ASE 382R.6/ME 381Q.4 Molecular Gas Dynamics

Frequently occurring definite integrals

When dealing with distribution functions, several integrals appear regularly. The integrals tabulated in the back of the text are for limits of *0* and ±∞. When dealing with finite upper (or lower) bounds a few other integrals are useful - (1) the error function *erf(x)* and its complement *erfc(x),* and (2) the incomplete gamma function, $\Gamma(j,\alpha)$.

As noted in Problem II 5.1, the error function is defined by

$$erf(x) = \frac{2}{\sqrt{\pi}}\int_0^x \exp(-t^2)dt\,.$$

The complementary error function is given by

$$erfc(x) = 1 - erf(x).$$

Note the following:

$$erf(-x) = -\,erf(x)$$

$$erf(0) = 0$$

$$erf(\infty) = 1$$

Computer subroutines (and even spread-sheet functions) are available for computing *erf(x)*. Sketch a graph of e^{-t^2} and interpret *erf(x)* and *erfc(x)* graphically.

The incomplete gamma function $\Gamma(j,\alpha)$ arises when evaluating integrals of the form

$$\int_a^\infty v^n \exp(-\beta v^2)dv\,.$$

Such integrals are often referred to as *moments* of the distribution function. It is defined by

$$\Gamma(j,\alpha) = \int_a^\infty x^{j-1}e^{-x}dx$$

and one can show by direct substitution that

$$\int_{|a|}^\infty v^n \exp(-\beta v^2)dv = \frac{1}{2\beta^{(\frac{n+1}{2})}}\Gamma(\frac{n+1}{2},\beta a^2)$$

A recurrence relation exists for the incomplete gamma function that permits one to reduce *j* in steps when one wishes to do a numerical calculation.

$$\Gamma(j,\alpha) = (j-1)\Gamma(j-1,\alpha) + \alpha^{j-1}e^{-\alpha}$$

For odd powers of v (n odd) in the original integral, j becomes an integer and one finally has to use:

$$\Gamma(1,\alpha) = \int_a^\infty x^{1-1} e^{-x} dx = \int_a^\infty e^{-x} dx = e^{-\alpha}$$

Equivalently, using the substitution $\beta v^2 = y$ one could transform the integral to the form

$$\int^\infty y^m e^{-y} dy$$

where $m = (n-1)/2$ is an integer, and then integrate by parts. For even n, j is half-integral, and the recurrence relation finally requires one to use

$$\Gamma(\frac{1}{2},\alpha) = \sqrt{\pi}\, erfc(\sqrt{\alpha})$$

For the special case $\alpha=0$ we get the *(complete) gamma function*, that satisfies the recurrence relation

$$\Gamma(j) = (j-1)\Gamma(j-1)$$

which gives the following simple results

$$\Gamma(j) = (j-1)! \quad \textit{for integer } j$$

$$\Gamma(j) = (j-1)(j-2)\ldots\left(\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right) = (j-1)(j-2)\ldots\left(\frac{1}{2}\right)\sqrt{\pi} \quad \textit{for half-integer } j$$

On any test you can leave results directly in terms of $\Gamma(j,\alpha)$ or $erf(\alpha)$. On homework problems you should evaluate them numerically to get a feeling for orders of magnitude. The following results are useful:

$$\int_{\pm a}^\infty \exp(-\beta v^2) dv = \frac{\pi^{1/2}}{2\beta^{1/2}}\{1 \pm \mathrm{erf}(\sqrt{\beta}\, a\}$$

$$\int_{\pm a}^\infty v \exp(-\beta v^2) dv = \frac{\exp(-\beta a^2)}{2\beta}$$

$$\int_{\pm a}^\infty v^2 \exp(-\beta v^2) dv = \frac{\pi^{1/2}}{4\beta^{3/2}}\{1 \pm erf(\sqrt{\beta}\, a\} \pm \frac{(\sqrt{\beta} a)\exp(-\beta a^2)}{2\beta^{3/2}}$$

$$\int_{\pm a}^\infty v^3 \exp(-\beta v^2) dv = \frac{\exp(-\beta a^2)}{2\beta^2}(1+\beta a^2)$$

$$\int_{\pm a}^\infty v^4 \exp(-\beta v^2) dv = \frac{3\pi^{1/2}}{8\beta^{5/2}}\ \{1 \pm erf(\sqrt{\beta}\, a\} \pm \frac{(\sqrt{\beta} a)\exp(-\beta a^2)}{2\beta^{5/2}}\left(\frac{3}{2} + \beta a^2\right)$$

$$\int_{\pm a}^{\infty} v^5 \exp(-\beta v^2)dv = \frac{\exp(-\beta a^2)}{2\beta^3}(2 + 2\beta a^2 + \beta^2 a^4)$$

The special case $a = 0$, is dealt with in Appendix 1 of Vincenti and Kruger.
Occasionally one needs

$$\Gamma(0,\alpha) = \int_{\alpha}^{\infty} \frac{e^{-x}}{x} dx = E_1(\alpha) \, ,$$

where $E_1(\alpha)$ is the *exponential integral* (a standard integral that is tabulated and available in computer routines).

$$E_1(\alpha) = \int_{\alpha}^{\infty} \frac{e^{-x}}{x} dx = -\gamma - \ln\alpha - \sum_{n=1}^{\infty} \frac{(-1)^n \alpha^n}{n\, n!} \; ; \; \gamma = 0.57721\ 56649\ldots \text{ is } \textit{Euler's constant} \, .$$

Note that all those significant figures above are meant facetiously, and perhaps for code checking. In any practical calculation one does not know the answer to better than 3 or 4 significant figures because ***the accuracy of the answer is limited by the data, model, and assumptions needed to solve the problem.***