Chem. 540

Notes on Integrals

Functions of the form

$$f(x) = e^{-ax^2+bx}, \quad \mathrm{Re}\, a > 0$$

are called Gaussian. Integrals of Gaussian functions occur frequently in quantum mechanics. It can be shown that

$$\int_{-\infty}^{\infty} e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}}\, e^{b^2/4a}.$$

One not so well known techniques for evaluating certain integrals is to take a derivative with respect to a parameter. For example, suppose we want to calculate

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx.$$

Notice that $x^2 = -\frac{\partial}{\partial a} e^{-ax^2}$, so we find

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = -\frac{\partial}{\partial a}\int_{-\infty}^{\infty} e^{-ax^2} dx = -\frac{\partial}{\partial a}\sqrt{\frac{\pi}{a}} = \frac{1}{2}\sqrt{\pi}\, a^{-\frac{3}{2}}.$$

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