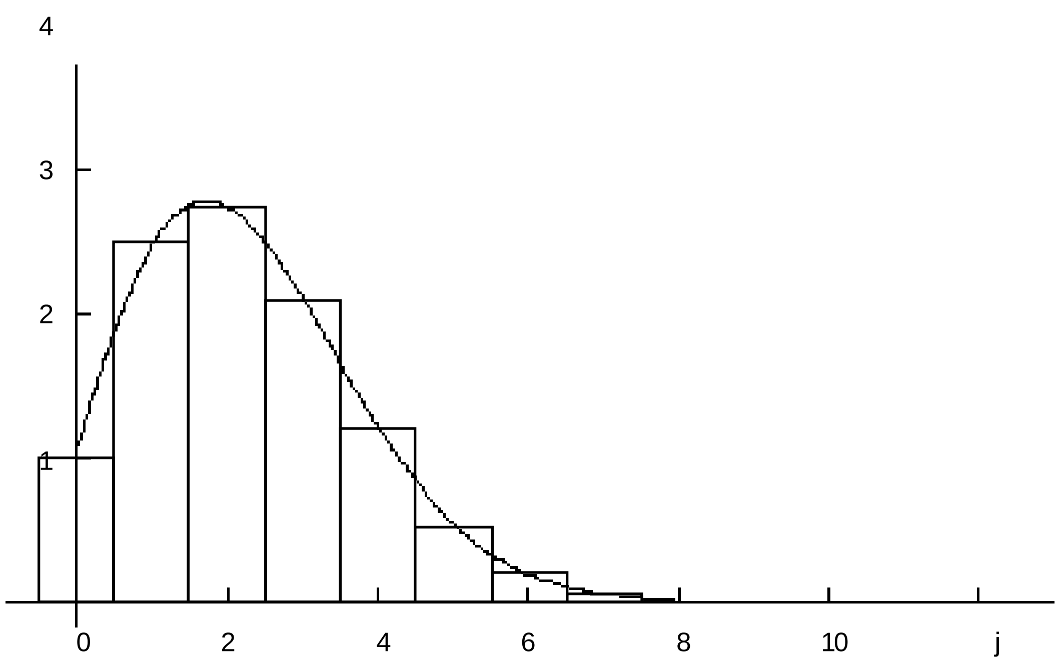
Converting Sums to Integrals

In physics one is occasionally faced with summations which cannot be evaluated exactly. In some cases these sums can be conveniently calculated on the computer. In other cases they can be rather accurately approximated by converting them to integrations.

Consider for example the following sum which arises (in statistical physics) in the evaluation of the partition function of a rotating (quantum) diatemic molecule.

$$Z = \sum_{j=o}^{\infty} (2j+1)\ e^{-j(j+1)\varepsilon_o / k_B T} \tag{1}$$

(k_B is Boltzmann's constant (T is the temperature) $\varepsilon_o = \hbar^2/2I$ where I is the moment of inertia of the molecule and j is the rotational quantum number. The factor (2j+1) arises from the degeneracy of the jth level.)



The sum as written cannot be evaluated exactly. Let $a=\varepsilon_o / k_B T$ for convenience and then note that when a is small (high temperature limit), the exponential in the sum varies rather slowly. The figure above shows the variation of the entire summand with j for the case a=0.1.

Superimposed on the plot is a histogram-like version of the plot with boxes of unit width. A little thought will convince you that the area under the histogram, is precisely the value of the sum in eg. (1). Since the area under the histogram and that under the curve are in reasonable agreement we could take

$$Z \quad \int_o^{\infty} (2j+1)\, e^{-aj(j+1)}\, dj \qquad (2)$$

This integral can be done by the technique of completing the square.
(See the Introduction to Integration section).