Appendix D: Partition Function, Polarization, and Moment Generating Function for N Isochronous Spins

D.1 Partition Function

The thermal-equilibrium density operator for a system of N isochronous spins ½ at temperature T is given by

$$\rho_0 = \frac{1}{Q} e^{-H/k_B T}, \tag{D.1}$$

where

$$Q \equiv Tr\left\{e^{-H/k_B T}\right\} \tag{D.2}$$

denotes the partition function, and

$$H = -\hbar\omega_0 I_z \tag{D.3}$$

denotes the Hamiltonian, with ω_0 the Larmor frequency of the spins and

$$I_z = \sum_{j=1}^{N} I_{z,j} \tag{D.4}$$

the z-component of the total dimensionless angular momentum. Let

$$x \equiv \frac{\hbar\omega_0}{k_B T} \,. \tag{D.5}$$

Then

$$Q = Tr\left\{e^{xI_z}\right\} = Tr\left\{\prod_{j=1}^{N} e^{xI_{z,j}}\right\}. \tag{D.6}$$

If we expand each exponential in powers of $I_{z,j}$ and note that, for spin ½ operators, $I_{z,j}^2 = \frac{1}{4}\mathbf{1}$, we find that

$$Q = Tr\left\{\prod_{j=1}^{N}\left(\mathbf{1}\cosh\left(\frac{x}{2}\right) + 2I_{z,j}\sinh\left(\frac{x}{2}\right)\right)\right\}. \tag{D.7}$$

Expansion of the product yields a sum of operators, only one of which, $\mathbf{1}$, has nonzero trace ($Tr\{\mathbf{1}\} = 2^N$). Thus,

$$Q = 2^N\left(\cosh\frac{x}{2}\right)^N. \tag{D.8}$$

D.2 Polarization

Let us consider a Boltzmann distribution of spins ½ in two energy levels $\varepsilon_\pm = \pm\frac{1}{2}\hbar\omega_0$. We define the polarization, p, as the difference in the populations of the energy levels, normalized to unity:

$$p \equiv \frac{n_- - n_+}{n_- + n_+} = \frac{e^{+\frac{1}{2}x} - e^{-\frac{1}{2}x}}{e^{+\frac{1}{2}x} + e^{-\frac{1}{2}x}} = \tanh\frac{x}{2}\,. \tag{D.9}$$

D.3 Moment generating function

The moment generating function, defined by

$$G(s) = \left\langle e^{isI_z} \right\rangle , \tag{D.10}$$

is used in Chapter 5 to calculate expectation values of powers of I_z. With the equilibrium density operator ρ_0 and the parameter x defined as above, we have

$$G(s) = \frac{1}{Q} Tr\left\{ e^{xI_z} e^{isI_z} \right\} = \frac{1}{Q} Tr\left\{ e^{(x+is)I_z} \right\}. \tag{D.11}$$

In correspondence with Equations D.6–D.8, this may be written

$$G(s) = \frac{1}{Q} Tr\left\{ e^{(x+is)I_z} \right\} = \frac{1}{Q} 2^N \cosh^N\left(\frac{x+is}{2}\right) = \frac{\cosh^N\left(\frac{x+is}{2}\right)}{\cosh^N\left(\frac{x}{2}\right)} = \left(\frac{\cosh\left(\frac{x+is}{2}\right)}{\cosh\left(\frac{x}{2}\right)} \right)^N . \tag{D.12}$$

The hyperbolic cosine in the numerator may be expanded:

$$\cosh\left(\frac{x+is}{2}\right) = \cosh\left(\frac{x}{2}\right)\cos\left(\frac{s}{2}\right) + i \sinh\left(\frac{x}{2}\right)\sin\left(\frac{s}{2}\right). \tag{D.13}$$

Substitution of Equations D.9 and D.13 into Equation D.12 yields the moment generating function in terms of the number of spins N and the polarization p:

$$G(s) = \left(\cos\frac{s}{2} + ip \sin\frac{s}{2} \right)^N . \tag{D.14}$$