**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.

   ---

   We have $U = -\frac{e^2}{4\pi\epsilon_0 r}$. The kinetic energy is $\frac{p^2}{2m}$. We'll replace $p^2$ with $\hbar^2/4r^2$ from the Heisenberg uncertainty principle (squared), so the kinetic energy is $\hbar^2/8mr^2$. We can write our total energy then as

   $$E = -\frac{e^2}{4\pi\epsilon_0 r} + \frac{\hbar^2}{8mr^2}$$

   Differentiate w.r.t. $r$, and we get

   $$\frac{dE}{dr} = \frac{e^2}{4\pi\epsilon_0 r^2} - \frac{\hbar^2}{4mr^3}$$

   At the energy minimum, the derivative is zero, so we have

   $$\frac{e^2}{4\pi\epsilon_0 r^2} = \frac{\hbar^2}{4mr^3}$$

That gives us

$$r = \frac{\pi\hbar^2\epsilon_0}{me^2}$$

This is exactly a factor of 4 smaller than the Bohr radius. This shouldn't be a surprise since the hydrogen atom is not a minimum-uncertainty state, so $\delta x\delta p \geq \hbar/2$. In fact, we get the exact answer if we set $\delta x \delta p = \hbar$ without the factor of 2.

It's often said that quantum effects become important on the scale of atoms. Instead, an electron "wants" to spiral into a proton. It will keep doing this *until* quantum mechanics stops it from spiraling further in. A more correct view is to say that atoms are the size they are *because* of quantum mechanics.

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.

---

We have

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

Pull the $ikx$ into the second exponential, and factor out a $\frac{1}{2\sigma^2}$ to get:

$$\int_{-\infty}^{\infty} \exp(-\frac{1}{2\sigma^2}(x^2 - 2\sigma^2 ikx))dx$$

To complete the square, we know that $x - 2b = x - 2b + b^2 - b^2 = (x-b)^2 - b^2$. We have $2b = -2\sigma^2 ik$, so we need to subtract $(ik\sigma^2)^2 = -k^2\sigma^4$ inside the exponential. That gives:

$$\int_{-\infty}^{\infty} \exp(-\frac{1}{2\sigma^2}((x - \sigma^2 ik)^2 + k^2\sigma^4))dx$$

The final term no longer depends on $x$, so we can pull it out front. Note that $-\frac{1}{2\sigma^2}k^2\sigma^4 = -\frac{k^2\sigma^2}{2}$, so we get

$$\exp(-\frac{k^2\sigma^2}{2})\int_{-\infty}^{\infty}\exp(-\frac{1}{2\sigma^2}(x-\sigma^2 ik)^2)dx$$

We can do a change-of-variable $x' = x - ik\sigma^2$ with $dx' = dx$ to write the integral part as

$$\int_{-\infty+ik\sigma^2}^{\infty+ik\sigma^2}\exp(-x'^2/2\sigma^2)dx'$$

That is now the integral of a gaussian, but shifted off of the real axis. There are no poles in this analytic function, so any closed path integral has to be equal to zero. Draw a rectangle with long sides along the real axis and where the imaginary part is $k\sigma^2$. If you stretch that rectangle out to be infinitely long, the short sides don't contibute because the exponential goes to zero for large real $x$, and an extra imaginary phase won't change that. That means the integral along each of the long sides has to be equal, and so the integral always evaluates to $\sqrt{2\pi\sigma^2}$. It may seem rather remarkable that there's no dependence on $k$, but there isn't! You can try this out numericaly if you don't believe it.

Just to recap, with all the factors put in:

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

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 $N-1$. First, show that

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

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.

———————————————————————————— There are lots of ways to show the first part. We can take a geometric series $\sum_{k=0}^{\infty} r^k = 1/(1-r)$. If you have a partial sum then you get $\sum_{\alpha=0}^{k} r^\alpha = (1-r^n)/(1-r)$ by noting that the sum from n to infinity is $r^n$ times sum from 0 to infinity. For the DFT, $r = \exp(-2\pi ix/N)$, so we have the numerator is $1 - \exp(-2\pi ix/N)^N = 1 - \exp(-2\pi ix)$. For integer $x$, this always equals zero, so the sum is zero. Unless, of course, the denominator also equals zero, which happens when $1 - \exp(-2\pi ix/N)$ equals zero. For that to happen the exponential has to be 1, which happens when $x$ is an integer multiple of $N$, including $x = 0$.

For the second part, we know $F(k) = \sum_0^{N-1} \exp(-2\pi ikx/N) f(x)$. We can write that as a dot product between $\exp(-2\pi ikx/N)$ and $f(x)$ when the $x$'x are discrete. For every $k$, the vector $f(x)$ is in common, so we can stack the rows $\exp(-2\pi ikx/N)$ to make a matrix that gives us the DFT with one matrix multiply. The $x, k$'th entry is $\exp(-2\pi ikx/N)$, so the matrix is symmetric because the value doesn't change when you swap $x$ and $k$.

Finally, we know that each row/column is orthogonal from the first part, so the matrix is very nearly it's own inverse. It's not quite, though, because we want the diagonal elements to be one. The simplest way to have that happen is to have the $k$'th row of the inverse be $\exp(2\pi ikx/N)$, because now when we dot that row with $\exp(-2\pi ikx/N)$, we get the sum of $\exp(0)$, which equals $N$. So, we can make the inverse by taking $\exp(2\pi ikx/N)$ and dividing by $N$. Since the matrix is symmetric, a dagger is equivalent to a conjugate, so $F^{-1} = 1/NF^\dagger$.