Lightning-quick introduction to dynamical mean field theory

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Abstract

This is a very short introduction to the philosophy and algorithm of dynamical mean field theory (DMFT). I brought these points together and wrote this up mostly to cement my own understanding of the topic.

1 Refresher on (static) mean field theory

The Curie-Weiss version of mean field theory involves replacing the spatial fluctuations in the Hamiltonian or the energy by an effective static field. The static field has to be determined self-consistently. To see what this means, we take the canonical example of the Ising model. Its Hamiltonian is given by

$$H = J\sum_{\langle ij\rangle} S_i^z S_j^z = J\sum_i S_i^z \sum_{j\in\text{NN of } i} S_j^z \tag{1}$$

In order to introduce the mean-field, we replace the spins S_j^z of the nearest-neighbour sites by their average value $\left\langle S_j^z\right\rangle \equiv m_j$:

$$H_{\text{MF}} = J\sum_i S_i^z \sum_{j\in\text{NN of } i} m_j \tag{2}$$

Because of translation symmetry, we expect the average local magnetisation to be independent of the position j: $m_j \equiv m_{\text{loc}}$. If z is the coordination number of the lattice, we get

$$H_{\text{MF}} = J\sum_i S_i^z zm = h_{\text{MF}} \sum_i S_i^z, \tag{3}$$

where we have defined the static mean field $h_{\text{MF}} \equiv Jzm_{\text{loc}}$. This mean field Hamiltonian is solvable, in terms of h_{MF}. The mean-field itself, however, is still unknown. To determine it, we will use the fact that if our approach is to be internally consistent, the average magnetisation $\langle S_i^z\rangle$ obtained from the mean-field Hamiltonian H_{MF} should be equal to that defined before, m_{loc}. This is again demanded on grounds of translation invariance. Since H_{MF} just consists of decoupled spins, the local Hamiltonian has two solutions: $S_i^z = \pm\frac{1}{2}$ with energies $\pm\frac{h_{\text{MF}}}{2}$. The local partition function Z_{MF} and hence the magnetisation at site i is then obtained easily:

$$Z_{\text{MF}} = 2\cosh\left(\beta h_{\text{MF}}/2\right), m = \frac{1}{Z_{\text{MF}}}\sum_{S_i^z=\pm\frac{1}{2}} S_i^z e^{-\beta h_{\text{MF}} S_i^z} = \tanh\left(\beta h_{\text{MF}}/2\right) \tag{4}$$

The self-consistency equation takes the form

$$m_{\text{loc}} = m = \tanh\left(\beta Jzm_{\text{loc}}/2\right) \tag{5}$$

This equation now has to be solved numerically, to obtain the value of the local magnetisation m_{loc}. This is the general approach to the mean field approximation:

- replace the fluctuations by an effective local mean field y_{loc}, in order to obtain a simpler problem (the simplified Hamiltonian H_{MF},
- solve the simpler problem at a particular local site i to calculate the mean field y_i from it, and
- demand that a self-consistent solution should have $y_i = y_{\text{loc}}$, and solve this equation.