Chemistry 60649 — Fall 2008
Professor J. Daniel Gezelter — Due Fri. 10/3/2008

Problem Set 3

This problem set will concentrate on Matrix properties that we will begin using shortly in class.

1. a) Prove, using the definition of matrix elements and their complex conjugates, that

$$(\mathbf{AB})^\dagger = \mathbf{B}^\dagger \mathbf{A}^\dagger$$

   b) Show that the product of two Hermitian operators need not be Hermitian. Under what condition is the product of two Hermitian operators Hermitian?

2. The Trace.

   Consider an operator $\hat{G}$ whose eigenstates and eigenvalues are $|g\rangle$ and $\lambda_g$ respectively. That is,

$$\hat{G}|g\rangle = \lambda_g |g\rangle$$

   The trace of an operator is defined as follows:

$$\text{Tr}\, \hat{G} \equiv \sum_g \lambda_g$$

   a) Prove that

$$\text{Tr}\, \hat{G} = \sum_g \langle g|\hat{G}|g\rangle$$

   b) Show that

$$\text{Tr}\, \hat{G} = \sum_n \langle n|\hat{G}|n\rangle$$

   for any basis $|n\rangle$. (Here you can assume that the states $|g\rangle$ are denumerable.)

   c) Re-analyze part (b) by proving that the trace of an operator is invariant under a unitary transformation of the operator. That is,

$$\mathbf{G} \rightarrow \mathbf{U}^\dagger \mathbf{G} \mathbf{U} \text{ where } \mathbf{U}^\dagger \mathbf{U} = 1.$$

3. Suppose we have, again,

$$\hat{G}|g\rangle = \lambda_g |g\rangle$$

   Let's define a new operator $\hat{F}(\hat{G})$ which has a power series expansion in $\hat{G}$ about some point. Prove that

$$\langle g|\hat{F}(\hat{G})|g\rangle = F(\lambda_g)$$

   and

$$\langle g|\hat{F}(\hat{G})|g'\rangle = \delta_{gg'} F(\lambda_g)$$

4. The Dirac Delta function. Using the properties of the Dirac delta function, show that:

   a) $\int_{-\infty}^{\infty} x\delta(x)f(x)dx = 0$

   b) $\int_{-\infty}^{\infty} f(x)\frac{d}{dx}\delta(x)dx = -\int_{-\infty}^{\infty} \frac{df(x)}{dx}\delta(x)dx$

   c) $\int_{-\infty}^{\infty} \delta(x)f(x)dx = \int_{-\infty}^{\infty} \delta(-x)f(x)dx$