THERMAL AVERAGE OF A HARMONIC OSCILLATOR

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Reference: Tom Lancaster and Stephen J. Blundell, *Quantum Field Theory for the Gifted Amateur*, (Oxford University Press, 2014), Problem 21.1.
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L&B define the density operator as

$$\rho = \frac{e^{-\beta H}}{Z} \tag{1}$$

where $\beta = k_B T$ (with k_B being the Boltzmann constant and T the temperature) and Z being the partition function, defined as

$$Z = \sum_\lambda \left\langle \lambda \middle| e^{-\beta H} \middle| \lambda \right\rangle \tag{2}$$

$$= \mathrm{Tr}\left[e^{-\beta H}\right] \tag{3}$$

where $|\lambda\rangle$ is an eigenstate of the Hamiltonian H and Tr indicates a matrix trace.

The thermal average of an operator A is given by

$$\langle A \rangle_t = \mathrm{Tr}\left[\rho A\right] \tag{4}$$

This is related to the density matrix we encountered earlier, although in that case, no mention was made of a partition function or temperature.

For a quantum harmonic oscillator, the Hamiltonian is given by

$$H = \omega a^\dagger a \tag{5}$$

where ω is the energy of a single quantum and $a^\dagger$ and a are the creation and annihilation operators of a quantum state. The number operator is

$$n = a^\dagger a \tag{6}$$

The thermal average of the number of excitations is therefore

$$\langle n\rangle_t = \left\langle a^\dagger a\right\rangle \tag{7}$$
$$= \mathrm{Tr}\left[\rho a^\dagger a\right] \tag{8}$$
$$= \frac{\sum_n \left\langle n\left|e^{-\beta\omega H}a^\dagger a\right|n\right\rangle}{Z} \tag{9}$$
$$= \frac{\sum_n e^{-\beta\omega n}n}{Z} \tag{10}$$

In this case, the set of eigenstates of the Hamiltonian are $|n\rangle$, the states with a number n of energy quanta ω. We can therefore work out the partition function as

$$Z = \sum_n \left\langle n\left|e^{-\beta\omega a^\dagger a}\right|n\right\rangle \tag{11}$$
$$= \sum_n e^{-\beta\omega n} \tag{12}$$

This is a geometric series so we can use the usual formula for summing the series (given that $e^{-\beta\omega} < 1$ so the series converges) to get

$$Z = \frac{1}{1-e^{-\beta\omega}} \tag{13}$$

The numerator in 10 can be found if we define a parameter $x \equiv \beta\omega$ so

$$Z = \sum_n e^{-xn} \tag{14}$$
$$\sum_n e^{-\beta\omega n}n = \sum_n ne^{-xn} \tag{15}$$
$$= -\frac{\partial Z}{\partial x} \tag{16}$$

From this and 13 we find

$$\sum_n e^{-xn}n = \frac{e^{-x}}{\left(1-e^{-x}\right)^2} \tag{17}$$
$$= \frac{e^{-\beta\omega}}{\left(1-e^{-\beta\omega}\right)^2} \tag{18}$$

Plugging this and 13 back into 10 we have

$$\langle n\rangle_t = \frac{e^{-\beta\omega}}{\left(1-e^{-\beta\omega}\right)^2}\left(1-e^{-\beta\omega}\right) \tag{19}$$

$$= \frac{e^{-\beta\omega}}{1-e^{-\beta\omega}} \tag{20}$$

$$= \frac{1}{e^{\beta\omega}-1} \tag{21}$$

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