7.4: Variational Density Matrix Method

The variational principle

Suppose we are given a Hamiltonian $\hat{H}$. From this we construct the free energy, F:

$$\begin{aligned} F &= E - TS \\ &= Tr\,(\varrho\,\hat{H}) + k_B T\, Tr\,(\varrho\,\ln\varrho)\,. \end{aligned}$$

Here, ϱ is the *density matrix*[13]. A physical density matrix must be (i) normalized ($Tr\,\varrho = 1$), (ii) Hermitian, and (iii) non-negative definite (all the eigenvalues of ϱ must be non-negative).

Our goal is to extremize the free energy subject to the various constraints on ϱ. Let us assume that ϱ is diagonal in the basis of eigenstates of $\hat{H}$,

$$\varrho = \sum_\gamma P_\gamma \,|\,\gamma\,\rangle\langle\,\gamma\,|\,, \tag{7.4.1}$$

where P_γ is the probability that the system is in state $|\,\gamma\,\rangle$. Then

$$F = \sum_\gamma E_\gamma\, P_\gamma + k_B T \sum_\gamma P_\gamma \ln P_\gamma\,. \tag{7.4.2}$$

Thus, the free energy is a function of the set $\{P_\gamma\}$. We now extremize F subject to the normalization constraint. This means we form the extended function

$$F^*\big(\{P_\gamma\},\lambda\big) = F\big(\{P_\gamma\}\big) + \lambda\Big(\sum_\gamma P_\gamma - 1\Big)\,, \tag{7.4.3}$$

and then freely extremize over both the probabilities $\{P_\gamma\}$ as well as the Lagrange multiplier λ. This yields the Boltzmann distribution,

$$P_\gamma^{eq} = \frac{1}{Z}\,\exp(-E_\gamma/k_B T)\,, \tag{7.4.4}$$

where $Z = \sum_\gamma e^{-E_\gamma/k_B T} = Tr\,e^{-\hat{H}/k_B T}$ is the canonical partition function, which is related to λ through

$$\lambda = k_B T\,(\ln Z - 1)\,. \tag{7.4.5}$$

Note that the Boltzmann weights are, appropriately, all positive.

If the spectrum of $\hat{H}$ is bounded from below, our extremum should in fact yield a minimum for the free energy F. Furthermore, since we have freely minimized over all the probabilities, subject to the single normalization constraint, *any distribution* $\{P_\gamma\}$ other than the equilibrium one must yield a greater value of F.

Alas, the Boltzmann distribution, while exact, is often intractable to evaluate. For one-dimensional systems, there are general methods such as the transfer matrix approach which do permit an exact evaluation of the free energy. However, beyond one dimension the situation is in general hopeless. A family of solvable (“integrable") models exists in two dimensions, but their solutions require specialized techniques and are extremely difficult. The idea behind the variational density matrix approximation is to construct a tractable *trial* density matrix ϱ which depends on a set of variational parameters $\{x_\alpha\}$, and to minimize with respect to this (finite) set.

Variational density matrix for the Ising model

Consider once again the Ising model Hamiltonian,

$$\hat{H} = -\sum_{i<j} J_{ij}\,\sigma_i\,\sigma_j - H\sum_i \sigma_i\,. \tag{7.4.6}$$

The states of the system $|\,\gamma\,\rangle$ may be labeled by the values of the spin variables: $|\,\gamma\,\rangle \longleftrightarrow |\,\sigma_1,\sigma_2,\ldots\,\rangle$. We assume the density matrix is diagonal in this basis,

$$\varrho_N(\gamma|\gamma') \equiv \varrho(\gamma)\,\delta_{\gamma,\gamma'}\ , \tag{7.4.7}$$

where

$$\delta_{\gamma,\gamma'} = \prod_i \delta_{\sigma_i,\sigma_i'}\ . \tag{7.4.8}$$

Indeed, this is the case for the exact density matrix, which is to say the Boltzmann weight,

$$\varrho_N(\sigma_1,\sigma_2,\ldots) = \frac{1}{Z}\,e^{-\beta\hat{H}(\sigma_1,\ldots,\sigma_N)}\ . \tag{7.4.9}$$

We now write a *trial density matrix* which is a product over contributions from independent single sites:

$$\varrho_N(\sigma_1,\sigma_2,\ldots) = \prod_i \varrho(\sigma_i)\ , \tag{7.4.10}$$

where

$$\varrho(\sigma) = \left(\frac{1+m}{2}\right)\delta_{\sigma,1} + \left(\frac{1-m}{2}\right)\delta_{\sigma,-1}\ . \tag{7.4.11}$$

Note that we've changed our notation slightly. We are denoting by $\varrho(\sigma)$ the corresponding diagonal element of the matrix

$$\varrho = \begin{pmatrix} \frac{1+m}{2} & 0 \\ 0 & \frac{1-m}{2} \end{pmatrix}\ , \tag{7.4.12}$$

and the full density matrix is a tensor product over the single site matrices:

$$\varrho_N = \varrho\otimes\varrho\otimes\cdots\otimes\varrho\ . \tag{7.4.13}$$

Note that ϱ and hence ϱ_N are appropriately normalized. The variational parameter here is m, which, if ρ is to be non-negative definite, must satisfy $-1\le m\le 1$. The quantity m has the physical interpretation of the average spin on any given site, since

$$\langle\sigma_i\rangle = \sum_\sigma \varrho(\sigma)\,\sigma = m. \tag{7.4.14}$$

We may now evaluate the average energy:

$$\begin{aligned} E &= \mathsf{Tr}\,(\varrho_N\hat{H}) = -\sum_{i<j} J_{ij}\,m^2 - H\sum_i m \\ &= -\frac{1}{2}N\hat{J}\,(0)\,m^2 - NHm\ , \end{aligned}$$

where once again $\hat{J}\,(0)$ is the discrete Fourier transform of $J(\mathbf{R})$ at wavevector $\mathbf{q}=0$. The entropy is given by

$$\begin{aligned} S &= -k_B\,\mathsf{Tr}\,(\varrho_N\ln\varrho_N) = -Nk_B\,\mathsf{Tr}\,(\varrho\ln\varrho) \\ &= -Nk_B\left\{\left(\frac{1+m}{2}\right)\ln\left(\frac{1+m}{2}\right) + \left(\frac{1-m}{2}\right)\ln\left(\frac{1-m}{2}\right)\right\}. \end{aligned}$$

We now define the dimensionless free energy per site: $f\equiv F/N\hat{J}\,(0)$. We have

$$f(m,h,\theta) = -\frac{1}{2}\,m^2 - hm + \theta\left\{\left(\frac{1+m}{2}\right)\ln\left(\frac{1+m}{2}\right) + \left(\frac{1-m}{2}\right)\ln\left(\frac{1-m}{2}\right)\right\}, \tag{7.4.15}$$

where $\theta\equiv k_BT/\hat{J}\,(0)$ is the dimensionless temperature, and $h\equiv H/\hat{J}\,(0)$ the dimensionless magnetic field, as before. We extremize $f(m)$ by setting

$$\frac{\partial f}{\partial m} = 0 = -m - h + \frac{\theta}{2}\ln\left(\frac{1+m}{1-m}\right). \tag{7.4.16}$$

Solving for m, we obtain

$$m = \tanh\left(\frac{m+h}{\theta}\right) , \tag{7.4.17}$$

which is precisely what we found in Equation [isingmft].

[ferg] Variational field free energy $\Delta f = f(m,h,\theta) + \theta\,\ln 2$ *versus* magnetization m at six equally spaced temperatures interpolating between 'high' ($\theta = 1.25$, red) and 'low' ($\theta = 0.75$, blue) values. Top panel: $h = 0$. Bottom panel: $h = 0.06$.

Note that the optimal value of m indeed satisfies the requirement $|m| \le 1$ of non-negative probability. This nonlinear equation may be solved graphically. For $h = 0$, the unmagnetized solution $m = 0$ always applies. However, for $\theta < 1$ there are two additional solutions at m=\pm m\nd_\ssr{A}(\theta), with m\nd_\ssr{A}(\theta) =\sqrt{3(1-\theta)} + \CO\big((1-\theta)^{3/2}\big) for t close to (but less than) one. These solutions, which are related by the $\mathbb{Z}_2$ symmetry of the $h = 0$ model, are in fact the low energy solutions. This is shown clearly in figure [ferg], where the variational free energy $f(m,t)$ is plotted as a function of m for a range of temperatures interpolating between 'high' and 'low' values. At the *critical temperature* $\theta_c = 1$, the lowest energy state changes from being unmagnetized (high temperature) to magnetized (low temperature).

For $h > 0$, there is no longer a $\mathbb{Z}_2$ symmetry ($\sigma_i \to -\sigma_i \;\forall\, i$). The high temperature solution now has $m > 0$ (or $m < 0$ if $h < 0$), and this smoothly varies as t is lowered, approaching the completely polarized limit $m = 1$ as $\theta \to 0$. At very high temperatures, the argument of the $\tanh$ function is small, and we may approximate $\tanh(x) \simeq x$, in which case

$$m(h,\theta) = \frac{h}{\theta - \theta_c} \; . \tag{7.4.18}$$

This is called the *Curie-Weiss law*. One can infer θ_c from the high temperature susceptibility $\chi(\theta) = (\partial m/\partial h)_{h=0}$ by plotting χ^{-1} *versus* θ and extrapolating to obtain the θ-intercept. In our case, $\chi(\theta) = (\theta - \theta_c)^{-1}$. For low θ and weak h, there are two inequivalent minima in the free energy.

When m is small, it is appropriate to expand $f(m,h,\theta)$, obtaining

$$f(m,h,\theta) = -\theta\,\ln 2 - hm + \frac{1}{2}\,(\theta - 1)\,m^2 + \frac{\theta}{12}\,m^4 + \frac{\theta}{30}\,m^6 + \frac{\theta}{56}\,m^8 + \ldots \; . \tag{7.4.19}$$

This is known as the *Landau expansion* of the free energy in terms of the *order parameter* m. An order parameter is a thermodynamic variable ϕ which distinguishes ordered and disordered phases. Typically $\phi = 0$ in the disordered (high temperature) phase, and $\phi \neq 0$ in the ordered (low temperature) phase. When the order sets in continuously, when ϕ is continuous across θ_c, the phase transition is said to be *second order*. When ϕ changes abruptly, the transition is *first order*. It is also quite commonplace to observe phase transitions between two ordered states. For example, a crystal, which is an ordered state, may change its lattice structure, say from a high temperature tetragonal phase to a low temperature orthorhombic phase. When the high T phase possesses the same symmetries as the low T phase, as in the tetragonal-to-orthorhombic example, the transition may be second order. When the two symmetries are completely unrelated, for example in a hexagonal-to-tetragonal transition, or in a transition between a ferromagnet and an antiferromagnet, the transition is in general first order.

Throughout this discussion, we have assumed that the interactions J_{ij} are predominantly *ferromagnetic*, $J_{ij} > 0$, so that all the spins prefer to align. When $J_{ij} < 0$, the interaction is said to be *antiferromagnetic* and prefers anti-alignment of the spins ($\sigma_i\,\sigma_j = -1$). Clearly not every pair of spins can be anti-aligned – there are two possible spin states and a thermodynamically extensive number of spins. But on the square lattice, for example, if the only interactions J_{ij} are between nearest neighbors and the interactions are antiferromagnetic, then the lowest energy configuration ($T = 0$ ground state) will be one in which spins on opposite sublattices are anti-aligned. The square lattice is *bipartite* – it breaks up into two interpenetrating sublattices A and B (which are themselves square lattices, rotated by 45° with respect to the original, and with a larger lattice constant by a factor of $\sqrt{2}$), such that any site in A has nearest neighbors in B, and *vice versa*. The honeycomb lattice is another example of a bipartite

lattice. So is the simple cubic lattice. The triangular lattice, however, is not bipartite (it is *tripartite*). Consequently, with nearest neighbor antiferromagnetic interactions, the triangular lattice Ising model is highly *frustrated*. The moral of the story is this: antiferromagnetic interactions can give rise to complicated magnetic ordering, and, when frustrated by the lattice geometry, may have finite specific entropy even at $T = 0$.

Mean Field Theory of the Potts Model

The Hamiltonian for the Potts model is

$$\hat{H} = -\sum_{i<j} J_{ij}\,\delta_{\sigma_i,\sigma_j} - H\sum_i \delta_{\sigma_i,1}\,. \tag{7.4.20}$$

Here, $\sigma_i \in \{1,\ldots,q\}$, with integer q. This is the so-called 'q-state Potts model'. The quantity H is analogous to an external magnetic field, and preferentially aligns (for $H > 0$) the local spins in the $\sigma = 1$ direction. We will assume $H \geq 0$.

The q-component set is conveniently taken to be the integers from 1 to q, but it could be anything, such as

$$\sigma_i \in \{\text{tomato, penny, ostrich, Grateful Dead ticket from 1987, } \ldots\}\,. \tag{7.4.21}$$

The interaction energy is $-J_{ij}$ if sites i and j contain the same object (q possibilities), and 0 if i and j contain different objects ($q^2 - q$ possibilities).

The two-state Potts model is equivalent to the Ising model. Let the allowed values of σ be ± 1. Then the quantity

\[\delta_{\sigma,\sigma'}=\half + \half\,\sigma\sigma'\\]

equals 1 if $\sigma = \sigma'$, and is zero otherwise. The three-state Potts model cannot be written as a simple three-state Ising model, one with a bilinear interaction $\sigma\,\sigma'$ where $\sigma \in \{-1, 0, +1\}$. However, it is straightforward to verify the identity

$$\delta_{\sigma,\sigma'} = 1 + \frac{1}{2}\,\sigma\sigma' + \frac{3}{2}\,\sigma^2\sigma'^2 - (\sigma^2 + \sigma'^2)\,. \tag{7.4.22}$$

Thus, the $q = 3$-state Potts model is equivalent to a $S = 1$ (three-state) Ising model which includes both bilinear $(\sigma\sigma')$ and biquadratic $(\sigma^2\sigma'^2)$ interactions, as well as a local field term which couples to the square of the spin, σ^2. In general one can find such correspondences for higher q Potts models, but, as should be expected, the interactions become increasingly complex, with bi-cubic, bi-quartic, bi-quintic, terms. Such a formulation, however, obscures the beautiful S_q symmetry inherent in the model, where S_q is the permutation group on q symbols, which has $q!$ elements.

Getting back to the mean field theory, we write the single site variational density matrix ϱ as a diagonal matrix with entries

$$\varrho(\sigma) = x\,\delta_{\sigma,1} + \left(\frac{1-x}{q-1}\right)\left(1 - \delta_{\sigma,1}\right)\,, \tag{7.4.23}$$

with $\varrho_N(\sigma_1,\ldots,\sigma_N) = \varrho(\sigma_1)\cdots\varrho(\sigma_N)$. Note that $\mathsf{Tr}\,(\varrho) = 1$. The variational parameter is x. When $x = q^{-1}$, all states are equally probable. But for $x > q^{-1}$, the state $\sigma = 1$ is preferred, and the other $(q-1)$ states have identical but smaller probabilities. It is a simple matter to compute the energy and entropy:

$$\begin{aligned} E = \mathsf{Tr}\,(\varrho_N \hat{H}) &= -\frac{1}{2}N\hat{J}\,(0)\left\{x^2 + \frac{(1-x)^2}{q-1}\right\} - NHx \\ S = -k_B\,\mathsf{Tr}\,(\varrho_N \ln \varrho_N) &= -Nk_B\left\{x\ln x + (1-x)\ln\left(\frac{1-x}{q-1}\right)\right\}\,. \end{aligned}$$

The dimensionless free energy per site is then

$$f(x,\theta,h) = -\frac{1}{2}\left\{x^2 + \frac{(1-x)^2}{q-1}\right\} + \theta\left\{x\ln x + (1-x)\ln\left(\frac{1-x}{q-1}\right)\right\} - hx\,, \tag{7.4.24}$$

where $h = H/\hat{J}\,(0)$. We now extremize with respect to x to obtain the mean field equation,

$$\frac{\partial f}{\partial x} = 0 = -x + \frac{1-x}{q-1} + \theta\,\ln x - \theta\,\ln\left(\frac{1-x}{q-1}\right) - h\,. \tag{7.4.25}$$

Note that for $h=0$, $x=q^{-1}$ is a solution, corresponding to a disordered state in which all states are equally probable. At high temperatures, for small h, we expect $x-q^{-1}\propto h$. Indeed, using Mathematica one can set

$$x\equiv q^{-1}+s\,, \tag{7.4.26}$$

and expand the mean field equation in powers of s. One obtains

$$h=\frac{q\,(q\theta-1)}{q-1}\,s+\frac{q^3\,(q-2)\,\theta}{2\,(q-1)^2}\,s^2+\mathcal{O}(s^3)\,. \tag{7.4.27}$$

For weak fields, $|h|\ll 1$, and we have

$$s(\theta)=\frac{(q-1)\,h}{q\,(q\theta-1)}+\mathcal{O}(h^2)\,, \tag{7.4.28}$$

which again is of the Curie-Weiss form. The difference $s=x-q^{-1}$ is the order parameter for the transition.

Finally, one can expand the free energy in powers of s, obtaining the Landau expansion,

$$\begin{aligned} f(s,\theta,h) \;=&-\frac{2h+1}{2q}-\theta\ln q-hs+\frac{q\,(q\theta-1)}{2\,(q-1)}\,s^2-\frac{(q-2)\,q^3\,\theta}{6\,(q-1)^2}\,s^3 \\ &+\frac{q^3\theta}{12}\Big[1+(q-1)^{-3}\Big]s^4-\frac{q^4\theta}{20}\Big[1-(q-1)^{-4}\Big]s^5 \\ &+\frac{q^5\theta}{30}\Big[1+(q-1)^{-5}\Big]s^6+\ldots\quad. \end{aligned}$$

Note that, for $q=2$, the coefficients of s^3, s^5, and higher order odd powers of s vanish in the Landau expansion. This is consistent with what we found for the Ising model, and is related to the $\mathbb{Z}_2$ symmetry of that model. For $q>3$, there is a cubic term in the mean field free energy, and thus we generically expect a first order transition, as we shall see below when we discuss Landau theory.

Mean Field Theory of the XY Model

Consider the so-called XY model, in which each site contains a continuous planar spin, represented by an angular variable $\phi_i\in[-\pi,\pi]$:

$$\hat{H}=-\frac{1}{2}\sum_{i\neq j}J_{ij}\cos\big(\phi_i-\phi_j\big)-H\sum_i\cos\phi_i\,. \tag{7.4.29}$$

We write the (diagonal elements of the) full density matrix once again as a product:

$$\varrho_N(\phi_1,\phi_2,\ldots)=\prod_i\varrho(\phi_i)\,. \tag{7.4.30}$$

Our goal will be to extremize the free energy with respect to the *function* $\varrho(\phi)$. To this end, we compute

$$E=\mathsf{Tr}\,(\varrho_N\,\hat{H})=-\frac{1}{2}N\hat{J}\,(0)\,\Big|\mathsf{Tr}\,\big(\varrho\,e^{i\phi}\big)\Big|^2-NH\,\mathsf{Tr}\,\big(\varrho\,\cos\phi\big)\,. \tag{7.4.31}$$

The entropy is

$$S=-Nk_B\,\mathsf{Tr}\,(\varrho\,\ln\varrho)\,. \tag{7.4.32}$$

Note that for any function $A(\phi)$, we have[14]

$$\mathsf{Tr}\;\,(\varrho\,A)\equiv\int_{-\pi}^{\pi}\frac{d\phi}{2\pi}\;\varrho(\phi)\,A(\phi)\,. \tag{7.4.33}$$

We now extremize the *functional* $F\big[\varrho(\phi)\big]=E-TS$ with respect to $\varrho(\phi)$, under the condition that $\mathsf{Tr}\;\varrho=1$. We therefore use Lagrange's method of undetermined multipliers, writing

$$F^*=F-Nk_BT\,\lambda\,\Big(\mathsf{Tr}\,\varrho-1\Big)\,. \tag{7.4.34}$$

Note that F^* is a *function* of the Lagrange multiplier λ and a *functional* of the density matrix $\varrho(\phi)$. The prefactor Nk_BT which multiplies λ is of no mathematical consequence – we could always redefine the multiplier to be $\lambda' \equiv Nk_BT\lambda$. It is present only to maintain homogeneity and proper dimensionality of F^* with λ itself dimensionless and of order N^0. We now have

$$\begin{aligned}\frac{\delta F^*}{\delta\varrho(\phi)} &= \frac{\delta}{\delta\varrho(\phi)}\Bigg\{-\frac{1}{2}N\hat{J}\,(0)\left|\mathsf{Tr}\big(\varrho\,e^{i\phi}\big)\right|^2 - NH\,\mathsf{Tr}\big(\varrho\,\cos\phi\big) \\ &\qquad + Nk_BT\;\mathsf{Tr}\,\big(\varrho\,\ln\varrho\big) - Nk_BT\,\lambda\,\Big(\mathsf{Tr}\,\varrho - 1\Big)\Bigg\}\,.\end{aligned}$$

To this end, we note that

$$\frac{\delta}{\delta\varrho(\phi)}\,\mathsf{Tr}\,(\varrho\,A) = \frac{\delta}{\delta\varrho(\phi)}\int_{-\pi}^{\pi}\frac{d\phi}{2\pi}\;\varrho(\phi)\,A(\phi) = \frac{1}{2\pi}\;A(\phi)\,. \tag{7.4.35}$$

Thus, we have

$$\begin{aligned}\frac{\delta\tilde{F}}{\delta\varrho(\phi)} &= -\frac{1}{2}N\hat{J}\,(0)\cdot\frac{1}{2\pi}\left[\mathop{\mathsf{Tr}}_{\phi'}\big(\varrho\,e^{i\phi'}\big)\;e^{-i\phi} + \mathop{\mathsf{Tr}}_{\phi'}\big(\varrho\,e^{-i\phi'}\big)\;e^{i\phi}\right] - NH\cdot\frac{\cos\phi}{2\pi} \\ &\qquad + Nk_BT\cdot\frac{1}{2\pi}\Big[\ln\varrho(\phi)+1\Big] - Nk_BT\cdot\frac{\lambda}{2\pi}\,.\end{aligned}$$

Now let us define

$$\mathop{\mathsf{Tr}}_{\phi}\big(\varrho\,e^{i\phi}\big) = \int_{-\pi}^{\pi}\frac{d\phi}{2\pi}\;\varrho(\phi)\,e^{i\phi} \equiv m\,e^{i\phi_0}\;. \tag{7.4.36}$$

We then have

$$\ln\varrho(\phi) = \frac{\hat{J}\,(0)}{k_BT}\;m\;\cos(\phi-\phi_0) + \frac{H}{k_BT}\;\cos\phi + \lambda - 1. \tag{7.4.37}$$

Clearly the free energy will be reduced if $\phi_0 = 0$ so that the mean field is maximal and aligns with the external field, which prefers $\phi = 0$. Thus, we conclude

$$\varrho(\phi) = \mathcal{C}\;\exp\left(\frac{H_{eff}}{k_BT}\;\cos\phi\right)\,, \tag{7.4.38}$$

where

$$H_{eff} = \hat{J}\,(0)\,m + H \tag{7.4.39}$$

and $\mathcal{C} = e^{\lambda-1}$. The value of λ is then determined by invoking the constraint,

$$\mathsf{Tr}\,\varrho = 1 = \mathcal{C}\int_{-\pi}^{\pi}\frac{d\phi}{2\pi}\;\exp\left(\frac{H_{eff}}{k_BT}\;\cos\phi\right) = \mathcal{C}\,I_0(H_{eff}/k_BT)\,, \tag{7.4.40}$$

where $I_0(z)$ is the Bessel function. We are free to define $\varepsilon \equiv H_{eff}/k_BT$, and treat ε as our single variational parameter. We then have the normalized single site density matrix

$$\varrho(\phi) = \frac{\exp(\varepsilon\cos\phi)}{\int_{-\pi}^{\pi}\frac{d\phi'}{2\pi}\;\exp(\varepsilon\cos\phi')} = \frac{\exp(\varepsilon\cos\phi)}{I_0(\varepsilon)}\;. \tag{7.4.41}$$

We next compute the following averages:

$$\left\langle\, e^{\pm i\phi}\,\right\rangle = \int\limits_{-\pi}^{\pi} \frac{d\phi}{2\pi}\,\varrho(\phi)\,e^{\pm i\phi} = \frac{I_1(\varepsilon)}{I_0(\varepsilon)}$$

$$\left\langle \cos(\phi-\phi')\right\rangle = \mathsf{Re}\,\left\langle e^{i\phi}\,e^{-i\phi'}\,\right\rangle = \left(\frac{I_1(\varepsilon)}{I_0(\varepsilon)}\right)^2 ,$$

as well as

$$\mathsf{Tr}\,(\varrho\,\ln\varrho) = \int\limits_{-\pi}^{\pi}\frac{d\phi}{2\pi}\,\frac{e^{\varepsilon\cos\phi}}{I_0(\varepsilon)}\,\Big\{\varepsilon\cos\phi - \ln I_0(\varepsilon)\Big\} = \varepsilon\,\frac{I_1(\varepsilon)}{I_0(\varepsilon)} - \ln I_0(\varepsilon)\,. \tag{7.4.42}$$

The dimensionless free energy per site is therefore

$$f(\varepsilon,h,\theta) = -\frac{1}{2}\left(\frac{I_1(\varepsilon)}{I_0(\varepsilon)}\right)^2 + (\theta\varepsilon - h)\,\frac{I_1(\varepsilon)}{I_0(\varepsilon)} - \theta\,\ln I_0(\varepsilon)\,, \tag{7.4.43}$$

with $\theta = k_{\scriptscriptstyle B}T/\hat{J}\,(0)$ and $h = H/\hat{J}\,(0)$ and $f = F/N\hat{J}\,(0)$ as before. Note that the mean field equation is $m = \theta\varepsilon - h = \left\langle\, e^{i\phi}\,\right\rangle$,

$$\theta\varepsilon - h = \frac{I_1(\varepsilon)}{I_0(\varepsilon)} \quad . \tag{7.4.44}$$

For small ε, we may expand the Bessel functions, using

$$I_\nu(z) = (\frac{1}{2}z)^\nu \sum_{k=0}^{\infty}\frac{(\frac{1}{4}z^2)^k}{k!\,\Gamma(k+\nu+1)}\,, \tag{7.4.45}$$

to obtain

$$f(\varepsilon,h,\theta) = \frac{1}{4}\,\big(\theta-\frac{1}{2}\big)\,\varepsilon^2 + \frac{1}{64}\,\big(2-3\theta\big)\,\varepsilon^4 - \frac{1}{2}\,h\varepsilon + \frac{1}{16}\,h\varepsilon^3 + \ldots\,. \tag{7.4.46}$$

This predicts a second order phase transition at $\theta_c = \frac{1}{2}$.[15] Note also the Curie-Weiss form of the susceptibility at high θ:

$$\frac{\partial f}{\partial\varepsilon} = 0 \quad\Longrightarrow\quad \varepsilon = \frac{h}{\theta-\theta_c} + \ldots\,. \tag{7.4.47}$$

XY model via neglect of fluctuations method

Consider again the Hamiltonian of Equation [XYmodel]. Define $z_i \equiv \exp(i\phi_i)$ and write

$$z_i = w + \delta z_i \quad , \tag{7.4.48}$$

where $w \equiv \langle z_i\rangle$ and $\delta z_i \equiv z_i - w$. Of course we also have the complex conjugate relations $z_i^* = w^* + \delta z_i^*$ and $w^* = \langle z_i^*\rangle$. Writing $\cos(\phi_i - \phi_j) = \mathsf{Re}\,(z_i^* z_j)$, by neglecting the terms proportional to $\delta z_i^*\,\delta z_j$ in $\hat{H}$ we arrive at the mean field Hamiltonian,

\HH^\ssr{MF}=\half N \HJ(0)\,|w|^2 - \half\HJ(0)\,|w|\sum_i\big(w^* z\ns_i + w z^*_i\big) - \half H\sum_i \big(z^*_i+z\ns_i\big)

It is clear that the free energy will be minimized if the mean field w breaks the $\mathsf{O}(2)$ symmetry in the same direction as the external field H, which means $w \in \mathbb{R}$ and

\HH^\ssr{MF}=\half N \HJ(0)\,|w|^2 - \big(H+\HJ(0)\,|w|\big)\sum_i\cos\phi\ns_i\quad.

The dimensionless free energy per site is then

$$f = \frac{1}{2}|w|^2 - \theta\ln I_0\left(\frac{h+|w|}{\theta}\right) \quad . \tag{7.4.49}$$

Differentiating with respect to $|w|$, one obtains

$$|w| \equiv m = \frac{I_1\left(\frac{h+m}{\theta}\right)}{I_0\left(\frac{h+m}{\theta}\right)} \quad , \tag{7.4.50}$$

which is the same equation as Equation [XYvdm]. The two mean field theories yield the same results in every detail (see §10).
