Quantum Mechanical Partition Function

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References

- Laine and Vuorinen, "Basics of Thermal Field Theory", Chapter 1:
  https://arxiv.org/pdf/1701.01554.pdf

Quantum Mechanics

- Schrödinger Equation, 1D (non-relativistic)

$$i\frac{\partial}{\partial t}\Psi(t,x) = \hat{\mathrm{H}}\,\Psi(t,x)\,, \quad \hat{\mathrm{H}} = -\frac{\partial_x^2}{2m} + \hat{\mathrm{V}}(x) \tag{2.1}$$

- Separation of Variables:

$$\Psi(t,x) = e^{-i\hat{\mathrm{H}}t}\psi(x) \tag{2.2}$$

- Time-independent Schrödinger Equation

$$\hat{\mathrm{H}}\psi(x) = E\psi(x)\,. \tag{2.3}$$

Partition Function

- Partition function Z(T) defines key thermodynamic properties of system at temperature T
- Having Z(T) allows one to calculate the free energy F and entropy S (and others):

$$F = -T \ln Z\,, \quad S = -\frac{\partial F}{\partial T}\,. \tag{2.4}$$

Partition Function

- In stat. mech., it is customary to denote the inverse temperature as

$$\beta \equiv \frac{1}{T} \tag{2.5}$$

- The partition function is defined as

$$\mathrm{Z}(T) = \mathrm{Tr}\left[e^{-\beta \hat{\mathrm{H}}}\right] . \tag{2.6}$$

Partition Function

- Using energy eigenstates $|n\rangle$ as basis we have

$$\hat{\mathrm{H}}|n\rangle = E_n|n\rangle\,. \tag{2.7}$$

- For simplicity, let's take basis to be labelled by discrete $n = 0, 1, 2, \ldots$
- Then $\mathrm{Z}(T) = \mathrm{Tr}\left[e^{-\beta\hat{\mathrm{H}}}\right]$ becomes

$$\mathrm{Z}(T) = \sum_{n=0}^{\infty}\langle n|e^{-\beta\hat{\mathrm{H}}}|n\rangle \tag{2.8}$$

Partition Function

- Using energy eigenstates $|n\rangle$ as basis we have

$$\hat{\mathrm{H}}|n\rangle = E_n|n\rangle\,. \tag{2.11}$$

- For simplicity, let's take basis to be labelled by discrete $n = 0, 1, 2, \ldots$
- Then $\mathrm{Z}(T) = \mathrm{Tr}\left[e^{-\beta\hat{\mathrm{H}}}\right]$ becomes

$$\mathrm{Z}(T) = \sum_{n=0}^{\infty}\langle n|e^{-\beta\hat{\mathrm{H}}}|n\rangle = \sum_{n=0}^{\infty}\langle n|e^{-\beta E_n}|n\rangle \tag{2.12}$$

Example 1

- Let's do an example for the QM partition function of the Harmonic Oscillator
- Harmonic Oscillator Hamiltonian

$$\hat{\mathrm{H}} = -\frac{1}{2m}\partial_x^2 + \frac{m\omega^2\hat{x}^2}{2}\,. \tag{2.13}$$

- Energy eigenstates are

$$E_n = \left(n + \frac{1}{2}\right)\omega\,. \tag{2.14}$$

- Therefore

$$Z(T) = \sum_{n=0}^{\infty} e^{-\beta\omega\left(n+\frac{1}{2}\right)} = e^{-\frac{\beta\omega}{2}}\sum_{n=0}^{\infty} e^{-\beta\omega n} = \frac{e^{-\frac{\beta\omega}{2}}}{1-e^{-\beta\omega}} \tag{2.15}$$

Example 1

- Make result look nicer:

$$Z(T) = \frac{e^{-\frac{\beta\omega}{2}}}{1 - e^{-\beta\omega}} = \frac{1}{e^{\frac{\beta\omega}{2}} - e^{-\frac{\beta\omega}{2}}} = \frac{1}{2\sinh\left[\frac{\beta\omega}{2}\right]} \tag{2.16}$$