Physics 606 -- Problem Set 1

Due Wednesday, February 4, 2009

Do the following problems from Merzbacher:

Chapter 1:	Problem 2
Chapter 2:	Problems 1 and 4
Chapter 3:	Exercises 3.2 and 3.4

Also do the following additional problems:

(1) Assume $\psi_1(x) = 1/\sqrt{(2a)}$ for $|x|<a$, and $\psi_1(x) = 0$ for $|x|>a$. Find the associated momentum-space wavefunction $\varphi_1(p)$. Show that $\varphi_1(p)$ is normalized to unity.

(2) Now consider a second wavefunction $\psi_2(x) = C\,(a - |x|)$ for $|x|<a$, and $\psi_2(x) = 0$ for $|x|>a$.

(a) Normalize ψ_2.

(b) Find the associated momentum-space wavefunction $\varphi_2(p)$.

(c) Show that, for large $|p|$, $\varphi_2(p)$ goes to zero much faster than $\varphi_1(p)$, even though $\psi_2(x)$ is more localized than $\psi_1(x)$.

(d) Explain, using a simple qualitative argument that builds on the discussion following Eq. 2.13 of Merzbacher, why the high-momentum behavior of $\varphi_1(p)$ is dominated by the discontinuities in $\psi_1(x)$.

Note: These problems illustrate the fact that the Heisenberg uncertainty principle only specifies a **lower limit** on $\Delta x \Delta p_x$.

Chapter 1, Problem 2

$$\lambda_{10^{-7}} = \frac{h}{p_x} = \frac{h}{\sqrt{2m\left(\frac{E}{3}\right)}} = \frac{h}{\sqrt{\cancel{2}m\left(\frac{1}{\cancel{2}}kT\right)}} = \frac{6.63*10^{-34}\,\mathrm{J\cdot s}}{\sqrt{(166*10^{-27}\,\mathrm{kg})\left(1.38*10^{-23}\,\frac{\mathrm{J}}{\mathrm{K}}\right)*10^{-7}\,\mathrm{K}}}$$

$$= 1.38*10^{-6}\,\mathrm{m}$$

$$\rho \sim \frac{1}{\lambda^3} = \boxed{\frac{3.8*10^{17}}{\mathrm{m}^3}}$$

Chapter 2, Problem 1

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ikx}\, \Psi(x, t=0)\, dx$$

$$= \frac{C}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \exp\left[-\frac{x^2}{4(\Delta x)^2} + i(\bar{k}_x - k)x\right] dx$$

Note: $\int_{-\infty}^{+\infty} e^{-\alpha^2 x^2} e^{\beta x}\, dx = \frac{\sqrt{\pi}}{\alpha} e^{\frac{\beta^2}{4\alpha^2}}$ when $Re(\alpha) > 0$

$$\Rightarrow \phi(k) = \frac{C}{\sqrt{2\pi}} \frac{\sqrt{\pi}}{\frac{1}{2(\Delta x)}} \exp\left[\frac{-(\bar{k}_x - k)^2}{4 \frac{1}{4(\Delta x)^2}}\right]$$

$$\Rightarrow \boxed{\phi(k) = \sqrt{2}\, C(\Delta x) \exp\left[-(\Delta x)^2 (k - \bar{k}_x)^2\right]}$$

Then $\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{i(kx - \omega t)}\, dk$

$$= \frac{C(\Delta x)}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp\left[-(\Delta x)^2 \left(k^2 - 2\bar{k}_x k + \bar{k}_x^2\right)\right] \exp\left[ikx - i\frac{\hbar k^2}{2m} t\right] dk$$

$$= \frac{C(\Delta x)}{\sqrt{\pi}} \exp\left[-(\Delta x)^2 \bar{k}_x^2\right] \int_{-\infty}^{+\infty} \exp\left[-\left((\Delta x)^2 + i\frac{\hbar t}{2m}\right) k^2\right] \exp\left[\left(2(\Delta x)^2 \bar{k}_x + ix\right) k\right] dk$$

$$= \frac{C(\Delta x)}{\sqrt{\pi}} \exp\left[-(\Delta x)^2 \bar{k}_x^2\right] \frac{\sqrt{\pi}}{\sqrt{(\Delta x)^2 + i\frac{\hbar t}{2m}}} \exp\left[\frac{\left(2(\Delta x)^2 \bar{k}_x + ix\right)^2}{4\left((\Delta x)^2 + i\frac{\hbar t}{2m}\right)}\right]$$

$$\Rightarrow \boxed{\Psi(x,t) = \frac{C(\Delta x)\, e^{-(\Delta x)^2 \bar{k}_x^2}}{\sqrt{(\Delta x)^2 + i\frac{\hbar t}{2m}}} \exp\left[\frac{-x^2 + i4(\Delta x)^2 \bar{k}_x x + 4(\Delta x)^4 (\bar{k}_x)^2}{4\left((\Delta x)^2 + i\frac{\hbar t}{2m}\right)}\right]}$$

A little arithmetic confirms $\Psi(x, t=0)$ matches the input function.

CH2.P1.2

For $|\psi|^2$ as a fn of x, the x-independent terms just serve to provide the time-dependent normalization of ψ.

The x-dependence of $|\psi|^2$ comes entirely from:

$$|\psi(x)|^2 \propto \left| \exp\left[\frac{\left(-x^2 + i4(\Delta x)^2 \bar{k}_x x\right)\left((\Delta x)^2 - i\frac{\hbar t}{2m}\right)}{2\left((\Delta x)^2 + i\frac{\hbar t}{2m}\right)\left((\Delta x)^2 - i\frac{\hbar t}{2m}\right)}\right]\right|$$

$$= \exp\left[-\frac{1}{2}\left\{\frac{(\Delta x)^2}{(\Delta x)^4 + \left(\frac{\hbar t}{2m}\right)^2} x^2 - \frac{2(\Delta x)^2 \bar{k}_x \frac{\hbar}{m} t}{(\Delta x)^4 + \left(\frac{\hbar t}{2m}\right)^2}\right\}\right]$$

$$= \exp\left[-\frac{1}{2}\frac{(\Delta x)^2}{(\Delta x)^4 + \left(\frac{\hbar t}{2m}\right)^2}\left(x - \frac{\hbar \bar{k}_x}{m} t\right)^2\right] \times \text{x-independent Normalization constant}$$

This is a Gaussian with width $\sigma = \sqrt{(\Delta x)^2 + \left(\frac{\hbar t}{2m\Delta x}\right)^2}$,

centered at $x = \frac{\hbar \bar{k}_x}{m} t = \frac{\bar{p}}{m} t = \bar{v} t$, which illustrates both the spreading and the classical average motion.

Note: The problem never asked, but $|C|^2 = \frac{1}{\sqrt{2\pi}(\Delta x)}$

CH2. P1-3

Electron, localized to 1 A, typical of the H atom		A bowling ball, localized to 1 A	
Dx_0 =	1.00E-10	Dx_0 =	1.00E-10
hbar/2mDx_0 =	5.79E+05	hbar/2mDx_0 =	7.25E-26
t (sec)	Dx(t) (cm)	t (sec)	Dx(t) (cm)
0.00E+00	1.00E-10	0.00E+00	1.00E-10
1.00E-16	1.16E-10	1.00E+15	1.24E-10
2.00E-16	1.53E-10	2.00E+15	1.76E-10
3.00E-16	2.00E-10	3.00E+15	2.39E-10
4.00E-16	2.52E-10	4.00E+15	3.07E-10
5.00E-16	3.06E-10	5.00E+15	3.76E-10
6.00E-16	3.62E-10	6.00E+15	4.47E-10
7.00E-16	4.17E-10	7.00E+15	5.17E-10
8.00E-16	4.74E-10	8.00E+15	5.89E-10
9.00E-16	5.31E-10	9.00E+15	6.60E-10
1.00E-15	5.88E-10	1.00E+16	7.32E-10

The wave packet of a 16# bowling ball initially localized to 1 Å spreads to 2 Å in ~76M years!

Chapter 2, Problem 4

$$p = \sqrt{2mE} = \sqrt{2 \cdot 1838.7 * 9.11 * 10^{-31}\,\text{kg} \cdot 0.02 \cdot 1.60 * 10^{-19}\,\text{J}}$$

$$= 3.27 * 10^{-24}\,\frac{\text{kg m}}{\text{s}}$$

$$\Rightarrow \Delta p \sim \frac{\Delta\lambda}{\lambda} p \approx 3.27 * 10^{-33}\,\frac{\text{kg m}}{\text{s}}$$

$$\Delta x\,\Delta p \sim \hbar \Rightarrow \Delta x \sim \frac{1.055 * 10^{-34}\,\text{J}\cdot\text{s}}{3.27 * 10^{-33}\,\frac{\text{kg m}}{\text{s}}} \boxed{= 0.0322\,\text{m}}$$

The wave packet will spread when

$$|t| \sim \frac{m\hbar}{(\Delta p_x)^2} \sim \frac{(1838.7 * 9.11 * 10^{-31}\,\text{kg})(1.055 * 10^{-34}\,\text{J}\cdot\text{s})}{\left(3.27 * 10^{-33}\,\frac{\text{kg m}}{\text{s}}\right)^2}$$

$$= 1.65 * 10^{4}\,\text{s} \quad \text{(about } 4\tfrac{1}{2} \text{ hours)}$$

Chapter 3, Exercise 3.2

$$i\hbar\,\Psi_1^*\frac{\partial\Psi_2}{\partial t} = -\frac{\hbar^2}{2m}\Psi_1^*\vec{\nabla}^2\Psi_2 + \Psi_1^* V\Psi_2 \quad \text{and} \quad [\Psi_1^* \circledast 3.1]$$

$$-i\hbar\frac{\partial\Psi_1^*}{\partial t}\Psi_2 = -\frac{\hbar^2}{2m}(\nabla^2\Psi_1^*)\Psi_2 + \Psi_1^* V\Psi_2 \quad [(3.1)^* \circledast \Psi_2]$$

The difference gives:

$$i\hbar\left\{\Psi_1^*\frac{\partial\Psi_2}{\partial t} + \frac{\partial\Psi_1^*}{\partial t}\Psi_2\right\} = \frac{\hbar^2}{2m}\left[(\nabla^2\Psi_1^*)\Psi_2 - \Psi_1^*\nabla^2\Psi_2\right]$$

$$\Rightarrow \frac{\partial}{\partial t}(\Psi_1^*\Psi_2) = \frac{\hbar}{2mi}\left[(\nabla^2\Psi_1^*)\Psi_2 + \vec{\nabla}\Psi_1^*\cdot\vec{\nabla}\Psi_2 - \Psi_1^*\nabla^2\Psi_2 - \vec{\nabla}\Psi_1^*\cdot\vec{\nabla}\Psi_2\right]$$

$$= \frac{\hbar}{2mi}\left[\vec{\nabla}\cdot\left[(\vec{\nabla}\Psi_1^*)\Psi_2\right] - \vec{\nabla}\cdot\left[\Psi_1^*\vec{\nabla}\Psi_2\right]\right]$$

$$= \frac{\hbar}{2mi}\vec{\nabla}\cdot\left[(\vec{\nabla}\Psi_1^*)\Psi_2 - \Psi_1^*(\vec{\nabla}\Psi_2)\right] \Rightarrow$$

$$\frac{\partial}{\partial t}(\Psi_1^*\Psi_2) + \frac{\hbar}{2mi}\vec{\nabla}\cdot\left[\Psi_1^*(\vec{\nabla}\Psi_2) - (\nabla\Psi_1^*)\Psi_2\right] = 0$$

Chapter 3, Exercise 3.4

$$\psi(\vec{r}, t=0) = \frac{1}{(2\pi)^{3/2}} \int \phi(\vec{k})\, e^{i\vec{k}\cdot\vec{r}}\, d^3k$$

Focus on $\int_{-\infty}^{+\infty} \phi(k_x)\, e^{ik_x x}\, dk_x$. $\phi(k_x) = \phi_2^{*}(k_x - \bar{k})$

where ϕ_2 is real and symmetric about zero. Let $k = k_x - \bar{k} \Rightarrow$

$$\int_{-\infty}^{+\infty} \phi_2(k)\, e^{i(k+\bar{k})x}\, dk = e^{i\bar{k}x} \int_{-\infty}^{+\infty} \phi_2(k) \left[\cos kx + i \sin kx\right] dk$$

The real part of the integrand is an even fn of k, while the imaginary part is an odd fn of k $\Rightarrow$ the integral is real, and

$\psi(\vec{r}, t=0) = e^{i\vec{\bar{k}}\cdot\vec{r}}\, \psi_0(\vec{r})$, with $\psi_0(\vec{r})$ real.

$\rho = |\psi|^2 = \psi_0^2$ (at $t=0$)

$$\vec{j} = \frac{\hbar}{2mi}\left[\psi^* \vec{\nabla}\psi - (\vec{\nabla}\psi)^* \psi\right]$$

$$= \frac{\hbar}{2mi}\left\{ e^{-i\bar{k}\cdot\vec{r}}\psi_0 \left[i\bar{k}\psi + \cancel{e^{i\bar{k}\cdot\vec{r}} \vec{\nabla}\psi_0} \right] - \left[-i\bar{k}\psi^* + \cancel{e^{-i\bar{k}\cdot\vec{r}} \vec{\nabla}\psi_0} \right]\psi \right\}$$

$$= \frac{\hbar}{2mi}\left\{ \cancel{e^{-i\bar{k}\cdot\vec{r}}}\psi_0\, i\bar{k}\, \cancel{e^{i\bar{k}\cdot\vec{r}}}\psi_0 + i\bar{k}\, \cancel{e^{-i\bar{k}\cdot\vec{r}}}\psi_0\, \cancel{e^{i\bar{k}\cdot\vec{r}}}\psi_0 \right\}$$

$$= \frac{\hbar}{\cancel{2}m\cancel{i}}\, \cancel{2i}\bar{k}\, \psi_0^2 = \frac{\bar{p}}{m}\rho \checkmark$$

Problem Set 1, Extra Problem 1

$$\phi_1(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-a}^{+a} e^{-i\frac{px}{\hbar}} \frac{1}{\sqrt{2a}}\, dx$$

$$= \frac{1}{2\sqrt{\pi\hbar a}} \left[\frac{e^{-i\frac{px}{\hbar}}}{-i\frac{p}{\hbar}}\right]_{x=-a}^{a} = \frac{1}{2\sqrt{\pi\hbar a}}\, \frac{e^{-i\frac{pa}{\hbar}} - e^{+i\frac{pa}{\hbar}}}{-i\frac{p}{\hbar}}$$

$$= \boxed{\sqrt{\frac{\hbar}{\pi a}}\, \frac{\sin\left(\frac{pa}{\hbar}\right)}{p}}$$

$$\int_{-\infty}^{+\infty} |\phi_1(p)|^2\, dp = \frac{\hbar}{\pi a} \int_{-\infty}^{+\infty} \frac{\sin^2\left(\frac{pa}{\hbar}\right)}{p^2}\, dp = \frac{\cancel{\hbar}}{\pi \cancel{a}} \int_{-\infty}^{+\infty} \frac{\sin^2(y)}{\left(\frac{\cancel{\hbar} y}{\cancel{a}}\right)^2}\, \frac{\cancel{\hbar}}{\cancel{a}}\, dy$$

$$= \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\sin^2 y}{y^2}\, dy = 1$$

Problem Set 1, Extra Problem 2

(a) $\int_{-\infty}^{+\infty} |\psi_2(x)|^2 dx = 2|C|^2 \int_0^a (a-x)^2 dx = 2|C|^2 \int_0^a (a^2-2ax+x^2)\, dx$

$= 2|C|^2 \left[a^3 - 2a\frac{a^2}{2} + \frac{a^3}{3} \right] = \frac{2}{3}|C|^2 a^3 = 1$

$\Rightarrow C = \sqrt{\frac{3}{2a^3}}$

(b) $\phi_2(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{-i\frac{px}{\hbar}} \psi_2(x)\, dx = \sqrt{\frac{3}{4\pi\hbar a^3}} \left\{ \int_{-a}^{0} e^{-i\frac{px}{\hbar}} (a+x)\, dx \right.$

$\left. + \int_0^a e^{-i\frac{px}{\hbar}} (a-x)\, dx \right\}$

$\int_{-a}^{0} e^{-i\frac{px}{\hbar}} (a+x)\, dx = \int_a^0 e^{i\frac{py}{\hbar}} (a-y)(-dy)$

$\Rightarrow \phi_2(p) = \sqrt{\frac{3}{4\pi\hbar a^3}} \int_0^a \left(e^{i\frac{px}{\hbar}} + e^{-i\frac{px}{\hbar}}\right)(a-x)\, dx$

$= \sqrt{\frac{3}{\pi\hbar a^3}} \int_0^a \cos\left(\frac{px}{\hbar}\right)(a-x)\, dx$

$= \sqrt{\frac{3}{\pi\hbar a^3}} \underbrace{\int_0^a a\cos\left(\frac{px}{\hbar}\right) dx}_{a\frac{\sin\frac{pa}{\hbar}}{p/\hbar}} - \sqrt{\frac{3}{\pi\hbar a^3}} \int_0^a x\cos\left(\frac{px}{\hbar}\right) dx$

$\int_0^a x\cos\left(\frac{px}{\hbar}\right) dx = \left[x\frac{\sin\left(\frac{px}{\hbar}\right)}{p/\hbar} \right]_{x=0}^{a} - \int_0^a \frac{\sin\left(\frac{px}{\hbar}\right)}{p/\hbar}\, dx$

$= a\frac{\sin\left(\frac{pa}{\hbar}\right)}{p/\hbar} - \left[\frac{-\cos\left(\frac{px}{\hbar}\right)}{(p/\hbar)^2} \right]_{x=0}^{a} = \frac{\hbar a}{p}\sin\left(\frac{pa}{\hbar}\right) + \frac{\cos\left(\frac{pa}{\hbar}\right) - 1}{\left(\frac{p}{\hbar}\right)^2}$

$\Rightarrow \boxed{\phi_2(p) = \sqrt{\frac{3}{\pi\hbar a^3}}\, \hbar^2\, \frac{1-\cos\left(\frac{pa}{\hbar}\right)}{p^2}}$

PS1. EP2.2

(c) At large $|p|$, $\phi_1 \to \frac{1}{|p|} \gg \phi_2 \to \frac{1}{|p|^2}$

(d) The complex exponential has period $\frac{2\pi\hbar}{p}$. Over each full period, the integral is zero. This leaves a segment of length $\Delta x < \frac{2\pi\hbar}{p}$ to give a finite contribution to $\phi_1(p)$. This produces the $\frac{1}{|p|}$ behavior at large $|p|$.