Sept. 10, 2007

Chem. 1410

Problem Set 2, due Sept. 17, 2007

Do the following problems from Engel; these are *not* to be handed in for grading; solutions will be distributed via .pdf.

Chapter 1: P2.5, P2.10, P2.15, P2.18, P2.23, P.2.30

The following two problems are to be handing in for grading:

(1) **Fundamental Commutation Relation.** Show that for an arbitrary (differentiable) function $F(x)$:

$$[\hat{x}\hat{p} - \hat{p}\hat{x}]F(x) = i\hbar F(x) \qquad [1]$$

Note: $\hat{x}\hat{p}F(x) = \frac{\hbar}{i} x\partial F(x)/dx$; $\hat{p}\hat{x}F(x) = \frac{\hbar}{i}\partial\left[xF(x)\right]/dx$.

(Since Eq. 1 holds for any $F(x)$, we can say that $[\hat{x}\hat{p} - \hat{p}\hat{x}] = i\hbar$. This is known as the fundamental commutation relation, which is discussed further in Engel Chapt. 6.)

(2) **Fourier Series**. Consider the function $f(x) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp(\frac{-x^2}{2\sigma^2})$, i.e., a unit normed Gaussian of width σ. Here we will carry out a Fourier series expansion of this function on the fundamental interval $[-\pi,\pi]$. That is, consider the expansion:

$$f_N(x) = a_0 + \sum_{j=1}^{N}\left[b_j \sin(jx) + c_j \cos(jx)\right]$$

In the limit $N \to \infty$, and with the superposition coefficients chosen appropriately, then according to Fourier's Theorem $f_N(x) \to f(x)$ on the interval $[-\pi,\pi]$, and generates periodically repeating replicas of $f(x)$ on the interval $[-3\pi,-\pi]$, $[\pi,3\pi]$, etc.

Recall the formula for determining the superposition coefficient:

$$a_0 = \frac{1}{2\pi}\int_{-\pi}^{\pi} dx f(x) \;\; ; \;\; b_j = \frac{1}{\pi}\int_{=\pi}^{\pi} dx f(x)\sin(jx) \;\; ; \;\; c_j = \frac{1}{\pi}\int_{-\pi}^{\pi} dx f(x)\cos(jx) \qquad [2]$$

a) Show that $b_j = 0$ for all *j=1,2,…*

b) To evaluate a_0 and c_j, let us specialize to the case that $\sigma \ll \pi$, i.e. the Gaussian is well-localized in the interval $[-\pi, \pi]$. Then we can extend the integrals in Eq. 2 from $-\infty$ to ∞. [Why?]

c) Now, using the integral identity $\frac{1}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty} dx \exp(\frac{-x^2}{2\sigma^2})\cos(\gamma x) = \exp(-\gamma^2\sigma^2/2)$, show that:

i) $a_0 = \frac{1}{2\pi}$

ii) $c_j = \frac{1}{\pi}\exp(-j^2\sigma^2/2)$, $j=1,2,\ldots$

d) Consider the numerical value of $\sigma = 0.5$. This is the case that was plotted in the Supplemental notes. Plot $f(x), f_2(x), f_6(x)$ on the same graph. Verify that the Fourier series converges to the exact function by roughly *N=6*.

e) Finally, consider the numerical value $\sigma = 0.25$. (This Gaussian is twice as narrow as that considered in part d.) Is the Fourier series converged by *N*=6 in this case? If not, what value of *N* (roughly) is required for convergence? Can you give a qualitative reason for the trend you observe in the relation between the narrowness of the function *f(x)* and the number of Fourier components (value of *N*) required to represent it accurately via a Fourier series?