Mathematics 18: Quantum Spins: Mean-Field Equations

In 'Maths12' some of the mathematics of spin-half is developed. Here we develop a bit more. *It is not crucial to understand this analysis, only the resulting self-consistent equations and their meaning.*

The original basis suggested is $|\uparrow>$ and $|\downarrow>$. It is much more useful to use a new basis for this problem, where:

$$|\uparrow> \mapsto b^\dagger \mid 0 >$$
$$|\downarrow> \mapsto \mid 0 >$$

where we interpret the $b^\dagger$ as a 'particle' creation operator, and invent a 'particle' annihilation operator b which destroys the particles:

$$bb^\dagger \mid 0 >= \mid 0 > \qquad b \mid 0 >= 0$$

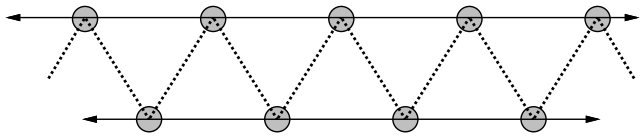
This representation in terms of 'particles' is really just $S^\pm$ in disguise, with $b^\dagger \sim S^+$ and $b \sim S^-$. The Hamiltonian in this new representation is quite simple however, and this is the main strength to the idea. The x-y model becomes simply:

$$H_{x-y} = \frac{1}{4} \sum_{ij} J_{ij} \left[b_i^\dagger b_j + b_j^\dagger b_i \right]$$

and the Heisenberg model is augmented by:

$$H_{Heis} = \frac{1}{4} \sum_{ij} J_{ij} \left[b_i^\dagger b_j + b_j^\dagger b_i \right] + \frac{1}{2} \sum_{ij} J_{ij} \left(b_i^\dagger b_i - \frac{1}{2} \right) \left(b_j^\dagger b_j - \frac{1}{2} \right)$$

where you can see from the last term that this contributes either $\pm\frac{1}{4}$ depending on whether there are an even or odd number of particles on the two sites. The particles involved in this description may be seen to be bosons, and so one might presume that the problem is easy: Just use the Bose-Einstein occupation number! Unfortunately, you can only have one boson per site, so called *hard-core* bosons (forced by $(b^\dagger)^2 = 0$), which are very subtle to deal with. Fortunately, in one dimension, the hard-core constraint can be handled using *Fermi statistics* and Pauli exclusion to prohibit more than one particle per site, and then the erroneous Fermi minus sign can be absorbed into a change in the Hamiltonian. For the 'Railroad Trestle' geometry:



RAILROAD TRESTLE

——— J_2

..... J_1

the Hamiltonian becomes:

$$H_1 = \frac{J_1}{2} \sum_i \left[b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i \right] + \mu J_1 \sum_i \left(b_i^\dagger b_i - \frac{1}{2} \right) \left(b_{i+1}^\dagger b_{i+1} - \frac{1}{2} \right)$$

for nearest-neighbour hopping and:

$$H_2 = \frac{J_2}{2}\sum_i \left[b_i^\dagger b_{i+2} + b_{i+2}^\dagger b_i\right] + \mu J_2 \sum_i \left(b_i^\dagger b_i - \frac{1}{2}\right)\left(b_{i+2}^\dagger b_{i+2} - \frac{1}{2}\right)$$

for second-nearest-neighbour hopping, and we use $\mu = 0$ or 1 to give the x-y model or Heisenberg model respectively.

The extension to using a fermionic basis is simply:

$$H_1 = \frac{J_1}{2}\sum_i \left[f_i^\dagger f_{i+1} + f_{i+1}^\dagger f_i\right] + \mu J_1 \sum_i \left(f_i^\dagger f_i - \frac{1}{2}\right)\left(f_{i+1}^\dagger f_{i+1} - \frac{1}{2}\right)$$

which is the same, because the particles cannot pass each-other using this term, and:

$$H_2 = \frac{J_2}{2}\sum_i \left[f_i^\dagger f_{i+2} + f_{i+2}^\dagger f_i\right]\left[1 - 2f_{i+1}^\dagger f_{i+1}\right] + \mu J_2 \sum_i \left(f_i^\dagger f_i - \frac{1}{2}\right)\left(f_{i+2}^\dagger f_{i+2} - \frac{1}{2}\right)$$

and there is now an inclusion of $\left[1 - 2f_{i+1}^\dagger f_{i+1}\right]$ which supplies the erroneous minus sign if two fermions pass each other.

There are *two* types of term: Single-particle:

$$f_2^\dagger f_1$$

which moves a particle from site 1 to site 2. This particle moves independently from all the others and is easy to deal with, since each particle can be treated independently. There are also two-particle terms:

$$f_4^\dagger f_3^\dagger f_2 f_1$$

which moves a pair of particles from sites 1 and 2 to sites 3 and 4. The motion of one of the particles depends on the existence of the other and is much more difficult to control. The basic reason is that we do not know which of the other particles might be the other one promoting the interaction, and so we need to know what *all* of the other particles are doing to assess whether the interaction will apply. In other words you need to consider either one particle alone or *all* the particles. In practice, interactions cannot be solved unless it *is* possible to work out unambiguously which of the other particles you will interact with (using an order for example). When you cannot solve the problem you need to *approximate!*

The 'simplest' approach to interactions between particles is to replace one of the particles by the *average* probability that a particle would be there. This is the so-called *mean-field* approximation or *Hartree-Fock* approximation. Technically:

$$f_4^\dagger f_3^\dagger f_2 f_1 \mapsto f_4^\dagger f_1 < f_3^\dagger f_2 > + f_3^\dagger f_2 < f_4^\dagger f_1 > - f_4^\dagger f_2 < f_3^\dagger f_1 > - f_3^\dagger f_1 < f_4^\dagger f_2 >$$

$$- < f_4^\dagger f_1 >< f_3^\dagger f_2 > + < f_4^\dagger f_2 >< f_3^\dagger f_1 >$$

where $< \ldots >$ denotes average. The original problem is replaced by an 'effective' single-particle problem which is solvable. The *difficulty* is that the quantities $< f_i^\dagger f_j >$ which

appear in the single-particle problem are unknown and must be *found* by requiring that the $< f_i^\dagger f_j >$ input to the potential must be equal to the $< f_i^\dagger f_j >$ induced in the single-particle problem. The requirement amounts to *self-consistent* equations for the quantities $< f_i^\dagger f_j >$.

For the current problem, the parameters involved in the potential are:

$$\begin{aligned} < f_i^\dagger f_i > &= N_0 + (-1)^i n_0 \\ < f_i^\dagger f_{i+1} > &= N_1 + (-1)^i n_1 \\ < f_i^\dagger f_{i+2} > &= N_2 + (-1)^i n_2 \end{aligned}$$

where:

$$< S_i^z > = < f_i^\dagger f_i - \frac{1}{2} > = N_0 - \frac{1}{2} + (-1)^i n_0$$

and *ferromagnetism* occurs when $N_0 \neq \frac{1}{2}$ while *antiferromagnetism* occurs when $n_0 \neq 0$. As well as this style of order, also $n_1 \neq 0$ is possible and is known as a *bond-order wave*.

Although the analysis is involved, in the region of interest the self-consistent equations are:

$$\begin{aligned} N_0 &= \frac{1}{2} \int_0^1 dx \;\; T_0[A, X] \\ N_1 &= \frac{1}{2} \int_0^1 dx \, \frac{a}{X} \cos \pi x \;\; T_1[A, X] \\ N_2 &= \frac{1}{2} \int_0^1 dx \cos 2\pi x \;\; T_0[A, X] \\ n_0 &= \frac{1}{2} \int_0^1 dx \, \frac{B}{X} \;\; T_1[A, X] \\ n_1 &= \frac{1}{2} \int_0^1 dx \, \frac{b}{X} \sin \pi x \;\; T_1[A, X] \\ n_2 &= \frac{1}{2} \int_0^1 dx \, \frac{B}{X} \cos 2\pi x \;\; T_1[A, X] \end{aligned}$$

with:

$$X^2 = a^2 + B^2 + b^2$$

$$\begin{aligned} A &= -2N_2\lambda + (2N_0 - 1)\mu(1 + \lambda) - (2N_0 - 1)\lambda \cos 2\pi x \\ a &= -[1 + 4N_1\lambda - 2N_1\mu] \cos \pi x \\ B &= -2n_2\lambda + 2n_0\mu(1 - \lambda) - [2n_0\lambda - 2n_2\lambda\mu] \cos 2\pi x \\ b &= [4n_1\lambda + 2n_1\mu] \sin \pi x \end{aligned}$$

where we use $J_2/J_1 \equiv \lambda$ and for the range of parameters of present interest you may assume that: $T_0[A, X] = 1 = T_1[A, X]$.

The total energy of the state is:

$$\epsilon \equiv \frac{E}{J_1 N} = N_1 + \left[N_2(1-2N_0) + 2N_1^2 + 2(n_0 n_2 - n_1^2)\right] \lambda$$

$$+ \left[\left(\frac{1}{2} - N_0\right)^2 - N_1^2 - n_0^2 - n_1^2\right] \mu$$

$$+ \left[\left(\frac{1}{2} - N_0\right)^2 - N_2^2 + n_0^2 - n_2^2\right] \lambda\mu$$

from which the potentials can be independently deduced:

$$\begin{aligned} A &= \left[\frac{\partial}{\partial N_0} + \cos 2\pi x \frac{\partial}{\partial N_2}\right] \epsilon \\ a &= -\cos \pi x \frac{\partial}{\partial N_1} \epsilon \\ B &= -\left[\frac{\partial}{\partial n_0} + \cos 2\pi x \frac{\partial}{\partial n_2}\right] \epsilon \\ b &= -\sin \pi x \frac{\partial}{\partial n_1} \epsilon \end{aligned}$$

The excitation spectrum in the model is non-interacting fermions with dispersion:

$$\epsilon_{\pm}(x) = A(x) \pm X(x)$$

which can be analysed to predict the low-temperature behaviour of the system.