Evaluation of $\bar{u}_{phn}$ requires that the Debye integral be evaluated over a range of arguments.[16] To facilitate its evaluation Table IIID-2, at the conclusion of the unit, lists values of the function

$$D(x_D) \equiv \frac{3}{x_D^3}\int_0^{x_D} \frac{x^3 dx}{(e^x-1)} \quad \text{where} \quad x_D = \frac{\theta_D}{T} \qquad \text{(IIID-14)}$$

When it is written in terms of $D(x_D)$ the phonon energy is

$$\bar{u}_{phn}(T,\theta_D) = 3\,\bar{R}T\,D(x_D) \qquad \text{(IIID-13b)}$$

The lattice contribution to the specific heat (see Exmp. 6) and the entropy (see Exer. 12) can be formulated in terms of the same function.[17]

$$\bar{c}_{v,phn}(x_D) = \left(\frac{\partial \bar{u}_{phn}}{\partial T}\right)_{\bar{v}} = 3\bar{R}\left[4D(x_D) - \frac{3x_D}{e^{x_D}-1}\right] \qquad \text{(IIID-15)}$$

$$\bar{s}_{phn} = \bar{R}\left[4D(x_D) - 3\,ln\,(1-e^{-x_D})\right] \qquad \text{(IIID-16)}$$

Note to the Student. The first of these developments requires differentiation of an integral, viz., the use of Leibnitz Rule. The purpose of these developments is to aid the student in understanding eqns IIID-15 and 16. Neither of these developments is representative of student requirements. The use of the relationships to determine properties is a student objective, see Exer. 13.

Example 6. Differentiate eqn. IIID-13a to derive eqn. IIID-15.

The development consists of the following differentiation

$$\bar{c}_{v,phn} = \left(\frac{\partial \bar{u}_{phn}}{\partial T}\right)_{\bar{v}} = \frac{\partial}{\partial T}\left[+\frac{9\bar{R}}{\theta_D^3}T^4\int_0^{\theta_D/T}\frac{x^3dx}{(e^x-1)}\right]_v$$

$$= 9\bar{R}\left\{4\left(\frac{T}{\theta_D}\right)^3\int_0^{\theta_D/T}\frac{x^3dx}{(e^x-1)} + \frac{T^4}{\theta_D^3}\frac{d}{dT}\left[\int_0^{\theta_D/T}\frac{x^3dx}{(e^x-1)}\right]\right\}$$

In the second term the variable appears in the upper limit of the integral. Its differentiation requires the use of Leibnitz Rule.

$$\frac{d}{dx}\int_{a(x)}^{b(x)} f(x,\xi)d\xi = f[(x,\ b(x)]\frac{db(x)}{dx} - f[x,\ a(x)]\frac{da(x)}{dx} + \int_{a(x)}^{b(x)}\frac{\partial}{\partial x}[f(x,\xi)d\xi$$

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[16] Eqn. IIID-12 implies that the minimum lattice energy is zero. But in fact, the minimum energy of each linear oscillator is $h\nu/2$. Thus the zero point energy is

$$U^\circ_{phn} = \int_0^{\nu_D}\frac{h\nu}{2}g(\nu)d\nu \quad \text{or} \quad \bar{u}^\circ_{phn} = \frac{9}{8}\bar{R}\theta_D$$

We omit this term for simplicity, since it affects only the level of energy not its change with temperature.

[17] As formulated, the Debye model predicts the specific heat at constant volume, c_v. Applications to solids require the specific heat at constant pressure, c_p, almost exclusively. A prediction of the difference between these two functions can be made based on the Debye model, but this requires that we predict the variation of the Debye temperature with volume, see Ref. 5. We omit this development and continue to depend on eqn. ID-6 to account for the difference between specific heats.

$$c_p - c_v = \frac{Tv\beta^2}{\kappa}$$