Statistical field theory

Tutorial n°2

Mean field approach: variational method

1) One considers a system of Hamiltonian H and of free energy F. Show the equality:

$$F = F_0 - k_B T \log\langle e^{-\beta(H-H_0)}\rangle_0$$

where H_0 is a Hamiltonian, F_0 the associated free energy and $\langle A\rangle_0$ the mean value of A in the canonical ensemble defined by H_0. In what follows H_0 will be chosen in such a way that all quantities computed in this ensemble will be particularly simple.

2) Show that for any function f one has:

$$\langle e^f\rangle \geq e^{\langle f\rangle}$$

and deduce an upper bound, F_{var}, of the free energy F in terms of F_0 and $\langle H - H_0\rangle_0$.

The idea of the method is to use this property to find the best approximation of the genuine free energy F for the Ising model in a uniform magnetic field h:

$$H = -J\sum_{\langle i,j\rangle} S_i S_j - h\sum_i S_i$$

considering, for H_0, the Hamiltonian of a system of N *free* spins:

$$H_0 = -\lambda\sum_i S_i$$

where λ should be determined to optimize F_{var}, *i.e.* to find its *lowest* value.

3) Compute the partition function Z_0 associated to the Hamiltonian H_0. Deduce the value of $\langle S_i\rangle_0$.

4) Use the result of the previous question to show that the mean value $\langle H - H_0\rangle_0$ is given by:

$$\langle H - H_0\rangle_0 = -\frac{JNz}{2}\tanh^2\beta\lambda + (\lambda - h)N\tanh\beta\lambda$$

5) Give the expression of F_{var} and find the optimal value λ_{min} of λ making F_{var} minimal.

6) Determine, from this value of F_{var}, the magnetization m and the equation that it obeys. Comment.

7) Give the expression of the Gibbs free energy $\Gamma(m)$ as a function of m. After some algebra show that:

$$\Gamma[m] = -Nk_BT\log 2 - \frac{JNz}{2}m^2 + \frac{Nk_BT}{2}[(1-m)\log(1-m) + (1+m)\log(1+m)]$$