PHYS 357 Pset 8. Due 11:59 PM Thursday Nov. 14

1. Townsend 6.1.
2. Townsend 6.3.
3. Size of the hydrogen atom. The potential between a proton and electron is $U = -\frac{e^2}{4\pi\epsilon_0 r}$. If we work in a frame where $<x>=<p>=0$, then the Heisenberg uncertainty principle tells us we'll have some minimum kinetic energy for a fixed r (remember, the electron can "move" in angular directions, so even if we know say it's at fixed radius, there's still uncertainty in the 3-D position). Find the radius r that minimizes the total energy, in terms of elementary constants, and a constant of order unity (at this level of accuracy, reasonable people may get different values for this constant). Evaluate your radius, and compare to the accepted value for the radius of the ground-state hydrogen, $5.3 \times 10^{-11} m$.

   Note - Like many things in quantum mechanics, what we mean by "the" radius is rather fuzzy. This is the Bohr radius, which is the average distance of a ground-state electron from the nucleus for an isolated atom. You'd get a different number if you made molecular hydrogen (H_2), and yet another number if you froze hydrogen into a solid and measured the per-atom volume of that solid.

4. Fourier transform of a Gaussian. Gaussian wave packets get used repeatedly in QM, and so practice with integrals is very valuable. The Fourier transform $F(k)$ of $f(x)$ is defined to be $\int f(x)\exp(ikx)dx$. For a Gaussian, we have $f(x) = \exp(-x^2/2\sigma^2$. By completing the square, show that

   $$\int_{-\infty}^{\infty} \exp(ikx)\exp(-x^2/2\sigma^2)dx = \exp(-k^2\sigma^2/2)\int(something)dx$$

   Then show that $\int(something)dx = \int_{-\infty}^{\infty}\exp(-x^2/2\sigma^2)dx$. As a reminder, all closed path integrals in the complex plane are zero if the function has no poles. That integral evaluates to $\sqrt{2\pi\sigma^2}$, giving us the Fourier tranform of a Gaussian.

5. Discrete Fourier transform. The discrete Fourier transform of $f(x)$ is defined to be

   $$F(k) \equiv \sum_{x=0}^{N-1} f(x)\exp(-2\pi ikx/N)$$

for some integer N, and x, k integers running from 0 to $N-1$. First, show that

$$\sum_{x=0}^{N-1} \exp(-2piikx/N) = 0$$

unless $k = 0$ (technically, any integer multiple of N, but we restricted k to be between 0 and $N-1$). As a reminder, the sum of a geometric series $\sum_{m=m_0}^{\infty} r^m = r^{m_0}/(1-r)$.

Now show that we can get $F(k) = \mathrm{F} f(x)$ for the symmetric matrix F that has $F_{m,n} = \exp(-2\pi imn/N)$.

Finally, show that $\mathrm{F}^{-1} = \frac{1}{N}\mathrm{F}^{\dagger}$. This means for the discrete case, the inverse Fourier transform is just the conjugate of the Fourier transform, with a $1/N$ normalization factor. We'll be able to use this to go easily between position and momentum representations of wave functions.

6.1.

(a) Use induction to show that $[\hat{x}^n, \hat{p}_x] = i\hbar n\hat{x}^{n-1}$. *Suggestion:* Take advantage of the commutation relation $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$ in working out the commutators.

We know $[\hat{x}, \hat{p}] = i\hbar$ $(n=1)$

Assume $[\hat{x}^m, \hat{p}] = i\hbar m\hat{x}^{m-1}$ for $n=m$, then for $n=m+1$, we have

$$[\hat{x}^{m+1}, \hat{p}] = [\hat{x}\hat{x}^m, \hat{p}] = \hat{x}\underbrace{[\hat{x}^m, \hat{p}]}_{\substack{i\hbar m\hat{x}^{m-1} \\ \text{by induction} \\ \text{hypothesis}}} + \underbrace{[\hat{x}, \hat{p}]}_{i\hbar}\hat{x}^m$$

$$= \hat{x}\, i\hbar m\hat{x}^{m-1} + i\hbar\hat{x}^m$$

$$= i\hbar m\hat{x}^m + i\hbar\hat{x}^m$$

$$= i\hbar(m+1)\hat{x}^m$$

$\Rightarrow$ by induction, $[\hat{x}^n, \hat{p}] = i\hbar n\hat{x}^{n-1}$

(b) Using the expansion

$$F(x) = F(0) + \left(\frac{dF}{dx}\right)_{x=0} x + \frac{1}{2!}\left(\frac{d^2F}{dx^2}\right)_{x=0} x^2 + \cdots \frac{1}{n!}\left(\frac{d^nF}{dx^n}\right)_{x=0} x^n + \cdots$$

show that

$$[F(\hat{x}), \hat{p}_x] = i\hbar\frac{\partial F}{\partial x}(\hat{x})$$

all evaluated at $x=0$

$$[f(\hat{x}), \hat{p}] = [f(0) + (d_x f)\hat{x} + \frac{1}{2!}(d_x^2 f)\hat{x}^2 + \cdots + \frac{1}{n!}(d_x^n f)\hat{x}^n + \cdots, \hat{p}]$$

$$= \underbrace{[f(0), \hat{p}]}_{\substack{f(0) = \text{cst so commutes} \\ \text{w/ } \hat{p} \to [f(0), \hat{p}] = 0}} + \frac{df}{dx}[\hat{x}, \hat{p}] + \frac{1}{2!}\frac{d^2f}{dx^2}[\hat{x}^2, \hat{p}] + \cdots + \frac{1}{n!}\frac{d^nf}{dx^n}[\hat{x}^n, \hat{p}] + \cdots$$

and $[\hat{x}^n, \hat{p}] = i\hbar n\hat{x}^{n-1}$

$$= i\hbar\frac{df}{dx} + \frac{1}{2!}\frac{d^2f}{dx^2}\cdot i\hbar 2\hat{x} + \cdots + \frac{1}{n!}\frac{d^nf}{dx^n}\cdot i\hbar n\hat{x}^{n-1} + \cdots$$

$$= \sum_{n=1}^{\infty}\frac{i\hbar}{n!}n\hat{x}^{n-1}\frac{d^nf}{dx^n}$$

$$\frac{n}{n!} = \frac{1}{(n-1)!}$$

$$= \sum_{n=0}^{\infty}\frac{i\hbar}{n!}\hat{x}^n\frac{d^{n+1}f}{dx^{n+1}}$$

$$= \frac{d}{dx}\underbrace{\left(\sum_{n=0}^{\infty}\frac{i\hbar}{n!}\frac{d^nf}{dx^n}\hat{x}^n\right)}_{\text{Taylor expansion of } f(\hat{x}) \times i\hbar}$$

$$[f(\hat{x}), \hat{p}] = i\hbar\frac{df(\hat{x})}{dx}$$

(c) For the one-dimensional Hamiltonian

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + V(\hat{x})$$

show that

$$\frac{d\langle p_x \rangle}{dt} = \left\langle -\frac{dV}{dx} \right\rangle$$

$$\frac{d\langle p\rangle}{dt} = \frac{i}{\hbar}[H, \hat{p}]$$

$$= \frac{i}{\hbar}\left[\frac{\hat{p}^2}{2m} + V(\hat{x}), \hat{p}\right]$$

$$= \underbrace{\frac{i}{\hbar}\left[\frac{\hat{p}^2}{2m}, \hat{p}\right]}_{\text{$\hat{p}$ commutes w/ powers of itself so this is $=0$}} + \underbrace{\frac{i}{\hbar}[V(\hat{x}), \hat{p}]}_{\text{from b) we've shown that $[f(\hat{x}), \hat{p}] = i\hbar \frac{df}{dx}(\hat{x})$}}$$

$$= \frac{i}{\hbar}\left(i\hbar \frac{dV}{dx}(\hat{x})\right)$$

$$\boxed{\frac{d\langle p\rangle}{dt} = -\frac{dV}{dx}}$$

6.3. Show for the infinitesimal translation

$$|\psi\rangle \to |\psi'\rangle = \hat{T}(\delta x)|\psi\rangle$$

that

$$\langle x\rangle \to \langle x\rangle + \delta x \quad \text{and} \quad \langle p_x\rangle \to \langle p_x\rangle.$$

we know $\hat{T}(\delta x)|x\rangle = |x+\delta x\rangle$ so $|\psi'\rangle = \hat{T}(\delta x)|\psi\rangle = \hat{T}(\delta x)\int dx|x\rangle\langle x|\psi\rangle$

$$= \int dx\, \underbrace{\hat{T}(\delta x)|x\rangle}_{|x+\delta x\rangle}\langle x|\psi\rangle$$

$$= \int dx\, |x+\delta x\rangle\langle x|\psi\rangle$$

and we have $\psi'(x) = \langle x|\psi'\rangle = \langle x|\hat{T}(\delta x)|\psi\rangle = \psi(x-\delta x)$

$\to \langle x\rangle' = \langle\psi'|\hat{x}|\psi'\rangle = \int dx\, \langle\psi'|\hat{x}|x\rangle\langle x|\psi'\rangle$

$\hat{x}|x\rangle = x|x\rangle$

$$= \int dx\, \langle\psi'|x\rangle x\langle x|\psi'\rangle$$

$$= \int dx\, \psi'(x)^* x\, \psi'(x)$$

$\psi'(x) = \psi(x-\delta x)$

$$= \int dx\, \psi(x-\delta x)^* x\, \psi(x-\delta x)$$

$\partial_x = \frac{\partial}{\partial x}$

we can Taylor expand $\psi(x-\delta x) \approx \psi(x) - \partial_x\psi(x)\,\delta x$

(similar for ψ^*)

$$= \int dx\left[\psi^*(x) - \partial_x\psi(x)^*\delta x\right] x \left[\psi(x) - \partial_x\psi(x)\,\delta x\right]$$

$$= \underbrace{\int dx\, \psi^*(x)\, x\, \psi(x)}_{\langle x\rangle} - \int x\,\delta x\, dx\, (\underbrace{\psi^*(x)\partial_x\psi(x) + \psi(x)\partial_x\psi^*(x)}_{\text{product rule} \to\ = \partial_x(\psi(x)^*\psi(x))}] + \int \cancel{\delta x^2 \text{ term}}^{\,0}$$

0, drop higher order

$$= \langle x\rangle - \delta x \underbrace{\int dx\, x\frac{\partial}{\partial x}(\psi^*\psi)}$$

$u = x$, $dv = \partial_x(\psi^*\psi)\,dx$

$du = dx$, $v = \psi^*\psi = |\psi|^2$

so we have

0 when evaluated at $\int$ bounds

$uv - \int v\,du = \cancel{x|\psi|^2} - \int|\psi|^2 dx$

$$= \langle x\rangle - \delta x(-\underbrace{\int|\psi|^2 dx}_{=1})$$

$\langle x\rangle' = \langle x\rangle + \delta x$

$\to \langle p\rangle' = \langle\psi'|\hat{p}|\psi'\rangle = \int dx\, \langle\psi'|x\rangle\frac{\hbar}{i}\partial_x\langle x|\psi'\rangle$

$$= \int dx\, \psi'(x)^*\frac{\hbar}{i}\partial_x\psi'(x)$$

$\psi'(x) = \psi(x-\delta x) \approx \psi(x) - \partial_x\psi(x)\cdot\delta x$

$$= \int dx\left[\psi^* - \partial_x\psi^*\delta x\right]\frac{\hbar}{i}\partial_x\left[\psi - \partial_x\psi\cdot\delta x\right]$$

drop higher order δx terms

$$= \int dx\frac{\hbar}{i}\left[\psi^*\partial_x\psi - \psi^*\partial_x^2\psi\,\delta x - \partial_x\psi\,\partial_x\psi^*\delta x + \cancel{\partial_x\psi^*\partial_x\psi\,\delta x^2}\right]$$

$$= \underbrace{\int dx\, \psi^*(x)\frac{\hbar}{i}\partial_x\psi(x)}_{\langle p\rangle} - \frac{\hbar}{i}\delta x\int dx\,(\underbrace{\psi^*\partial_x^2\psi + \partial_x\psi\,\partial_x\psi^*}_{\text{product rule w/ }\psi^*\text{ and }\partial_x\psi\ = \partial_x(\psi^*\partial_x\psi)})$$

$$\langle p \rangle' = \langle p \rangle - \frac{\hbar}{i}\delta x \int dx \cdot \partial_x (\psi^* \partial_x \psi)$$

$$= \langle p \rangle - \frac{\hbar}{i}\delta x \, \underbrace{\cancel{(\psi^* \partial_x \psi)}\Big|_{-\infty}^{\infty}}_{0}$$

0 since ψ & $\partial_x \psi$ vanish at inf.

$\langle p \rangle' = \langle p \rangle$

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① $\sigma(x) = \sqrt{\langle x^2\rangle - \langle \underbrace{x}_{0}\rangle^2} = \sqrt{\langle x^2 \rangle} \sim r$

$\sigma(p) = \sqrt{\langle p^2\rangle - \langle \underbrace{p}_{0}\rangle^2} = \sqrt{\langle p^2 \rangle} \rightarrow \sigma(p)^2 \sim p^2$

so we have $\sigma(x)\sigma(p) \geq \frac{\hbar}{2}$

$$\sigma(x)^2\sigma(p)^2 \geq \frac{\hbar^2}{4}$$

$$r^2 p^2 \approx \frac{\hbar^2}{4}$$

$$p^2 \approx \frac{\hbar^2}{4r^2}$$

② $E = K + U$

$$E = \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 r}$$

↓ minimize

$$\frac{dE}{dr} = \frac{d}{dr}\left(\frac{\hbar^2}{2m4} r^{-2} - \frac{e^2}{4\pi\varepsilon_0} r^{-1}\right)$$

$$0 = \frac{\hbar^2}{8m}(-2)r^{-3} - \frac{e^2}{4\pi\varepsilon_0}(-1)r^{-2}$$

$$0 = \frac{-\hbar^2}{4m}\frac{1}{r^3} + \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r^2}$$

$$0 = \frac{-\hbar^2}{m}\frac{1}{r} + \frac{e^2}{\pi\varepsilon_0}$$

$$\frac{\hbar^2}{m}\frac{1}{r} = \frac{e^2}{\pi\varepsilon_0}$$

$$r = \frac{\pi\varepsilon_0\hbar^2}{me^2}$$

↓ wolfram

$r \approx 1.32 \times 10^{-11}$ m → The accepted value is 5.3×10^{-11}m so r is off by a factor of ~5 (but we have the right order of magnitude)

4. Fourier transform of a Gaussian. Gaussian wave packets get used repeatedly in QM, and so practice with integrals is very valuable. The Fourier transform $F(k)$ of $f(x)$ is defined to be $\int f(x)\exp(ikx)dx$. For a Gaussian, we have $f(x) = \exp(-x^2/2\sigma^2$. By completing the square, show that

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$f(k) = \mathcal{F}\{f(x)\} = \int f(x)e^{ikx}dx$

gaussian $\rightarrow f(x) = e^{-x^2/2\sigma^2}$ so we have ...

$$f(k) = \int e^{-x^2/2\sigma^2} e^{ikx} dx$$
$$= \int e^{ikx - x^2/2\sigma^2} dx$$

complete the square

$$b(x+c)^2 = bx^2 + 2bcx + bc^2$$

so $b = \frac{-1}{2\sigma^2}$, $2bc = ik$

$$-\frac{c}{\sigma^2} = ik$$
$$c = -ik\sigma^2$$

$$\Rightarrow \underbrace{\frac{-1}{2\sigma^2}}_{b}x^2 + \underbrace{ikx}_{2bc} + \underbrace{\left(\frac{-1}{2\sigma^2}\right)}_{b}\underbrace{(-ik\sigma^2)^2}_{c^2} = \underbrace{\frac{-1}{2\sigma^2}}_{b}\underbrace{(x-ik\sigma^2)^2}_{(x+c)^2}$$

$$\frac{-1}{2\sigma^2}x^2 + ikx = \frac{-1}{2\sigma^2}(x-ik\sigma^2)^2 - \frac{1}{2\cancel{\sigma^2}}\cdot k^2\sigma^{\cancel{4}\,2}$$
$$= \frac{-1}{2\sigma^2}(x-ik\sigma^2)^2 - \frac{k^2\sigma^2}{2}$$

$$f(k) = \int e^{\frac{-1}{2\sigma^2}(x-ik\sigma^2)^2} e^{-k^2\sigma^2/2} dx$$
$$= e^{-k^2\sigma^2/2}\underbrace{\int_{-\infty}^{\infty} e^{\frac{-1}{2\sigma^2}(x-ik\sigma^2)^2} dx}$$

General gaussian : $\int_{-\infty}^{\infty} e^{-a(x-b)^2}dx = \sqrt{\frac{\pi}{a}}$

so this is $= \sqrt{2\pi\sigma^2}$

$$f(k) = \sqrt{2\pi\sigma^2}\, e^{-k^2\sigma^2/2}$$

5. Discrete Fourier transform. The discrete Fourier transform of $f(x)$ is defined to be

$$F(k) \equiv \sum_{x=0}^{N-1} f(x)\exp(-2\pi ikx/N)$$

for some integer N, and x, k integers running from 0 to $N-1$. ① First, show that

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② Now show that we can get $F(k) = \mathrm{F}f(x)$ for the symmetric matrix F that has $F_{m,n} = \exp(-2\pi imn/N)$.

③ Finally, show that $\mathrm{F}^{-1} = \frac{1}{N}\mathrm{F}^\dagger$. This means for the discrete case, the inverse Fourier transform is just the conjugate of the Fourier transform, with a $1/N$ normalization factor. We'll be able to use this to go easily between position and momentum representations of wave functions.

① $\displaystyle\sum_{x=0}^{N-1} e^{-2\pi ikx/N} = \sum_{x=0}^{N-1} (e^{-2\pi ik/N})^x$

$\downarrow$ $\displaystyle\sum_0^n ar^x = a\left(\frac{1-r^{n+1}}{1-r}\right)$ for $r \neq 1$

$$= \frac{1-(e^{-2\pi ik/N})^N}{1-e^{-2\pi ik/N}} \quad \text{for } k \neq 0$$

$$= \frac{1-e^{-2\pi ik}}{1-e^{-2\pi ik/N}}$$

$e^{-2\pi ik} = 1$ since $k = $ int (for any k)

$$= \frac{1-1}{1-e^{-2\pi ik/N}}$$

$= 0$

② we know $f(k) = \displaystyle\sum_{x=0}^{N-1} f(x) e^{-2\pi ikx/N}$ and $F_{m,n} = e^{-2\pi imn/N}$ $\rightarrow$ F - symmetric matrix

we can write $f(x) = \begin{pmatrix} f(x_0) \\ \vdots \\ f(x_{N-1}) \end{pmatrix}$, and we have $f(k_j) = \displaystyle\sum_{n=0}^{N-1} f(x_n) e^{-2\pi ik_j x_n/N}$

Writing this with matrices, we have

$$\underbrace{\begin{pmatrix} f(k_0) \\ \vdots \\ f(k_{N-1}) \end{pmatrix}}_{f(k)} = \begin{pmatrix} \sum_{n=0}^{N-1} f(x_n) e^{-2\pi ik_0 x_n/N} \\ \vdots \\ \sum_{n=0}^{N-1} f(x_n) e^{-2\pi ik_{N-1} x_n/N} \end{pmatrix}$$

$$= \underbrace{\begin{pmatrix} e^{-2\pi ik_0 x_0/N} & e^{-2\pi ik_0 x_1/N} & \cdots \\ \vdots & & \end{pmatrix}}_{\substack{k \to m \text{ \& } x \to n \text{ with } x \\ \text{and } k \text{ both ranging from} \\ 0 \text{ to } N-1 \text{ (so } x_0 = k_0 = 0\text{, etc)} \\ \text{Then this is just } F}} \underbrace{\begin{pmatrix} f(x_0) \\ \vdots \\ f(x_{N-1}) \end{pmatrix}}_{f(x)}$$

$f(k) = F f(x)$

③ $F^{\dagger}_{m,n} = \overline{F_{n,m}} = e^{2\pi i mn/N}$ so we can write:

$$(FF^{\dagger})_{m,n} = \left(e^{-2\pi i mn/N}\right)\left(e^{2\pi i mn/N}\right)$$
$$= \sum_{k=0}^{N-1} e^{-2\pi i mk/N} e^{2\pi i kn/N}$$
$$= \sum_{k=0}^{N-1} e^{2\pi i k(n-m)/N}$$

from ①, this is $=0$ unless $n-m=0$

if $n=m$, then $r = e^{2\pi i/N \cdot 0} = e^0 = 1$

so we have $\sum_0^n ar^x = (n+1)a$

if $m=n$

$= (N-1)+1$

$= N$

so $FF^{\dagger} = \begin{pmatrix} \ddots & & 0 \\ & N & \\ 0 & & \ddots \end{pmatrix} = NI$ and we know $FF^{-1} = I$

$\rightarrow FF^{\dagger} = NFF^{-1}$

$\Rightarrow \boxed{F^{-1} = \frac{1}{N}F^{\dagger}}$