

Figure 3.9 Heat capacity at constant volume of one molecule of H_2 in the gas phase. The vertical scale is in fundamental units; to obtain a value in conventional units, multiply by k_B . The contribution from the three translational degrees of freedom is $\frac{3}{2}$; the contribution at high temperatures from the two rotational degrees of freedom is 1; and the contribution from the potential and kinetic energy of the vibrational motion in the high temperature limit is 1. The classical limits are attained when $\tau \gg$ relevant energy level separations.

applies to the harmonic oscillator in the classical limit. The quantum results for the harmonic oscillator and for the diatomic rotator are derived in Problems 3 and 6, respectively. At high temperatures the classical limits are attained, as in Figure 3.9.

Example: Entropy of mixing. In Chapter 1 we calculated the number of possible arrangements of A and B in a solid made up of N-t atoms A and t atoms B. We found in (1.20) for the number of arrangements:

$$g(N,t) = \frac{N!}{(N-t)! \ t!}.$$
 (78)

The entropy associated with these arrangements is

$$\sigma(N,t) = \log g(N,t) = \log N! - \log(N-t)! - \log t!, \qquad (79)$$

and is plotted in Figure 3.10 for N = 20. This contribution to the total entropy of an alloy