7.6: Mean Field Theory of Fluctuations

Correlation and response in mean field theory

Consider the Ising model,

$$\hat{H} = -\frac{1}{2}\sum_{i,j} J_{ij}\,\sigma_i\,\sigma_j - \sum_k H_k\,\sigma_k\ , \tag{7.6.1}$$

where the local magnetic field on site k is now H_k. We assume without loss of generality that the diagonal terms vanish: $J_{ii} = 0$. Now consider the partition function $Z = \mathsf{Tr}\ e^{-\beta\hat{H}}$ as a function of the temperature T and the local field values $\{H_i\}$. We have

$$\begin{aligned} \frac{\partial Z}{\partial H_i} &= \beta\,\mathsf{Tr}\,\Big[\sigma_i\,e^{-\beta\hat{H}}\Big] = \beta Z\cdot\langle\sigma_i\rangle \\ \frac{\partial^2 Z}{\partial H_i\,\partial H_j} &= \beta^2\,\mathsf{Tr}\,\Big[\sigma_i\,\sigma_j\,e^{-\beta\hat{H}}\Big] = \beta^2 Z\cdot\langle\sigma_i\,\sigma_j\rangle\ . \end{aligned}$$

Thus,

$$\begin{aligned} m_i &= -\frac{\partial F}{\partial H_i} = \langle\sigma_i\rangle \\ \chi_{ij} &= \frac{\partial m_i}{\partial H_j} = -\frac{\partial^2 F}{\partial H_i\partial H_j} = \frac{1}{k_B T}\cdot\Big\{\langle\sigma_i\,\sigma_j\rangle - \langle\sigma_i\rangle\,\langle\sigma_j\rangle\Big\}\ . \end{aligned}$$

Expressions such as $\langle\sigma_i\rangle$, $\langle\sigma_i\,\sigma_j\rangle$, are in general called *correlation functions*. For example, we define the *spin-spin correlation function* C_{ij} as

$$C_{ij} \equiv \langle\sigma_i\,\sigma_j\rangle - \langle\sigma_i\rangle\,\langle\sigma_j\rangle\ . \tag{7.6.2}$$

Expressions such as $\frac{\partial F}{\partial H_i}$ and $\frac{\partial^2 F}{\partial H_i\,\partial H_j}$ are called *response functions*. The above relation between correlation functions and response functions, $C_{ij} = k_B T\,\chi_{ij}$, is valid *only for the equilibrium distribution*. In particular, this relationship is *invalid* if one uses an approximate distribution, such as the variational density matrix formalism of mean field theory.

The question then arises: within mean field theory, which is more accurate: correlation functions or response functions? A simple argument suggests that the *response functions* are more accurate representations of the real physics. To see this, let's write the variational density matrix ϱ^{var} as the sum of the exact equilibrium (Boltzmann) distribution $\varrho^{eq} = Z^{-1}\exp(-\beta\hat{H})$ plus a deviation $\delta\varrho$:

$$\varrho^{var} = \varrho^{eq} + \delta\varrho\ . \tag{7.6.3}$$

Then if we calculate a correlator using the variational distribution, we have

$$\begin{aligned} \langle\sigma_i\,\sigma_j\rangle_{var} &= \mathsf{Tr}\,\Big[\varrho^{var}\,\sigma_i\,\sigma_j\Big] \\ &= \mathsf{Tr}\,\Big[\varrho^{eq}\,\sigma_i\,\sigma_j\Big] + \mathsf{Tr}\,\Big[\delta\varrho\,\sigma_i\,\sigma_j\Big]\ . \end{aligned}$$

Thus, the variational density matrix gets the correlator right to first order in $\delta\varrho$. On the other hand, the free energy is given by

$$F^{var} = F^{eq} + \sum_\sigma \frac{\partial F}{\partial\varrho_\sigma}\bigg|_{\varrho^{eq}}\delta\varrho_\sigma + \frac{1}{2}\sum_{\sigma,\sigma'}\frac{\partial^2 F}{\partial\varrho_\sigma\,\partial\varrho_{\sigma'}}\bigg|_{\varrho^{eq}}\delta\varrho_\sigma\,\delta\varrho_{\sigma'} + \ldots\ . \tag{7.6.4}$$

Here σ denotes a state of the system, $|\,\sigma\,\rangle = |\,\sigma_1,\ldots,\sigma_N\,\rangle$, where every spin polarization is specified. Since the free energy is an extremum (and in fact an absolute minimum) with respect to the distribution, the second term on the RHS vanishes. This means that the free energy is accurate to second order in the deviation $\delta\varrho$.

Calculation of the response functions

Consider the variational density matrix

$$\varrho(\sigma) = \prod_i \varrho_i(\sigma_i)\ , \tag{7.6.5}$$

where

$$\varrho_i(\sigma_i) = \bigg(\frac{1+m_i}{2}\bigg)\,\delta_{\sigma_i,1} + \bigg(\frac{1-m_i}{2}\bigg)\,\delta_{\sigma_i,-1}\ . \tag{7.6.6}$$

The variational energy $E = \mathsf{Tr}\,(\varrho\,\hat{H})$ is

$$E = -\frac{1}{2}\sum_{ij} J_{i,j}\,m_i\,m_j - \sum_i H_i\,m_i \tag{7.6.7}$$

and the entropy $S = -k_B T\,\mathsf{Tr}\,(\varrho\ln\varrho)$ is

$$S = -k_B\sum_i\left\{\left(\frac{1+m_i}{2}\right)\ln\left(\frac{1+m_i}{2}\right) + \left(\frac{1-m_i}{2}\right)\ln\left(\frac{1-m_i}{2}\right)\right\}. \tag{7.6.8}$$

Setting the variation $\frac{\partial F}{\partial m_i} = 0$, with $F = E - TS$, we obtain the mean field equations,

$$m_i = \tanh\left(\beta J_{ij}\,m_j + \beta H_i\right), \tag{7.6.9}$$

where we use the summation convention: $J_{ij}\,m_j \equiv \sum_j J_{ij}\,m_j$. Suppose $T > T_c$ and m_i is small. Then we can expand the RHS of the above mean field equations, obtaining

$$\left(\delta_{ij} - \beta J_{ij}\right)m_j = \beta H_i\,. \tag{7.6.10}$$

Thus, the susceptibility tensor χ is the inverse of the matrix $(k_B T\cdot\mathbb{I} - \mathbb{J})$:

$$\chi_{ij} = \frac{\partial m_i}{\partial H_j} = \left(k_B T\cdot\mathbb{I} - \mathbb{J}\right)^{-1}_{ij}, \tag{7.6.11}$$

where $\mathbb{I}$ is the identity. Note also that so-called *connected averages* of the kind in Equation [connavg] vanish identically if we compute them using our variational density matrix, since all the sites are independent, hence

$$\langle\sigma_i\,\sigma_j\rangle = \mathsf{Tr}\,\left(\varrho^{var}\,\sigma_i\,\sigma_j\right) = \mathsf{Tr}\,\left(\varrho_i\,\sigma_i\right)\cdot\mathsf{Tr}\,\left(\varrho_j\,\sigma_j\right) = \langle\sigma_i\rangle\cdot\langle\sigma_j\rangle\,, \tag{7.6.12}$$

and therefore $\chi_{ij} = 0$ if we compute the correlation functions themselves from the variational density matrix, rather than from the free energy F. As we have argued above, the latter approximation is more accurate.

Assuming $J_{ij} = J(\mathbf{R}_i - \mathbf{R}_j)$, where $\mathbf{R}_i$ is a Bravais lattice site, we can Fourier transform the above equation, resulting in

$$\hat{m}(\mathbf{q}) = \frac{\hat{H}(\mathbf{q})}{k_B T - \hat{J}(\mathbf{q})} \equiv \hat{\chi}(\mathbf{q})\,\hat{H}(\mathbf{q})\,. \tag{7.6.13}$$

Once again, our definition of lattice Fourier transform of a function $\phi(\mathbf{R})$ is

$$\begin{aligned}\hat{\phi}(\mathbf{q}) &\equiv \sum_{\mathbf{R}}\phi(\mathbf{R})\,e^{-i\mathbf{q}\cdot\mathbf{R}}\\ \phi(\mathbf{R}) &= \Omega\int_{\hat{\Omega}}\frac{d^dq}{(2\pi)^d}\,\hat{\phi}(\mathbf{q})\,e^{i\mathbf{q}\cdot\mathbf{R}}\,,\end{aligned}$$

where Ω is the unit cell in real space, called the *Wigner-Seitz cell*, and $\hat{\Omega}$ is the first Brillouin zone, which is the unit cell in *reciprocal space*. Similarly, we have

$$\begin{aligned}\hat{J}(\mathbf{q}) &= \sum_{\mathbf{R}} J(\mathbf{R})\left(1 - i\mathbf{q}\cdot\mathbf{R} - \frac{1}{2}(\mathbf{q}\cdot\mathbf{R})^2 + \ldots\right)\\ &= \hat{J}(0)\cdot\left\{1 - q^2R_*^2 + \mathcal{O}(q^4)\right\},\end{aligned}$$

where

$$R_*^2 = \frac{\sum_{\mathbf{R}}\mathbf{R}^2\,J(\mathbf{R})}{2d\sum_{\mathbf{R}}J(\mathbf{R})}\,. \tag{7.6.14}$$

Here we have assumed inversion symmetry for the lattice, in which case

$$\sum_{\mathbf{R}} R^\mu R^\nu\,J(\mathbf{R}) = \frac{1}{d}\cdot\delta^{\mu\nu}\sum_{\mathbf{R}}\mathbf{R}^2\,J(\mathbf{R})\,. \tag{7.6.15}$$

On cubic lattices with nearest neighbor interactions only, one has $R_* = a/\sqrt{2d}$, where a is the lattice constant and d is the dimension of space.

Thus, with the identification $k_BT_c = \hat{J}(0)$, we have

$$\begin{aligned}\hat{\chi}(\mathbf{q}) &= \frac{1}{k_B(T-T_c) + k_BT_c\,R_*^2\,\mathbf{q}^2 + \mathcal{O}(q^4)} \\ &= \frac{1}{k_BT_c\,R_*^2}\cdot\frac{1}{\xi^{-2}+q^2+\mathcal{O}(q^4)}\ ,\end{aligned}$$

where

$$\xi = R_*\cdot\left(\frac{T-T_c}{T_c}\right)^{-1/2} \tag{7.6.16}$$

is the *correlation length*. With the definition

$$\xi(T) \propto |T-T_c|^{-\nu} \tag{7.6.17}$$

as $T\to T_c$, we obtain the mean field correlation length exponent $\nu=\frac{1}{2}$. The exact result for the two-dimensional Ising model is $\nu=1$, whereas $\nu\approx 0.6$ for the $d=3$ Ising model. Note that $\hat{\chi}(\mathbf{q}=0,T)$ diverges as $(T-T_c)^{-1}$ for $T>T_c$.

In real space, we have

$$m_i = \sum_j \chi_{ij}\,H_j\ , \tag{7.6.18}$$

where

$$\chi_{ij} = \Omega\!\int\!\frac{d^dq}{(2\pi)^d}\,\hat{\chi}(\mathbf{q})\,e^{i\mathbf{q}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\ . \tag{7.6.19}$$

Note that $\hat{\chi}(\mathbf{q})$ is properly periodic under $\mathbf{q}\to\mathbf{q}+\mathbf{G}$, where $\mathbf{G}$ is a reciprocal lattice vector, which satisfies $e^{i\mathbf{G}\cdot\mathbf{R}}=1$ for any direct Bravais lattice vector $\mathbf{R}$. Indeed, we have

$$\begin{aligned}\hat{\chi}^{-1}(\mathbf{q}) &= k_BT - \hat{J}(\mathbf{q}) \\ &= k_BT - J\sum_{\delta} e^{i\mathbf{q}\cdot\delta}\ ,\end{aligned}$$

where δ is a nearest neighbor separation vector, and where in the second line we have assumed nearest neighbor interactions only. On cubic lattices in d dimensions, there are $2d$ nearest neighbor separation vectors, $\delta=\pm a\,\hat{\mathbf{e}}_\mu$, where $\mu\in\{1,\ldots,d\}$. The real space susceptibility is then

$$\chi(\mathbf{R}) = \int\limits_{-\pi}^{\pi}\!\frac{d\theta_1}{2\pi}\cdots\int\limits_{-\pi}^{\pi}\!\frac{d\theta_d}{2\pi}\;\frac{e^{in_1\theta_1}\cdots e^{in_d\theta_d}}{k_BT-(2J\cos\theta_1+\ldots+2J\cos\theta_d)}\ , \tag{7.6.20}$$

where $\mathbf{R}=a\sum_{\mu=1}^d n_\mu\,\hat{\mathbf{e}}_\mu$ is a general direct lattice vector for the cubic Bravais lattice in d dimensions, and the $\{n_\mu\}$ are integers.

The long distance behavior was discussed in chapter 6 (see §6.5.9 on Ornstein-Zernike theory[18]). For convenience we reiterate those results:

- In $d=1$,

$$\chi_{d=1}(x) = \left(\frac{\xi}{2k_BT_cR_*^2}\right)e^{-|x|/\xi}\ . \tag{7.6.21}$$

- In $d>1$, with $r\to\infty$ and ξ fixed,

  \xhiOZ_d(\Br)\simeq C\ns_d\cdot{\xi^{(3-d)/2}\over \kT\,R_*^2}\cdot{e^{-r/\xi}\over r^{(d-1)/2}}\cdot\left\{1+\CO\bigg({d-3\over r/\xi}\bigg)\right\}\,

  where the C_d are dimensionless constants.
- In $d>2$, with $\xi\to\infty$ and r fixed ($T\to T_c$ at fixed separation $\mathbf{r}$),

$$\chi_d(\mathbf{r}) \simeq \frac{C_d'}{k_BTR_*^2}\cdot\frac{e^{-r/\xi}}{r^{d-2}}\cdot\left\{1+\mathcal{O}\left(\frac{d-3}{r/\xi}\right)\right\}\ . \tag{7.6.22}$$

  In $d=2$ dimensions we obtain

$$\chi_{d=2}(\mathbf{r}) \simeq \frac{C_2'}{k_BTR_*^2}\cdot\ln\left(\frac{r}{\xi}\right)e^{-r/\xi}\cdot\left\{1+\mathcal{O}\left(\frac{1}{\ln(r/\xi)}\right)\right\}\ , \tag{7.6.23}$$

where the C_d' are dimensionless constants.

Beyond the Ising model

Consider a general spin model, and a variational density matrix ϱ_{var} which is a product of single site density matrices:

$$\varrho_{var}\big[\{\mathbf{S}_i\}\big]=\prod_i \varrho_1^{(i)}(\mathbf{S}_i) \quad , \tag{7.6.24}$$

where $\mathsf{Tr}\,\big(\varrho_{var}\,\mathbf{S}\big)=\mathbf{m}_i$ is the local magnetization and $\mathbf{S}_i$, which may be a scalar (, σ_i in the Ising model previously discussed), is the local spin operator. Note that $\varrho_1^{(i)}(\mathbf{S}_i)$ depends parametrically on the variational parameter(s) $\mathbf{m}_i$. Let the Hamiltonian be

$$\hat{H}=-\frac{1}{2}\sum_{i,j} J_{ij}^{\mu\nu}\, S_i^\mu\, S_j^\nu+\sum_i h(\mathbf{S}_i)-\sum_i \mathbf{H}_i\cdot\mathbf{S}_i \quad . \tag{7.6.25}$$

The variational free energy is then

$$F_{var}=-\frac{1}{2}\sum_{i,j} J_{ij}^{\mu\nu}\, m_i^\mu\, m_j^\nu+\sum_i \varphi(\mathbf{m}_i,T)-\sum_i H_i^\mu\, m_i^\mu \quad , \tag{7.6.26}$$

where the single site free energy $\varphi(\mathbf{m}_i,T)$ in the absence of an external field is given by

$$\varphi(\mathbf{m}_i,T)=\mathsf{Tr}\Big[\varrho_1^{(i)}(\mathbf{S})\,h(\mathbf{S})\Big]+k_{B}T\,\mathsf{Tr}\Big[\varrho_1^{(i)}(\mathbf{S})\ln\varrho_1^{(i)}(\mathbf{S})\Big] \tag{7.6.27}$$

We then have

$$\frac{\partial F_{var}}{\partial m_i^\mu}=-\sum_j J_{ij}^{\mu\nu}\, m_j^\nu-H_i^\mu+\frac{\partial\varphi(\mathbf{m}_i,T)}{\partial m_i^\mu} \quad . \tag{7.6.28}$$

For the noninteracting system, we have $J_{ij}^{\mu\nu}=0$, and the weak field response must be linear. In this limit we may write $m_i^\mu=\chi_{\mu\nu}^0(T)\,H_i^\nu+\mathcal{O}(H_i^3)$, and we conclude

$$\frac{\partial\varphi(\mathbf{m}_i,T)}{\partial m_i^\mu}=\big[\chi^0(T)\big]^{-1}_{\mu\nu}\, m_i^\nu+\mathcal{O}\big(m_i^3\big) \quad . \tag{7.6.29}$$

Note that this entails the following expansion for the single site free energy in zero field:

$$\varphi(\mathbf{m}_i,T)=\frac{1}{2}\,\big[\chi^0(T)\big]^{-1}_{\mu\nu}\, m_i^\nu\, m_i^\nu+\mathcal{O}(m^4) \quad . \tag{7.6.30}$$

Finally, we restore the interaction term and extremize F_{var} by setting $\partial F_{var}/\partial m_i^\mu=0$. To linear order, then,

$$m_i^\mu=\chi_{\mu\nu}^0(T)\,\Big(H_i^\nu+\sum_j J_{ij}^{\nu\lambda}\, m_j^\lambda\Big) \quad . \tag{7.6.31}$$

Typically the local susceptibility is a scalar in the internal spin space, $\chi_{\mu\nu}^0(T)=\chi^0(T)\,\delta_{\mu\nu}$, in which case we obtain

$$\big(\delta^{\mu\nu}\,\delta_{ij}-\chi^0(T)\,J_{ij}^{\mu\nu}\big)\, m_i^\nu=\chi^0(T)\,H_i^\mu \quad . \tag{7.6.32}$$

In Fourier space, then,

$$\hat{\chi}_{\mu\nu}(\mathbf{q},T)=\chi^0(T)\,\Big(1-\chi^0(T)\,\hat{\mathbb{J}}(\mathbf{q})\Big)^{-1}_{\mu\nu} \quad , \tag{7.6.33}$$

where $\hat{\mathbb{J}}(\mathbf{q})$ is the matrix whose elements are $\hat{J}^{\mu\nu}(\mathbf{q})$. If $\hat{J}^{\mu\nu}(\mathbf{q})=\hat{J}\,(\mathbf{q})\,\delta^{\mu\nu}$, then the susceptibility is isotropic in spin space, with

$$\hat{\chi}(\mathbf{q},T)=\frac{1}{\big[\chi^0(T)\big]^{-1}-\hat{J}\,(\mathbf{q})} \quad . \tag{7.6.34}$$

Consider now the following illustrative examples:

- Quantum spin S with $h(\mathbf{S})=0$: We take the $\hat{\mathbf{z}}$ axis to be that of the local external magnetic field, $\hat{\mathbf{H}}_i$. Write $\varrho_1(\mathbf{S})=z^{-1}\,\exp(uS^z/k_BT)$, where $u=u(m,T)$ is obtained implicitly from the relation $m(u,T)=\mathsf{Tr}(\varrho_1\,S^z)$. The normalization constant is

$$z=\mathsf{Tr}\,e^{uS^z/k_BT}=\sum_{j=-S}^{S} e^{ju/k_BT}=\frac{\sinh\big[(S+\frac{1}{2})\,u/k_BT\big]}{\sinh\big[u/2k_BT\big]} \tag{7.6.35}$$

The relation between m, u, and T is then given by

$$\begin{aligned} m &= \langle S^z \rangle = k_B T \, \frac{\partial \ln z}{\partial u} = (S + \frac{1}{2}) \, ctnh\big[(S+\frac{1}{2}) \, u / k_B T\big] - \frac{1}{2} \, ctnh\big[u/2k_B T\big] \\ &= \frac{S(S+1)}{3k_B T} \, u + \mathcal{O}(u^3) \quad . \end{aligned}$$

The free-field single-site free energy is then

$$\varphi(\mathbf{m},T) = k_B T \, \mathsf{Tr}\, \big(\varrho_1 \ln \varrho_1\big) = um - k_B T \ln z \quad , \tag{7.6.36}$$

whence

$$\frac{\partial\varphi}{\partial m} = u + m \, \frac{\partial u}{\partial m} - k_B T \, \frac{\partial \ln z}{\partial u} \, \frac{\partial u}{\partial m} = u \equiv \chi_0^{-1}(T) \, m + \mathcal{O}(m^3) \quad , \tag{7.6.37}$$

and we thereby obtain the result

$$\chi_0(T) = \frac{S(S+1)}{3k_B T} \quad , \tag{7.6.38}$$

which is the Curie susceptibility.

- Classical spin $\mathbf{S} = S\,\hat{\mathbf{n}}$ with $h=0$ and $\hat{\mathbf{n}}$ an N-component unit vector : We take the single site density matrix to be $\varrho_1(\mathbf{S}) = z^{-1} \exp(\mathbf{u}\cdot\mathbf{S}/k_B T)$. The single site field-free partition function is then

$$z = \int \frac{d\hat{\mathbf{n}}}{\Omega_N} \, \exp(\mathbf{u}\cdot\mathbf{S}/k_B T) = 1 + \frac{S^2 \, \mathbf{u}^2}{N(k_B T)^2} + \mathcal{O}(u^4) \tag{7.6.39}$$

and therefore

$$\mathbf{m} = k_B T \, \frac{\partial \ln z}{\partial \mathbf{u}} = \frac{S^2 \, \mathbf{u}}{N k_B T} + \mathcal{O}(u^3) \quad , \tag{7.6.40}$$

from which we read off $\chi_0(T) = S^2/Nk_BT$. Note that this agrees in the classical ($S\to\infty$) limit, for $N=3$, with our previous result.

- Quantum spin S with $h(\mathbf{S}) = \Delta(S^z)^2$: This corresponds to so-called *easy plane anisotropy*, meaning that the single site energy $h(\mathbf{S})$ is minimized when the local spin vector $\mathbf{S}$ lies in the (x,y) plane. As in example (i), we write $\varrho_1(\mathbf{S}) = z^{-1} \, \exp(uS^z/k_B T)$, yielding the same expression for z and the same relation between z and u. What is different is that we must evaluate the local energy,

$$\begin{aligned} e\,(u,T) &= \mathsf{Tr}\,\big(\varrho_1 \, h(\mathbf{S})\big) = \Delta \, (k_B T)^2 \, \frac{\partial^2 \ln z}{\partial u^2} \\ &= \frac{\Delta}{4}\left[\frac{1}{\sinh^2\big[u/2k_BT\big]} - \frac{(2S+1)^2}{\sinh^2\big[(2S+1)u/2k_BT\big]}\right] = \frac{S(S+1)\Delta\, u^2}{6(k_BT)^2} + \mathcal{O}(u^4) \quad . \end{aligned}$$

We now have $\varphi = e + um - k_B T \ln z$, from which we obtain the susceptibility

$$\chi^0(T) = \frac{S(S+1)}{3(k_B T + \Delta)} \quad . \tag{7.6.41}$$

Note that the local susceptibility no longer diverges as $T\to 0$, because there is always a gap in the spectrum of $h(\mathbf{S})$.