1, V_2, \ldots\rangle$

$\propto |V_1-1, \ldots\rangle$

And this part says

$\Delta V_2 = +2, 0, 0, \text{ or } -2$

by similar arguments

selection rules

b) The influence of the anharmonic coupling is by far the largest on the states that are closest in energy because of the energy denominators that appear in perturbation theory

$$|\psi_n^{(1)}\rangle = \sum_m \frac{\langle \psi_m^{(0)} | \hat{U} | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} |\psi_m^{(0)}\rangle$$

When $E_n - E_m$ is close to zero, this term dominates the sum, so we don't need to consider other terms.

c) The thing to do is diagonalize the Hamiltonian in the (nearly) degenerate subspace

$$\hat{H} = \hat{H}_0 + \hat{U}'$$

$$\langle 100 | \hat{H} | 100 \rangle = E_{100}^{(0)} \qquad b/c \quad \langle 100 | \hat{U}' | 100 \rangle$$

$$\langle 020 | \hat{H} | 020 \rangle = E_{020}^{(0)}$$

$$\langle 100 | \hat{H}_0 | 020 \rangle = \langle 020 | \hat{H}_0 | 100 \rangle = 0$$

$$V \equiv \langle 100 | \hat{U}' | 020 \rangle$$

So in the nearly degenerate subspace

$$\mathbf{H} = \begin{bmatrix} E_{100}^{(0)} & V \\ V & E_{020}^{(0)} \end{bmatrix}$$

Finding the new energy eigenvalues

$$\det(H - EI) = \begin{vmatrix} E_{100}^{(0)} - E & V \\ V & E_{020}^{(0)} - E \end{vmatrix} = 0$$

$$(E_{100}^{(0)} - E)(E_{020}^{(0)} - E) - V^2 = 0$$

Now write

$$E_{100}^{(0)} = \bar{E}_0 + \Delta \qquad \bar{E} = \frac{E_{100}^{(0)} + E_{020}^{(0)}}{2}$$

$$E_{020}^{(0)} = \bar{E}_0 - \Delta \qquad \Delta = \frac{E_{100}^{(2)} - E_{020}^{(2)}}{2}$$

$$(\bar{E}_0 + \Delta - E)(\bar{E}_0 - \Delta - E) - V^2 = 0$$

$$(E_0^2 - \Delta^2) - E(\bar{E}_0 - \cancel{\Delta}) - E(\bar{E}_0 + \cancel{\Delta}) + E^2 - V^2 = 0$$

$$\bar{E}_0^2 - \Delta^2 - V^2 - 2E\bar{E}_0 + E^2 = 0$$

$$E^2 - 2E\bar{E}_0 - (\Delta^2 + V^2) + \bar{E}_0^2 = 0$$

$$E = +\frac{2\bar{E}_0}{2} \pm \frac{\sqrt{\cancel{4\bar{E}_0^2} - 4(1)(\cancel{\bar{E}_0^2} - \Delta^2 - V^2)}}{2}$$

$$\boxed{E_{\pm} = \bar{E}_0 \pm [\Delta^2 + V^2]^{1/2}}$$

So for E_+, $E_{100} - E_+ = \cancel{E_0} + \Delta - (\cancel{E_0} + (\Delta^2 + V^2)^{1/2})$

$$= \Delta - (\Delta^2 + V^2)^{1/2}$$

$$E_{020} - E_+ = \cancel{E_0} - \Delta - (\cancel{E_0} + (\Delta^2 + V^2)^{1/2})$$

$$= -\Delta - (\Delta^2 + V^2)^{1/2}$$

$$\begin{bmatrix} \Delta - (V^2+\Delta^2)^{1/2} & V \\ V & -\Delta - (\Delta^2+V^2)^{1/2} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = 0$$

$c_1(\Delta - (V^2+\Delta^2)^{1/2}) + c_2 V = 0$ for E_+

$$\boxed{\frac{c_1}{c_2} = \frac{V}{(V^2+\Delta^2)^{1/2} - \Delta}}$$

Now if we take $c_1 = -\sin\theta$ $c_2 = \cos\theta$, then we get

$$\tan\theta = \frac{V}{(V^2+\Delta^2)^{1/2} - \Delta}$$

Using the trig identity $\tan^2(2\theta) = \dfrac{2\tan\theta}{1-\tan^2\theta}$, this can be rearranged to

$$\boxed{\tan(2\theta) = \frac{V}{\Delta}}$$ and $E_+ \rightarrow |\beta\rangle$

$E_- \rightarrow |\alpha\rangle$

See Nesbitt Paper for d)

TOPS 35500

a)

$$\psi = e^{-\alpha x^2}$$

Using the integral tables in the back of Levine

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} dx\, e^{-2\alpha x^2}$$

$u = \sqrt{2\alpha}\, x$

$du = \sqrt{2\alpha}\, dx$

$$= \frac{1}{\sqrt{2\alpha}} \underbrace{\int_{-\infty}^{\infty} du\, e^{-u^2}}_{\sqrt{\pi}}$$

$$\boxed{\langle\psi|\psi\rangle = \frac{\sqrt{\pi}}{\sqrt{2\alpha}}} \qquad (1)$$

$$\langle\psi|\hat{H}|\psi\rangle = \frac{-\hbar^2}{2m}\int_{-\infty}^{\infty} dx\, \psi \frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 \int_{-\infty}^{\infty} dx\, \psi x^2 \psi$$

$$\frac{d^2\psi}{dx^2} = \frac{d}{dx}\left(-2\alpha x\, e^{-\alpha x^2}\right)$$

$$= -2\alpha\left(e^{-\alpha x^2} + (-2\alpha x)x\, e^{-\alpha x^2}\right)$$

$$= -2\alpha\, e^{-\alpha x^2}\left(1 - 2\alpha x^2 e^{-\alpha x^2}\right)$$

So

$$\langle\psi|\hat{H}|\psi\rangle = \frac{2\hbar^2\alpha}{2m}\int_{-\infty}^{\infty} dx\, e^{-2\alpha x^2}$$

$$+ \left(\frac{1}{2}m\omega^2 - \frac{2\hbar^2\alpha^2}{m}\right)\int_{-\infty}^{\infty} dx\, x^2 e^{-2\alpha x^2}$$

Integral Table

$$= \frac{\hbar^2\alpha}{m}\sqrt{\frac{\pi}{2\alpha}} + \left(\frac{1}{2}m\omega^2 - \frac{2\hbar^2\alpha^2}{m}\right)\cancel{2}\left(\frac{2!}{2^3\, 1!}\right)\left(\frac{\pi}{(2\alpha)^3}\right)^{1/2}$$

$$\frac{\hbar^2}{m}\sqrt{\frac{\pi}{2}}\,\alpha^{+1/2} + \left(\frac{1}{2}m\omega^2 - \frac{2\hbar^2}{m}\alpha^2\right)\left(\frac{\pi^{1/2}}{2^{5/2}}\right)\alpha^{-3/2}$$

$$\left(\frac{\hbar^2}{m}\sqrt{\frac{\pi}{2}} - \frac{\hbar^2}{m}\frac{\pi^{1/2}}{2^{3/2}}\right)\alpha^{+1/2} + \frac{1}{2}m\omega^2\frac{\pi^{1/2}}{2^{5/2}}\alpha^{-3/2}$$

$$\boxed{\frac{\hbar^2}{2m}\sqrt{\frac{\pi}{2}}\,\alpha^{1/2} + m\omega^2\frac{\pi^{1/2}}{2^{7/2}}\alpha^{-3/2}} \qquad (2)$$

So

$$\frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\frac{\hbar^2}{2m}\cancel{\sqrt{\frac{\pi}{2}}}\,\alpha^{\cancel{1/2}\;1} + m\omega^2\frac{\cancel{\sqrt{\pi}}}{2^{\cancel{7/2}\;3}}\alpha^{\cancel{-3/2}\;-1}}{\cancel{\sqrt{\frac{\pi}{2}}}\,\cancel{\alpha^{-1/2}}}$$

$$\boxed{\frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\hbar^2}{2m}\alpha + \frac{m\omega^2}{8}\alpha^{-1}} \qquad (3)$$

So now we minimize this w/ respect to α by setting the derivative of eqn (3) to zero

$$\frac{\partial}{\partial\alpha}(3) \to 0 \Rightarrow \frac{\hbar^2}{2m} - \frac{m\omega^2}{8}\alpha^{-2} = 0$$

$$\alpha^{-2} = \frac{8\hbar^2}{2m^2\omega^2} = \frac{4\hbar^2}{m^2\omega^2} \qquad (4)$$

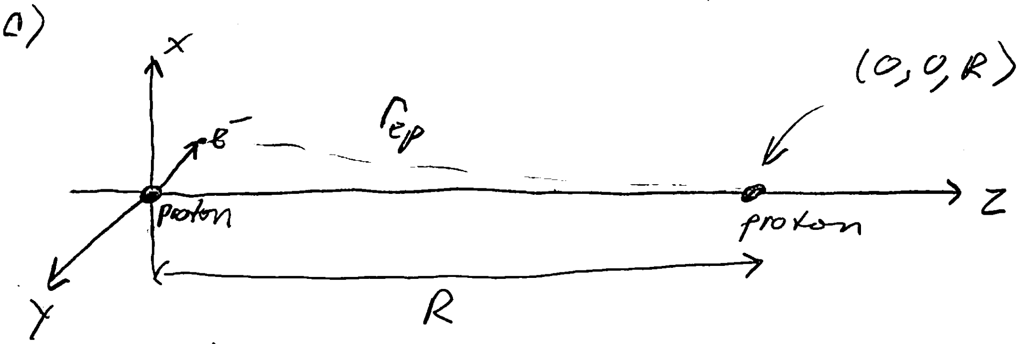
$$\Rightarrow \boxed{\alpha = \frac{m\omega}{2\hbar}}$$

The (−) solution to the quadratic eqn (4) is nonsense because then ψ would not be normalizable

This is the exact result because the basis function chosen is of the same functional form as the harmonic oscillator ground state. Usually we are not so lucky.

b) SEE MATLAB CODE

a)



Neglecting Nuclear kinetic energy

$$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}}_{\text{Hydrogen atom}} + \frac{1}{4\pi\varepsilon_0}\frac{e^2}{R} - \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r_{ep}}$$

$$= \vec{H}_0 + \underbrace{\frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{R} - \frac{1}{r_{ep}}\right)}_{\hat{V}}$$

$$\vec{r}_{ep} = x\hat{e}_x + y\hat{e}_y + (R-z)\hat{e}_z$$

$$|\vec{r}_{ep}|^2 = x^2 + y^2 + (R-z)^2$$

$$= x^2+y^2+z^2 + R^2 - 2Rz$$

keeping only terms to first order in z, x, y and lower

$$|\vec{r}_{ep}| \simeq \sqrt{R^2 - 2Rz} \simeq R\left(1 - 2\frac{z}{R}\right)^{1/2}$$

$$\simeq R\left(1 - \frac{z}{R}\right)$$

$$\frac{1}{|\vec{r}_{ep}|} \simeq \frac{1}{R(1 - z/R)} = \left(\frac{1}{R}\right)\left(1 + \frac{z}{R} + \dots\right)$$

to first order

$$\Rightarrow \hat{H}' = \frac{e^2}{4\pi\varepsilon_0}\left(\frac{1}{R} - \frac{1}{R}\left(1 + \frac{z}{R}\right)\right)$$

$$\boxed{\hat{H}' = \frac{e^2}{4\pi\varepsilon_0}\left(\frac{-z}{R^2}\right)}$$

b) Taking $\psi^{(0)}$ = ground state of H-atom $= \psi_{1s}$

$$E^{(1)} = \langle \psi_{1s} | \frac{e^2}{4\pi\varepsilon_0} \frac{-z}{R^2} | \psi_{1s} \rangle$$

$$= \frac{-e^2}{4\pi\varepsilon_0 R^2} \cancel{\langle \psi^{(0)} | z | \psi^{(0)} \rangle} \rightarrow 0 \text{ by symmetry}$$

So we have to go to second order

$$E_1^{(2)} = \sum_{m \neq n} \frac{|\langle \psi_m | \hat{H}' | \psi_n \rangle|^2}{E_1 - E_m}$$

$$= \left(\frac{-e^2}{4\pi\varepsilon_0 R^2}\right)^2 \sum_{m \neq 1} \frac{|\langle \psi_m | z | \psi_1 \rangle|^2}{E_1 - E_m}$$

Now since E_1 is the ground state, all $E_{m\neq 1}$ are higher in energy and thus all terms in the sum are negative and we have

$$\boxed{E^{(2)} = \frac{-C}{R^4}} \quad \text{with} \quad \boxed{C = \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \sum_{m \neq 1} \frac{|\langle \psi_m | z | \psi_1 \rangle|^2}{|E_1 - E_m|}}$$

c) With $E_1 - E_m \approx E_1$ the sum can be evaluated with a trick. Expanding...

$$C = \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{1}{|E_1|} \sum_{m\neq 1} \langle\psi_1|z|\psi_m\rangle\langle\psi_m|z|\psi_1\rangle$$

Since $\langle\psi_1|z|\psi_1\rangle = 0$, might as well include $m=1$, in the sum, then you have the identity operator to work with! Viz.

$$\sum_{m=1,2,\ldots} \langle\psi_1|\hat{z}|\psi_m\rangle\langle\psi_m|\hat{z}|\psi_1\rangle$$

$$= \langle\psi_1|\hat{z}\left(\sum_m |\psi_m\rangle\langle\psi_m|\right)\hat{z}|\psi_1\rangle$$

$$= \langle\psi_1|\hat{z}^2|\psi_1\rangle$$

Now we just have one integral to do.

$$\psi_1 = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$$

$$z = r\cos\theta \Rightarrow \langle z^2\rangle = \int_0^\pi d\theta \int_0^{2\pi} d\phi \int_0^\infty dr\, r^2\sin\theta\, r^2\cos^2\theta\, \frac{e^{-2r/a_0}}{\pi a_0^3}$$

$$= \frac{2\cancel{\pi}}{\cancel{\pi} a_0^3} \underbrace{\int_0^\pi d\theta \sin\theta\cos^2\theta}_{I_1} \underbrace{\int_0^\infty dr\, r^4 e^{-2r/a_0}}_{I_2}$$

$$I_1 = -\int_1^{-1} du\, u^2 \qquad \begin{aligned} u &= \cos\theta \\ du &= -\sin\theta\, d\theta \end{aligned}$$

$$= \int_{-1}^{1} du\, u^2 = \left.\frac{u^3}{3}\right|_{-1}^{1} = \frac{2}{3}$$

$$I_2 = \int_0^\infty \frac{a_0}{2} dz \left(\frac{a_0}{2} z\right)^4 e^{-z} \qquad \begin{aligned} z &= 2r/a_0 \\ dz &= \frac{2}{a_0} dr \end{aligned}$$

$$= \left(\frac{a_0}{2}\right)^5 \underbrace{\int_0^\infty dz\, z^4 e^{-z}}_{\Gamma(5) = 4! = 24}$$

$$= \frac{24 a_0^5}{32} = \frac{3}{4} a_0^5$$

So

$$\langle z^2 \rangle = \frac{\cancel{2}}{a_0^3} \frac{\cancel{2}}{\cancel{3}} \frac{\cancel{3}}{\cancel{4}} a_0^5$$

$$= a_0^2$$

$$\Rightarrow \boxed{C = \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 a_0^2} = 1 \text{ in atomic units!}$$

Problem 6.36

(a)

$$|1\,0\,0\rangle = \frac{1}{\sqrt{\pi a^3}}e^{-r/a}\ \text{(Eq. 4.80)},\ \ E_s^1 = \langle 1\,0\,0|H'|1\,0\,0\rangle = eE_{\text{ext}}\frac{1}{\pi a^3}\int e^{-2r/a}(r\cos\theta)r^2\sin\theta\,dr\,d\theta\,d\phi.$$

But the θ integral is zero: $\displaystyle\int_0^\pi \cos\theta\sin\theta\,d\theta = \left.\frac{\sin^2\theta}{2}\right|_0^\pi = 0.$ So $E_s^1 = 0.$ QED

(b) From Problem 4.11:
$$\begin{cases} |1\rangle = \psi_{2\,0\,0} = \dfrac{1}{\sqrt{2\pi a}}\dfrac{1}{2a}\left(1-\dfrac{r}{2a}\right)e^{-r/2a} \\ |2\rangle = \psi_{2\,1\,1} = -\dfrac{1}{\sqrt{\pi a}}\dfrac{1}{8a^2}re^{-r/2a}\sin\theta e^{i\phi} \\ |3\rangle = \psi_{2\,1\,0} = \dfrac{1}{\sqrt{2\pi a}}\dfrac{1}{4a^2}re^{-r/2a}\cos\theta \\ |4\rangle = \psi_{2\,1\,-1} = \dfrac{1}{\sqrt{\pi a}}\dfrac{1}{8a^2}re^{-r/2a}\sin\theta e^{-i\phi} \end{cases}$$

$$\left.\begin{aligned} \langle 1|H_s'|1\rangle &= \{\dots\}\int_0^\pi \cos\theta\sin\theta\,d\theta = 0 \\ \langle 2|H_s'|2\rangle &= \{\dots\}\int_0^\pi \sin^2\theta\cos\theta\sin\theta\,d\theta = 0 \\ \langle 3|H_s'|3\rangle &= \{\dots\}\int_0^\pi \cos^2\theta\cos\theta\sin\theta\,d\theta = 0 \\ \langle 4|H_s'|4\rangle &= \{\dots\}\int_0^\pi \sin^2\theta\cos\theta\sin\theta\,d\theta = 0 \\ \langle 1|H_s'|2\rangle &= \{\dots\}\int_0^{2\pi} e^{i\phi}\,d\phi = 0 \\ \langle 1|H_s'|4\rangle &= \{\dots\}\int_0^{2\pi} e^{-i\phi}\,d\phi = 0 \\ \langle 2|H_s'|3\rangle &= \{\dots\}\int_0^{2\pi} e^{-i\phi}\,d\phi = 0 \\ \langle 2|H_s'|4\rangle &= \{\dots\}\int_0^{2\pi} e^{-2i\phi}\,d\phi = 0 \\ \langle 3|H_s'|4\rangle &= \{\dots\}\int_0^{2\pi} e^{-i\phi}\,d\phi = 0 \end{aligned}\right\}$$

All matrix elements of H_s' are zero except $\langle 1|H_s'|3\rangle$ and $\langle 3|H_s'|1\rangle$ (which are complex conjugates, so only one needs to be evaluated).

$$\begin{aligned} \langle 1|H_s'|3\rangle &= eE_{\text{ext}}\frac{1}{\sqrt{2\pi a}}\frac{1}{2a}\frac{1}{\sqrt{2\pi a}}\frac{1}{4a^2}\int\left(1-\frac{r}{2a}\right)e^{-r/2a}re^{-r/2a}\cos\theta(r\cos\theta)r^2\sin\theta\,dr\,d\theta\,d\phi \\ &= \frac{eE_{\text{ext}}}{2\pi a 8a^3}(2\pi)\left[\int_0^\pi\cos^2\theta\sin\theta\,d\theta\right]\int_0^\infty\left(1-\frac{r}{2a}\right)e^{-r/a}r^4\,dr \\ &= \frac{eE_{\text{ext}}}{8a^4}\frac{2}{3}\left\{\int_0^\infty r^4e^{-r/a}\,dr - \frac{1}{2a}\int_0^\infty r^5e^{-r/a}\,dr\right\} = \frac{eE_{\text{ext}}}{12a^4}\left(4!a^5 - \frac{1}{2a}5!a^6\right) \\ &= \frac{eE_{\text{ext}}}{12a^4}24a^5\left(1-\frac{5}{2}\right) = eaE_{\text{ext}}(-3) = -3aeE_{\text{ext}}. \end{aligned}$$

$$\mathsf{W} = -3aeE_{\text{ext}}\begin{pmatrix} 0&0&1&0 \\ 0&0&0&0 \\ 1&0&0&0 \\ 0&0&0&0 \end{pmatrix}.$$

We need the eigenvalues of this matrix. The characteristic equation is:

$$\begin{vmatrix} -\lambda & 0 & 1 & 0 \\ 0 & -\lambda & 0 & 0 \\ 1 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & -\lambda \end{vmatrix} = -\lambda \begin{vmatrix} -\lambda & 0 & 0 \\ 0 & -\lambda & 0 \\ 0 & 0 & -\lambda \end{vmatrix} + \begin{vmatrix} 0 & -\lambda & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -\lambda \end{vmatrix} = -\lambda(-\lambda)^3 + (-\lambda^2) = \lambda^2(\lambda^2-1) = 0.$$

The eigenvalues are 0, 0, 1, and -1, so the perturbed energies are

$$\boxed{E_2,\ E_2,\ E_2 + 3aeE_{\text{ext}},\ E_2 - 3aeE_{\text{ext}}.\quad \text{Three levels.}}$$

(c) The eigenvectors with eigenvalue 0 are $|2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$ and $|4\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$; the eigenvectors with eigenvalues ± 1 are $|\pm\rangle \equiv \dfrac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ \pm 1 \\ 0 \end{pmatrix}$. So the "good" states are $\boxed{\psi_{2\,1\,1},\ \psi_{2\,1\,-1},\ \frac{1}{\sqrt{2}}(\psi_{2\,0\,0} + \psi_{2\,1\,0}),\ \frac{1}{\sqrt{2}}(\psi_{2\,0\,0} - \psi_{2\,1\,0}).}$

$$\langle \mathbf{p}_e \rangle_4 = -e \frac{1}{\pi a} \frac{1}{64 a^4} \int r^2 e^{-r/a} \sin^2\theta \left[r\sin\theta\cos\phi\,\hat{i} + r\sin\theta\sin\phi\,\hat{j} + r\cos\theta\,\hat{k} \right] r^2 \sin\theta\, dr\, d\theta\, d\phi.$$

But $\displaystyle\int_0^{2\pi} \cos\phi\, d\phi = \int_0^{2\pi} \sin\phi\, d\phi = 0, \quad \int_0^{\pi} \sin^3\theta\cos\theta\, d\theta = \left.\frac{\sin^4\theta}{4}\right|_0^{\pi} = 0,$ so

$$\boxed{\langle \mathbf{p}_e \rangle_4 = 0. \quad \text{Likewise} \quad \langle \mathbf{p}_e \rangle_2 = 0.}$$

$$\begin{aligned} \langle \mathbf{p}_e \rangle_\pm &= -\frac{1}{2} e \int (\psi_1 \pm \psi_3)^2 (\mathbf{r}) r^2 \sin\theta\, dr\, d\theta\, d\phi \\ &= -\frac{1}{2} e \frac{1}{2\pi a} \frac{1}{4a^2} \int \left[\left(1 - \frac{r}{2a}\right) \pm \frac{r}{2a}\cos\theta \right]^2 e^{-r/a} r (\sin\theta\cos\phi\,\hat{i} + \sin\theta\sin\phi\,\hat{j} + \cos\theta\,\hat{k}) r^2 \sin\theta\, dr\, d\theta\, d\phi \\ &= -\frac{e}{2} \frac{\hat{k}}{2\pi a} \frac{1}{4a^2} 2\pi \int \left[\left(1 - \frac{r}{2a}\right) \pm \frac{r}{2a}\cos\theta \right]^2 r^3 e^{-r/a} \cos\theta\sin\theta\, dr\, d\theta. \end{aligned}$$

But $\int_0^\pi \cos\theta\sin\theta\, d\theta = \int_0^\pi \cos^3\theta\sin\theta\, d\theta = 0$, so only the cross-term survives:

$$\begin{aligned} \langle \mathbf{p}_e \rangle_\pm &= -\frac{e}{8a^3} \hat{k} \left(\pm \frac{1}{a}\right) \int \left(1 - \frac{r}{2a}\right) r\cos\theta\, r^3 e^{-r/a} \cos\theta\sin\theta\, dr\, d\theta \\ &= \mp \left(\frac{e}{8a^4}\hat{k}\right) \left[\int_0^\pi \cos^2\theta\sin\theta\, d\theta\right] \int_0^\infty \left(1 - \frac{r}{2a}\right) r^4 e^{-r/a} dr = \mp \left(\frac{e}{8a^4}\hat{k}\right) \frac{2}{3} \left[4! a^5 - \frac{1}{2a} 5! a^6\right] \\ &= \mp e\hat{k} \left(\frac{1}{12a^4}\right) 24 a^5 \left(1 - \frac{5}{2}\right) = \boxed{\pm 3ae\hat{k}.} \end{aligned}$$

Problem 6.37

(a) The nine states are:

Version 2

PHY 308 Midterm 1, Spring 2017

Stony Brook University
Instructor: Prof. Thomas K. Allison

100 points total. The following information may or may not be useful

Planck's constant: $\hbar = 1.055 \times 10^{-34}$ J-s $= 6.582 \times 10^{-16}$ eV-s
Speed of light: $c = 3 \times 10^{8}$ m/s
Mass of the electron: $m_e = 9.1 \times 10^{-31}$ kg
The electron volt: 1 eV $= 1.6 \times 10^{-19}$ J
$\hbar^2/2m_e = 3.81$ eV-Å^2.

1 True/False (18 points)

Circle **T** if the statement is always true. Otherwise circle **F** for false. 2 points each

T F The state function of a quantum system is always equal to a function of time multiplied by a function of the coordinates.

T F Every linear combination of eigenfunctions of the Hamiltonian is an eigenfunction of the Hamiltonian.

T F The probability density is independent of time for a stationary state.

T F Eigenkets of a Hermitian operator with different eigenvalues are always orthogonal.

T F If the Hermitian operator $\hat{B}$ corresponds to a physical property of the quantum-mechanical system, the state function $|\Psi\rangle$ must be an eigenfunction of $\hat{B}$.

T F All eigenfunctions of Hermitian operators must be real functions.

T F When the state function $|\Psi\rangle$ is an eigenket of the Hermitian operator $\hat{B}$ with eigenvalue b, we are certain to measure b when the observable corresponding to $\hat{B}$ is measured.

T F The magnitude of the absorption coefficient for microwave radiation by a gas of NO molecules will be similar to that of a gas of O_2 molecules because their moments of inertia are similar.

T F The energy difference between the $n = 1$ and $n = 0$ states of the harmonic oscillator is the same as the energy difference between the $n = 2$ and $n = 1$ states of the harmonic oscillator.

2 Multiple Choice (18 points)

Circle **one** answer for each question. 3 points each.

Consider a particle moving in 1 dimension ~~at~~ described by the wave function $\Psi(x, t_0) = A(x)e^{ikx}$, with A(x) real. The probability current evaluated at t_0 is

at $t = t_0$

a) 0 everywhere.
b) $[\hbar k/m]|\Psi(x, t_0)|^2$
c) $[\hbar k/(2m)]|\Psi(x, t_0)|^2$
d) $-[\hbar k/m]|\Psi(x, t_0)|^2$
e) none of the above.

Consider a quantum bouncing ball, moving in one dimension with the potential $V(y) = mgy$ for $y > 0$ and $V(y) = \infty$ for $y \leq 0$. The boundary conditions on the stationary states $\psi_n(y)$ are

a) $\psi_n(y \leq 0) = 0$, $\psi_n(y = \infty) = 0$
b) $\psi_n(y \leq 0) = 0$, $\psi_n(y = \infty) = 0$, and $\frac{d\psi_n}{dy}$ continuous at $x = 0$
c) $\psi_n(y \leq 0) = 0$, $\psi_n(y = \infty) = 0$, $\frac{d\psi_n}{dy}$ continuous at $x = 0$, and ψ_n must be either an even or odd function of y
d) $\psi_n(y \leq 0) = 0$, $\psi_n(y = \infty) = 0$, and all derivatives of ψ_n continuous at $x = 0$

The simple harmonic oscillator potential, $V(x) = \frac{1}{2}m\omega^2x^2$, has which of the following properties:

a) The energy levels are evenly spaced and given by $(n + 1/2)\hbar\omega$, with $n = 0, 1, 2, ...$
b) With x the displacement from equilibrium, it is the lowest-order approximation to the potential energy of the nuclei in a diatomic molecule near equilibrium, with m the reduced mass
c) The number of nodes in the n^{th} energy eigenstate wavefunction, with corresponding energy $(n + 1/2)\hbar\omega$, is n.
d) all of the above.
e) a) and c) only.

For a particle moving in 1 dimension with Hamiltonian $\hat{H}(\hat{x}, \hat{p})$, the stationary states are:

a) Solutions to the time-independent Schrödinger equation, $\hat{H}\psi = E\psi$.
b) States with $\langle \hat{p} \rangle = 0$. e^{ikx}
c) Eigenfunctions of the position operator, $\hat{x}$.
d) all of the above
e) a) and c) only.
f) none of the above.

A system is in a quantum state $|\Psi\rangle$ and one makes a measurement of the observable $\hat{O}$. According to quantum theory, the result of the measurement will be

a) the expectation value of $\hat{O}$, given by $\langle\Psi|\hat{O}|\Psi\rangle$.
b) a random value ~~between~~ with probability given by a a normal (Gaussian) ~~probability~~ distribution with mean $\langle\Psi|\hat{O}|\Psi\rangle$ and standard deviation $\sqrt{\langle\Psi|\hat{O}^2|\Psi\rangle - \langle\Psi|\hat{O}|\Psi\rangle^2}$.
c) that the measurement will collapse the wavefunction to one of the stationary states $|\psi_n\rangle$, such that one will measure $\langle\psi_n|\hat{O}|\psi_n\rangle$.
d) one of the eigenvalues λ_n of $\hat{O}$ with probability $|\langle\lambda_n|\Psi\rangle|^2$, where $|\lambda_n\rangle$ are the normalized eigenkets of $\hat{O}$ with eigenvalues λ_n.
e) none of the above.

When an operator $\hat{A}$ commutes with the Hamiltonian $\hat{H}$ of a quantum system, it means that

✓ a) its expectation value $\langle\hat{A}\rangle$ is a constant of the motion.
✓ b) one can construct simultaneous eigenkets of $\hat{A}$ and $\hat{H}$.
c) The set of expectation values of $\hat{A}$ calculated using the stationary states, $\langle\psi_n|\hat{A}|\psi_n\rangle$, are non-degenerate.
d) all of the above.
e) a) and b) only.
f) b) and c) only.

3 The Classical Limit (12 points)

Explain when it is appropriate to use classical mechanics to describe the motion of a particle, and when quantum mechanics must be used. You are encouraged to use a combination of words, equations, and pictures, as appropriate.

The classical limit occurs when $xp \gg \hbar$, such that the uncertainty principle $\sigma_x \sigma_p \geq \hbar/2$ does not present practical limits. One can also think of CM as the $\hbar \to 0$ limit of QM.

For systems in thermal equilibrium, another useful metric is the probability of finding the system in any one quantum state. If $\frac{\Delta E}{kT} \ll 1$, then this probability is small, and one is probably OK w/ CM.

In terms of wave mechanics $xp \gg \hbar$ corresponds to $\frac{x}{\lambda_{DB}} \gg 2$. If a particle is confined to a dimension x, CM is appropriate when x is much larger than the particle's de Broglie wavelength.

4 Resonant Tunneling Diodes (15 points)

Consider an electron with kinetic energy $E = 0.1$ eV incident from the left ($x < 0$) on the potential shown in figure 1.

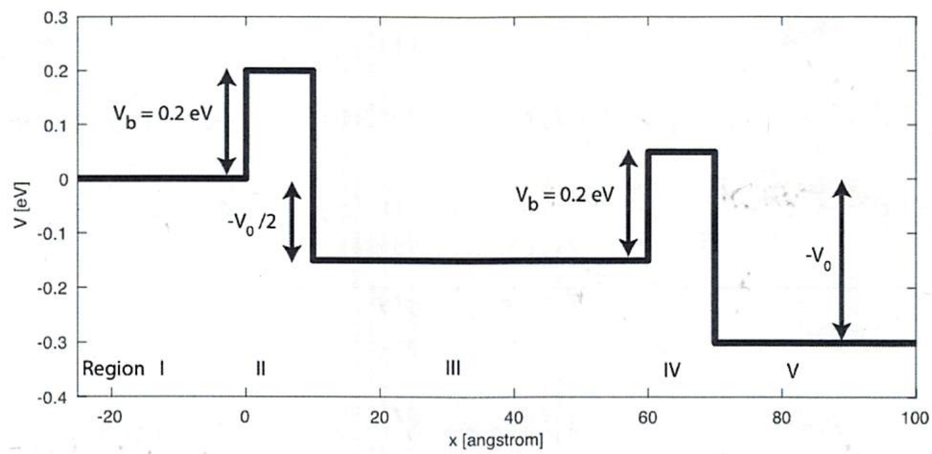


Figure 1: Scattering potential for problem 4. A 0.1 eV electron is incident from the left. The barriers are 0.2 eV high and 10 Å thick. The spacing between the barriers is 50 Å. The wave function has a different form in each labeled region.

a) Write down the general form of the wavefunction in each region of the potential in terms of plane waves or exponential decays. For example, in region I, we have $E > V$, so we can write the wave function as a sum of leftward (incident) and rightward (reflected) going plane waves $\psi(x) = Ae^{ikx} + Be^{-ikx}$, with $k = \sqrt{\frac{2mE}{\hbar^2}}$

b) Apply the boundary conditions at $x = 0$ to your answer to part a) to relate the parameters of the wave function in region I to the parameters of the wave function in region II. Just set up the equations, do not worry about solving them.

c) Why do you get the wrong answer for the transmission coefficient in this problem (and $R + T \neq 1$) if you simply use the square modulus of the amplitude of the wave function in region V to calculate T? How do you properly calculate T

d) As the bias potential is swept from 0 - 2 eV, one observes resonances in the transmission probability (I-V curve) of this device. Why?

e) Can this potential support bound states trapped between the two barriers? Why or why not?

a) I $\psi = Ae^{ik_1x} + Be^{-ik_1x}$ $\qquad k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

II $\psi = Ce^{-K_2x} + De^{+K_2x}$ $\qquad K_2 = \sqrt{\frac{2m(V_b - E)}{\hbar^2}}$

III $\psi = Fe^{ik_3x} + Ge^{-ik_3x}$ $\qquad k_3 = \sqrt{\frac{2m(E + V_0/2)}{\hbar^2}}$

More space for 4

IV $\psi = He^{-K_4 x} + Ie^{+K_4 x}$ $\quad K_4 = \sqrt{\frac{2m(V_6 - \frac{V_0}{2} - E)}{\hbar^2}}$

↑ Note that this still works for $E > V_6 - V_0/2$ b/c K becomes imaginary.

V $\psi = Le^{ik_5 x}$ w/ $K = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

Note that there is no reflected wave

b) $\psi_I(0) = \psi_{II}(0) \Rightarrow$ $A+B = C+D$

$\psi_I'(0) = \psi_{II}'(0) \Rightarrow$ $ik_1 A - ik_1 B = -KC + KD$

c) $T \neq \frac{|L|^2}{|A|^2}$ b/c phase $k_1 \neq k_5$. Phase velocities are different.

Have to use the probability current.

d) One observes resonances when an integer number of waves fit btwn. the barriers

e) No bound states b/c they will escape to $x = \infty$ by tunnelling.

5 Half Harmonic Oscillator (12 points)

Consider a particle of mass m moving in one dimension on the potential of half a harmonic oscillator

$$V(x) = \begin{cases} \infty, & x \leq 0 \\ m\omega^2 x^2/2, & x > 0 \end{cases}$$

What are the stationary states $\chi_n(x)$ in terms of the stationary state solutions of the full harmonic oscillator with the same vibrational frequency ω: $\psi_n(x)$? What is the energy level spacing? Sketch the ground state wave function of the half harmonic oscillator.

The diff. eqn. is the same as the SHO, just different b.c.'s, so the SHO sol^{n}s solve the problem, just that only the odd ones meet the b.c. $\psi_n(0)=0$, $\psi_n(+\infty)=0$

so

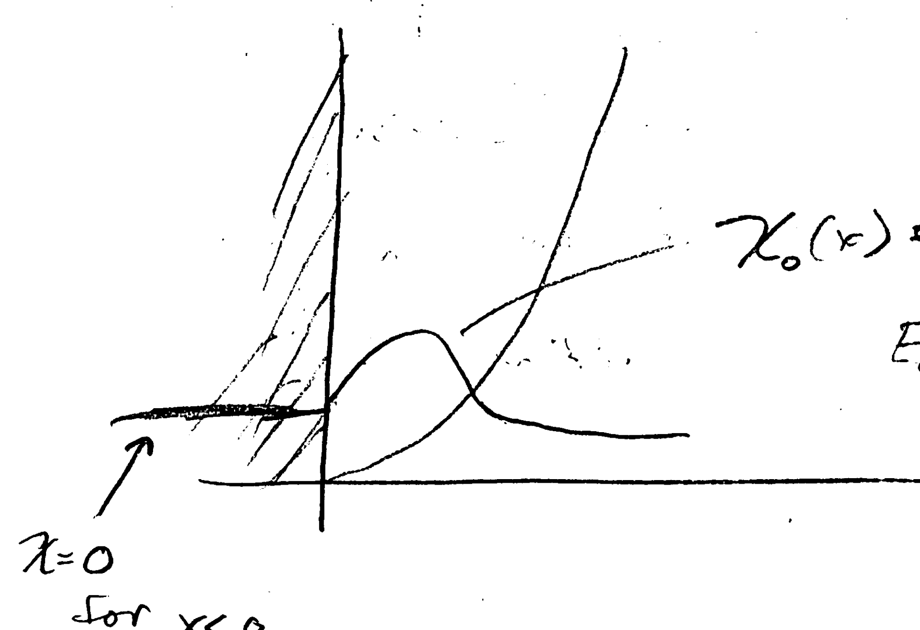
$$\boxed{\chi_m(x) = \begin{cases} \sqrt{2}\,\psi_{2m+1} & x \geq 0 \\ 0 & x < 0 \end{cases}}$$

where ψ_n are the SHO sol^n

$m = 0, 1, 2, \ldots$

$2m+1 = 1, 3, 5 \ldots$

The energy level spacing is now $\boxed{2\hbar\omega}$



$\chi_0(x) \propto x e^{-\frac{m\omega}{2\hbar}x^2}$ for $x > 0$

$E_0 = \frac{3}{2}\hbar\omega$

6 Two-Dimensional Harmonic Oscillator (14 points)

Consider a particle confined to a symmetric two-dimensional harmonic oscillator potential $V(x,y) = \frac{1}{2}m\omega^2(x^2 + y^2)$. The time-independent Schrödinger equation reads

$$\hat{H}\psi(x,y) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,y)}{\partial x^2} + \frac{1}{2}m\omega^2x^2\psi(x,y) - \frac{\hbar^2}{2m}\frac{\partial^2\psi(x,y)}{\partial y^2} + \frac{1}{2}m\omega^2y^2\psi(x,y) = E\psi(x,y) \qquad (6.1)$$

a) Solve the Schrödinger equation and provide formulae for the energy eigenvalues and stationary state wavefunctions. You may express your answers in terms of the solutions to the 1D harmonic oscillator (ψ_n) we have studied in class without re-deriving them.

If you can guess the answers without derivation that is fine, just write.

b) What is the degeneracy of the ground state, the first excited state, and the second excited state?

c) Show that the operator $\hat{L}_z = x\hat{p}_y - y\hat{p}_x$, commutes with the Hamiltonian.

d) Find one simultaneous eigenfunction of $\hat{H}$ and $\hat{L}_z$ and determine its eigenvalues.

Hint: For parts of this problem it may be helpful to use polar coordinates (r, ϕ). In ~~cylindrical~~ polar coordinates

$$\cancel{\nabla^2 f(r,\phi) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 f}{\partial \phi^2}}, \quad \hat{L}_z = -i\hbar\frac{\partial}{\partial \phi}$$

$[\hat{H}_x, \hat{H}_y] = 0 \Rightarrow$ sep. var.

a) TISE $\rightarrow$ $\left(\hat{H}_{SHO,x} + \hat{H}_{SHO,y}\right)\psi_x(x)\psi_y(y) = E\psi_x\psi_y$

$\psi_x(x) = \psi_n(x) \rightarrow$ Normal SHO wavefcns.

$\psi_y(y) = \psi_m(y)$

$$\boxed{\psi_{nm}(x,y) = \psi_n(x)\psi_m(y)}$$

$$E_{nm} = \left(n+m+\frac{1}{2}+\frac{1}{2}\right)\hbar\omega$$

$$\boxed{E_{nm} = (n+m+1)\hbar\omega}$$

b) ground state $E_{00} = \hbar\omega \rightarrow$ only one way (nondegenerate) $\boxed{g_0 = 1}$

First excited state $\underbrace{E_{01} = E_{10}}_{\text{two ways}} = 2\hbar\omega$ $\boxed{g_1 = 2}$

Second excited state

$3\hbar\omega = \underbrace{E_{02} = E_{20} = E_{11}}_{\text{three ways}}$ $\boxed{g_2 = 3}$

c) Using the hint $r^2 = x^2 + y^2$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2$$

Now one can see that $\left[\hat{H}, \frac{\partial}{\partial\phi}\right] = 0$ or $[\hat{H}, \hat{L}_z] = 0$

This makes sense since the potential is cylindrically symmetric!

d) the ground state $\psi_{00} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\frac{m\omega}{2\hbar}(x^2+y^2)}$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\frac{m\omega}{2\hbar}r^2}$$

does <u>not</u> depend on ϕ

so $L_z \psi_{00} = \underset{\substack{\uparrow \\ \text{eigenvalue}}}{0}\,\psi_{00}$ and $\hat{H}\psi_{00} = \hbar\omega\psi_{00}$

so this is a silmutaneous eigenket of $\hat{H}$ and $\hat{L}_z$

For higher n it is more complicated and one must derive the Laguerre Gaussian modes!

Sol$^{\underline{n}}$

PHY 308 Midterm 2, Spring 2017

Stony Brook University

Instructor: Prof. Thomas K. Allison

7 problems and 100 points total. The following information may or may not be useful

Planck's constant: $\hbar = 1.055 \times 10^{-34}$ J-s $= 6.582 \times 10^{-16}$ eV-s
Speed of light: $c = 3 \times 10^8$ m/s
Mass of the electron: $m_e = 9.1 \times 10^{-31}$ kg
The electron volt: 1 eV $= 1.6 \times 10^{-19}$ J
The fine structure constant $\alpha = 1/137$

Table 4.2: The first few spherical harmonics, $Y_l^m(\theta, \phi)$.

$Y_0^0 = \left(\frac{1}{4\pi}\right)^{1/2}$	$Y_2^{\pm 2} = \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta e^{\pm 2i\phi}$
$Y_1^0 = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$	$Y_3^0 = \left(\frac{7}{16\pi}\right)^{1/2} (5\cos^3\theta - 3\cos\theta)$
$Y_1^{\pm 1} = \mp\left(\frac{3}{8\pi}\right)^{1/2} \sin\theta e^{\pm i\phi}$	$Y_3^{\pm 1} = \mp\left(\frac{21}{64\pi}\right)^{1/2} \sin\theta(5\cos^2\theta - 1)e^{\pm i\phi}$
$Y_2^0 = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$	$Y_3^{\pm 2} = \left(\frac{105}{32\pi}\right)^{1/2} \sin^2\theta\cos\theta e^{\pm 2i\phi}$
$Y_2^{\pm 1} = \mp\left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta e^{\pm i\phi}$	$Y_3^{\pm 3} = \mp\left(\frac{35}{64\pi}\right)^{1/2} \sin^3\theta e^{\pm 3i\phi}$

TABLE 4.7: The first few radial wave functions for hydrogen, $R_{nl}(r)$.

$R_{10} = 2a^{-3/2}\exp(-r/a)$
$R_{20} = \frac{1}{\sqrt{2}} a^{-3/2}\left(1 - \frac{1}{2}\frac{r}{a}\right)\exp(-r/2a)$
$R_{21} = \frac{1}{\sqrt{24}} a^{-3/2}\frac{r}{a}\exp(-r/2a)$
$R_{30} = \frac{2}{\sqrt{27}} a^{-3/2}\left(1 - \frac{2}{3}\frac{r}{a} + \frac{2}{27}\left(\frac{r}{a}\right)^2\right)\exp(-r/3a)$
$R_{31} = \frac{8}{27\sqrt{6}} a^{-3/2}\left(1 - \frac{1}{6}\frac{r}{a}\right)\left(\frac{r}{a}\right)\exp(-r/3a)$
$R_{32} = \frac{4}{81\sqrt{30}} a^{-3/2}\left(\frac{r}{a}\right)^2\exp(-r/3a)$
$R_{40} = \frac{1}{4} a^{-3/2}\left(1 - \frac{3}{4}\frac{r}{a} + \frac{1}{8}\left(\frac{r}{a}\right)^2 - \frac{1}{192}\left(\frac{r}{a}\right)^3\right)\exp(-r/4a)$
$R_{41} = \frac{\sqrt{5}}{16\sqrt{3}} a^{-3/2}\left(1 - \frac{1}{4}\frac{r}{a} + \frac{1}{80}\left(\frac{r}{a}\right)^2\right)\frac{r}{a}\exp(-r/4a)$
$R_{42} = \frac{1}{64\sqrt{5}} a^{-3/2}\left(1 - \frac{1}{12}\frac{r}{a}\right)\left(\frac{r}{a}\right)^2\exp(-r/4a)$
$R_{43} = \frac{1}{768\sqrt{35}} a^{-3/2}\left(\frac{r}{a}\right)^3\exp(-r/4a)$

1 True/False (12 points)

Circle **T** if the statement is always true. Otherwise circle **F** for false. 2 points each

T F The wavefunction describing a many-body quantum system that is a mixture of Fermions and Bosons must be antisymmetric under exchange of any two particles.

T F Observables in quantum mechanics are represented by Hermitian Operators.

T F All operators used in quantum mechanics are Hermitian.

T F The wave function describing the positions of two identical deuterons (the nucleus of a deuterium atom), each with 1 proton and 1 neutron, must be symmetric with exchange of the two deuteron's position coordinates since the deuteron is a (composite) boson. → can have antisymmetric spin w.f.

T F The variational principle states that for any quantum system, the expectation value of the Hamiltonian evaluated using any normalized trial wave function will always be larger than the energy of the system's ground state. $\geq$

T F In the variational method, if one uses a normalized trial function ϕ orthogonal to the ground state wave function of a quantum system, then $\langle\phi|\hat{H}|\phi\rangle$ always gives an upper bound for the energy of the first excited state.

2 Multiple Choice (16 points)

Circle **one** answer for each question. 4 points each.

Which property applies to identical particles that are labeled "Fermions":
- a) they possess integer spin angular momentum
- b) their angular momentum cannot be added.
- c) they always have $\langle\hat{S}^2\rangle = 0$
- d) they obey the Pauli principle.

In atomic units, the mass of the proton is (circle the closest answer):
- a) 1
- b) 13.6
- c) 1.673 $\times 10^{-27}$
- d) 1836

Which of the following is *not* a valid set of quantum numbers for the orbitals of the hydrogen atom $\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_\ell^m(\theta,\phi)$:
- a) $n = 1, \ell = 0, m = 0$
- b) $n = 27, \ell = 0, m = 0$
- c) $n = 2, \ell = 1, m = -1$
- d) $n = 2, \ell = 2, m = -1$
- e) none of the above.

If the spin angular momenta of two spin-3/2 particles are added, the possible s values for the *total* spin angular momentum (such that $\hat{S}^2_{\text{tot}}|\psi\rangle = s(s+1)\hbar^2|\psi\rangle$) are
- a) s = -3, -2, -1, 0, 1, 2, or 3
- b) s = 3, 2, 1, or 0
- c) s = 3 or 0
- d) s = -3, -5/2, -2, -3/2, -1, -1/2, 0, 1/2, 1, 3/2, 2, 5/2, or 3
- e) s = 3/2 or 1/2
- f) Not enough information to answer the question because it depends on if the particles are identical or not.

3 Matrix Element Potpouri (18 points)

For each of the expressions below, indicate if the answer is 0, 1, or something else. If it is "something else", just write "something else" - you don't need to calculate it. 2 points each.

For the stationary state wave functions of the hydrogen atom in spherical coordinates $\psi_{n\ell m}(r,\theta,\phi) = R_{nl}(r)Y_\ell^m(\theta,\phi)$, with $\int d^3\vec{r}$ representing the volume integral over all three dimensional space.

a) $\int_0^\infty dr\; r^2 |R_{n\ell}(r)|^2 =$ 1

b) $\int_0^\infty dr\; r^2 |\psi_{n\ell m}|^2 =$ something else

c) $\langle 2s|\hat{r}^2|1s\rangle = \int d^3\vec{r}\; \psi_{200}^*\, r^2\, \psi_{100} =$ something else

d) $\langle 2p_z|\hat{r}^2|1s\rangle = \int d^3\vec{r}\; \psi_{210}^*\, r^2\, \psi_{100} =$ 0

e) $\langle 2p_z|\hat{z}|1s\rangle = \int d^3\vec{r}\; \psi_{210}^*\, r\cos\theta\, \psi_{100} =$ something else

For the spherical harmonics in spherical coordinates $Y_\ell^m(\theta,\phi)$, with $\int_{4\pi} d\Omega$ representing the integral over all 4π solid angle:

f) $\int_{4\pi} d\Omega\; (Y_1^0)^* Y_0^0 =$ 0

g) $\int_{4\pi} d\Omega\; (Y_1^0)^* \cos\theta\, Y_0^0 =$ something else

h) $\int_{4\pi} d\Omega\; (Y_2^0)^* \cos\theta\, Y_0^0 =$ 0

i) $\int_{4\pi} d\Omega\; (Y_0^0)^* \sin\phi\, Y_0^0 =$ 0

4 Addition of Angular Momenta (9 points)

For each expression below, give the Clebsch-Gordan coefficients $\langle j_1 j_2; m_1 m_2 | j_1 j_2; jm\rangle$ regarding the angular momentum addition of two spin-1/2 particles ($j_1 = 1/2, j_2 = 1/2$). 3 points each.

a) $\langle \frac{1}{2}\frac{1}{2}; \frac{+1}{2}\frac{+1}{2} | \frac{1}{2}\frac{1}{2}; 10\rangle =$ 0

b) $\langle \frac{1}{2}\frac{1}{2}; \frac{+1}{2}\frac{+1}{2} | \frac{1}{2}\frac{1}{2}; 11\rangle =$ 1

c) $\langle \frac{1}{2}\frac{1}{2}; \frac{+1}{2}\frac{-1}{2} | \frac{1}{2}\frac{1}{2}; 10\rangle =$ $1/\sqrt{2}$

5 The Pauli Exclusion Principle (13 points)

Consider two non-interacting spin-$\frac{1}{2}$ particles confined to a 1D box of length 1 ($V(x) = 0$ for $0 < x < 1$ and ∞ otherwise), with the two particles in the excited configuration represented by the following Slater determinant:

$$\Psi_e = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_{1\alpha}(x_1) & \phi_{2\alpha}(x_1) \\ \phi_{1\alpha}(x_2) & \phi_{2\alpha}(x_2) \end{vmatrix} \tag{5.1}$$

and the "α" designates spin "up", viz. $\phi_{1\alpha}(x) = \phi_1(x)\,|\uparrow\rangle$. Take $\phi_1 = \sqrt{2}\sin(\pi x)$ and $\phi_2 = \sqrt{2}\sin(2\pi x)$.

a) Verify that Ψ_e satisfies the time independent Schrödinger equation. To save writing, if you desire you can use the fact that ϕ_1 and ϕ_2 are eigenstates of the 1 particle Hamiltonian without re-deriving this.

b) Make a sketch illustrating the 2-dimensional $|\Psi_e(x_1, x_2)|^2$. You can draw a contour plot, a 3D surface plot, or use shading to represent magnitude, as long as you make yourself clear. What happens when $x_1 = x_2$? Interpret your results in the context of the Pauli exclusion principle.

a) $\hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2}$ btwn $x=0$ and $x=1$

$= \hat{H}_1 + \hat{H}_2$

$\Psi_e = \frac{1}{\sqrt{2}}\left(\phi_1(x_1)\phi_2(x_2) - \phi_2(x_1)\phi_1(x_2)\right)\alpha(1)\alpha(2)$

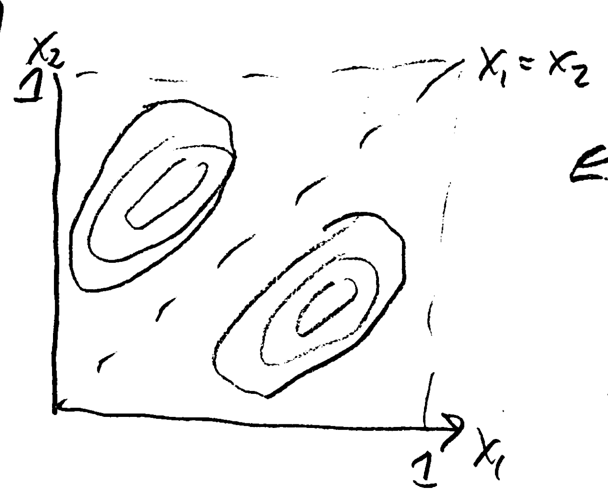
$\hat{H}_1 \Psi_e = \frac{1}{\sqrt{2}}\left(E_1\phi_1(x_1)\phi_2(x_2) - E_2\phi_2(x_1)\phi_1(x_2)\right)\alpha(1)\alpha(2)$

$\hat{H}_2 \Psi_e = \frac{1}{\sqrt{2}}\left(E_2\phi_1(x_1)\phi_2(x_2) - E_1\phi_2(x_1)\phi_1(x_2)\right)\alpha(1)\alpha(2)$

$\Rightarrow \hat{H}\Psi_e = (\hat{H}_1 + \hat{H}_2)\Psi_e = (E_1 + E_2)\Psi_e$ w/ $E_1 = \frac{\hbar^2}{2m}\left(\frac{\pi}{1}\right)^2$ $\leftarrow L=1$

$E_2 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{1}\right)^2$

b)



$\leftarrow |\Psi|^2$ is symmetric around $x_1 = x_2$ but must have a node at $x_1 = x_2$ since the two particles have the same spin. The Pauli Exc. principle requires $\Psi(x_1, x_1) = 0$ when $spin_1 = spin_2$

6 Half-Hydrogen Atom (12 points)

Consider an electron bound to a point impurity at the surface of an insulator. Taking the model potential for this problem in spherical coordinates (r, θ, ϕ) to be.

$$V(r,\theta,\phi) = \begin{cases} \infty, & \theta \geq \pi/2 \\ -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r} & \theta < \pi/2 \end{cases}$$

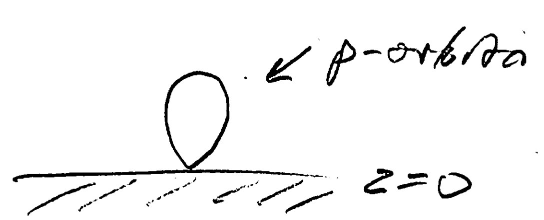
What is the normalized ground state wave function and ground state energy, both written in atomic units $(m_e = \hbar = e = 1/4\pi\epsilon_0 = 1)$?

The Hamiltonian for $z>0$ $(\theta < \pi/2)$ is the same as the Hydrogen atom, so the solns are the same, but not all soln's are able to meet the b.c.'s. The lowest energy soln that meets the b.c. $\psi \to 0$ at $\theta = \pi/2$ is ψ_{210}. We need to multiply by $\sqrt{2}$ since now we are only integrating over half of all space and we still need

$$\int_{z>0} d^3\vec{r}\, |\psi|^2 = 1$$

So

$$\psi_{ground} = \underset{\substack{\uparrow \\ \text{normalization}}}{\sqrt{2}}\, \overbrace{\frac{1}{\sqrt{24}}\, r e^{-r/2}}^{R_{21}} \overbrace{\left(\frac{3}{4\pi}\right)^{1/2} \cos\theta}^{Y_1^0}$$



7 Spin-Orbit Coupling (20 points)

For the hydrogen atom, the electron with spin $s = 1/2$ "orbits" the proton, and it is thus convenient to describe this system with states labeled by the angular momentum quantum numbers $|\ell s; m_\ell m_s\rangle$:

$$\hat{L}^2 |\ell s; m_\ell m_s\rangle = \hbar^2 \ell(\ell+1) \tag{7.1}$$

$$\hat{L}_z |\ell s; m_\ell m_s\rangle = \hbar m_\ell \tag{7.2}$$

$$\hat{S}^2 |\ell s; m_\ell m_s\rangle = \hbar^2 \frac{1}{2}\left(\frac{1}{2}+1\right) \tag{7.3}$$

$$\hat{S}_z |\ell s; m_\ell m_s\rangle = \hbar m_s \tag{7.4}$$

Consider, now an additional term in the Hamiltonian the couples the spin and orbital angular momentum together:

$$\hat{H}_{so} = \beta \hat{\vec{S}} \cdot \hat{\vec{L}} = \beta\left(\hat{S}_x \hat{L}_x + \hat{S}_y \hat{L}_y + \hat{S}_z \hat{L}_z\right) \tag{7.5}$$

where we'll take β as a positive constant (really it would be an operator of the spatial coordinates). This is called spin-orbit coupling. Note that since this term involves all of the components $\hat{L}_i$ and $\hat{S}_i$, the states $|\ell s; m_\ell m_s\rangle$ are *not* eigenstates of this term. The operators $\hat{L}_z$ and $\hat{S}_z$ do not commute with $\hat{H}_{so}$.

In this case, it is convenient to introduce a total angular momentum $\hat{\vec{J}} = \hat{\vec{S}} + \hat{\vec{L}}$, which has its own eigenstates $|\ell s; jm\rangle$, viz.

$$\hat{J}^2 |ls; jm\rangle = \left(\hat{S}^2 + \hat{L}^2 + 2\hat{\vec{S}} \cdot \hat{\vec{L}}\right) |\ell s; jm\rangle = \hbar^2 j(j+1) |\ell s; jm\rangle \tag{7.6}$$

$$\hat{J}_z |ls; jm\rangle = \left(\hat{S}_z + \hat{L}_z\right) |\ell s; jm\rangle = \hbar m |\ell s; jm\rangle \tag{7.7}$$

a) Show that the operator $\hat{J}_z = \hat{L}_z + \hat{S}_z$ commutes with $\hat{H}_{so}$

b) Show that the opperators $\hat{S}^2$ and $\hat{L}^2$ also commute with $\hat{H}_{so}$

c) Rewrite $\hat{H}_{so}$ in terms of $\hat{J}^2$, $\hat{L}^2$, and $\hat{S}^2$, what are the energy eigenvalues you get when you act this part of the Hamiltonian on the states $|ls; jm\rangle$?

d) For an $\ell = 1$ state (p-orbital), j can have only two possible values: $j = \frac{1}{2}$ and $j = \frac{3}{2}$. What are the $\ell = 1$ energy eigenstates? What are their degeneracies?

e) Draw an energy level diagram for the Hydrogen 2p energy level without the spin-orbit coupling and with the spin orbit coupling, what is the energy splitting between the states due to H_{so} in terms of β?

a) $\beta\left[\hat{S}_x \hat{L}_x + \hat{S}_y \hat{L}_y + \overset{\to 0}{\cancel{\hat{S}_z \hat{L}_z}},\ \hat{L}_z + \hat{S}_z\right]$

$= \beta\left(\hat{S}_x[\hat{L}_x, \hat{L}_z] + \hat{S}_y[\hat{L}_y, \hat{L}_z] + [\hat{S}_x, \hat{S}_z]\hat{L}_x + [\hat{S}_y, \hat{S}_z]\hat{L}_y\right)$

$= \beta\left(\cancel{\hat{S}_x(-i\hbar \hat{L}_y)} + \cancel{\hat{S}_y(+i\hbar \hat{L}_x)} + \cancel{(-i\hbar \hat{S}_y)\hat{L}_x} + \cancel{(i\hbar \hat{S}_x)\hat{L}_y}\right)$

$= 0$

More space for 7

b) $[\hat H_{so}, \hat S^2] = \beta\left(\cancelto{0}{[\hat S_x, \hat S^2]}\hat L_x + \cancelto{0}{[\hat S_y, \hat S^2]}\hat L_y + \cancelto{0}{[\hat S_z, \hat S^2]}\hat L_z\right)$

$\hat S^2$ commutes w/ all S's components.

similarly $[\hat H_{so}, \hat L^2] = \beta\left(\hat S_x\cancelto{0}{[\hat L_x, \hat L^2]} + \hat S_y[\hat L_y, \hat L^2] + \hat S_z\cancelto{0}{[\hat L_z, \hat L^2]}\right)$

c) $\hat H_{so} = \beta\vec S\cdot\vec L = \frac{\beta}{2}\left(\hat J^2 - \hat S^2 - \hat L^2\right)$

so $\hat H_{so}|ls;jm\rangle = \frac{\beta\hbar^2}{2}\left(j(j+1) - s(s+1) - l(l+1)\right)$

d) For $l=1$, $s=\frac12$ j can be $\frac32$ or $\frac12$

$\hat H_{so}|1\tfrac12;\tfrac32 m\rangle = \frac{\beta\hbar^2}{2}\left(\frac32\left(\frac32+1\right) - \frac12\left(\frac12+1\right) - 1(1+1)\right)$

$= \frac{\beta\hbar^2}{2}\left(\frac{15}{4} - \frac34 - 2\right) = +\frac{\beta\hbar^2}{2}$

$\hat H_{so}|1\tfrac12;\tfrac12 m\rangle = \frac{\beta\hbar^2}{2}\left(\cancel{\frac12\left(\frac12+1\right)} - \cancel{\frac12\left(\frac12+1\right)} - 2\right)$

$= -\beta\hbar^2$

e) 2x3-fold degenerat