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A Short Simple Evaluation of Expressions of the Debye–Waller Form

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Averages like those encountered in the theory of the Debye-Waller factor are evaluated in one sentence.

WHEN calculating absorption, emission, or scattering cross sections for crystalline matter in the harmonic approximation one needs the thermal equilibrium average of exponentials of operators linear in the atomic displacements and/or momenta:

$$\langle e^{\sum c_i a_i + d_i a_i^\dagger}\rangle = \mathrm{Tr}\, e^{-\beta H}\, e^{\sum c_i a_i + d_i a_i^\dagger}/\mathrm{Tr}\, e^{-\beta H},$$
$$H = \sum \omega_i(a_i^\dagger a_i + \tfrac{1}{2}),\quad \beta = 1/k_B T,\quad [a_i, a_j^\dagger] = \delta_{ij}. \tag{1}$$

This can be evaluated in a variety of ways,[1] some difficult, some direct, but all annoyingly cumbersome considering the simplicity of the final form. Here is a derivation as simple as the result:

As in most approaches, begin by using the well-known formula[1]

$$e^{A+B} = e^A\, e^B\, e^{-\frac{1}{2}[A,B]} \qquad ([A, B] \text{ a } c\text{-number}) \tag{2}$$

to reduce (1) to

$$\langle e^{\sum c_i a_i + d_i a_i^\dagger}\rangle = \langle e^{\sum c_i a_i}\, e^{\sum d_i a_i^\dagger}\rangle\, e^{-\frac{1}{2}\sum c_i d_i}, \tag{3}$$

but instead of proceeding with the clumsy direct evaluation of

$$g(c_i d_i) = \langle e^{\sum c_i a_i}\, e^{\sum d_i a_i^\dagger}\rangle, \tag{4}$$

note that (2) also entitles one to conclude

$$\langle e^{\sum c_i a_i + d_i a_i^\dagger}\rangle = \langle e^{\sum d_i a_i^\dagger}\, e^{\sum c_i a_i}\rangle\, e^{\frac{1}{2}\sum c_i d_i}, \tag{5}$$

which is consistent with (3) only if

$$g(c_i d_i) = e^{\sum c_i d_i}\langle e^{\sum d_i a_i^\dagger}\, e^{\sum c_i a_i}\rangle$$
$$= e^{\sum c_i d_i}\langle e^{\beta H}\, e^{\sum c_i a_i}\, e^{-\beta H}\, e^{\sum d_i a_i^\dagger}\rangle$$

(cyclical permutation within trace)

$$= e^{\sum c_i d_i}\langle e^{\sum c_i e^{\beta H} a_i e^{-\beta H}}\, e^{\sum d_i a_i^\dagger}\rangle$$
$$= e^{\sum c_i d_i}\langle e^{\sum c_i e^{-\beta\omega_i} a_i}\, e^{\sum d_i a_i^\dagger}\rangle$$

(harmonic approximation)

$$= e^{\sum c_i d_i} g(c_i\, e^{-\beta\omega_i}, d_i), \tag{6}$$

from which identity it follows at once (by iteration or induction on n) that

$$g(c_i d_i) = e^{\sum c_i d_i (1 + e^{-\beta\omega_i} + \cdots + e^{-n\beta\omega_i})} g(c_i\, e^{-(n+1)\beta\omega_i}, d_i), \tag{7}$$

and hence, taking the limit $n \to \infty$ (each ω_i is positive),

$$g(c_i d_i) = e^{\sum c_i d_i (1 - e^{-\beta\omega_i})^{-1}} g(0, d_i), \tag{8}$$

which, since it follows trivially from (4) that

$$g(0, d_i) = \langle e^{\sum d_i a_i^\dagger}\rangle = 1, \tag{9}$$

completes the derivation:

$$\langle e^{\sum c_i a_i + d_i a_i^\dagger}\rangle = e^{-\frac{1}{2}\sum c_i d_i} g(c_i d_i)$$
$$= e^{\frac{1}{2}\sum c_i d_i \coth \frac{1}{2}\beta\omega_i}. \tag{10}$$

[1] See, for instance, A. A. Maradudin, E. W. Montroll, and G. H. Weiss, Solid State Phys. Suppl. 3, 239 (1963).