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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:

\[ \langle e^{\sum \omega_ia_i^*a_i + \frac{1}{2}} \rangle = \text{Tr} \left( e^{-\beta H} \right) e^{\sum \omega_ia_i^*a_i} / \text{Tr} \left( e^{-\beta H} \right), \]

\[ H = \sum \omega_i(a_i^*a_i + \frac{1}{2}), \quad \beta = 1/k_BT, \quad [a_i, a_i^*] = \delta_{ij}. \]

(1)

This can be evaluated in a variety of ways, 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

\[ e^Ae^B = e^{A+B} \quad ([A, B] \text{ a c-number}) \]

to reduce (1) to

\[ \langle e^{\sum \omega_i^2a_i^*a_i + \frac{1}{2}} \rangle = \langle e^{\sum \omega_i^2a_i^*a_i} \rangle e^{-\frac{1}{2}\sum \omega_i^2}, \]

(3)

but instead of proceeding with the clumsy direct evaluation of

\[ g(c, d) = \langle e^{\sum \omega_i^2a_i^*a_i} \rangle, \]

(4)

note that (2) also entitles one to conclude

\[ \langle e^{\sum \omega_i^2a_i^*a_i + \frac{1}{2}} \rangle = \langle e^{\sum \omega_i^2a_i^*a_i} \rangle e^{\frac{1}{2}\sum \omega_i^2}, \]

(5)

which is consistent with (3) only if

\[ g(c, d) = e^{\sum \omega_i^2a_i^*a_i + \frac{1}{2}} g(c, d), \]

(6)

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

\[ g(c, d) = e^{\sum \omega_i^2a_i^*a_i + \frac{1}{2}} g(0, d), \]

(7)

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

\[ g(c, d) = e^{\sum \omega_i^2a_i^*a_i} g(0, d), \]

(8)

which, since it follows trivially from (4) that

\[ g(0, d) = \langle e^{\sum \omega_i^2a_i^*a_i} \rangle = 1, \]

(9)

completes the derivation:

\[ \langle e^{\sum \omega_i^2a_i^*a_i + \frac{1}{2}} \rangle = e^{\frac{1}{2}\sum \omega_i^2} g(c, d). \]