M2 ICFP
Theoretical Condensed Matter

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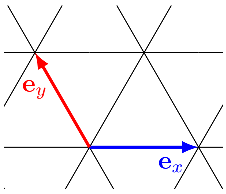
Problem: Schwinger boson mean-field theory

In Mott's insulators, the low energy behavior is described by a purely magnetic Hamiltonian: the Heisenberg Hamiltonian:

$$\hat{H} = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{1}$$

where $\mathbf{S}_i$ is the spin operator (S_i^x, S_i^y, S_i^z) on site i. Here we consider antiferromagnetic interactions between nearest neighboring spins $S = 1/2$ on a triangular lattice, whose basis vectors $\mathbf{e}_x$ and $\mathbf{e}_y$ are:



Despite the simplicity of $\hat{H}$, no exact expression of the ground state has been found (even if we can say that a numerical solution exists on the square lattice). Even its nature has a long time remained controversial and has led to many proposals (resonnating valence bonds, valence bond crystals, Néel states...).

Here we use the Schwinger boson mean-field theory to solve this model in a *large* N approximation.

1 Formalism

1. We first construct an equivalent model with bosonic particles. $a^\dagger_{\sigma i}$ is the creation operator of a boson of spin $\sigma = \pm 1/2$ on lattice site i. What are the conditions to respect to define spin operators in this model as:
$$\begin{cases} S_i^+ = a^\dagger_{\uparrow i} a_{\downarrow i}, \\ S_i^- = a^\dagger_{\downarrow i} a_{\uparrow i}, \\ S_i^z = \frac{1}{2}\left(a^\dagger_{\uparrow i} a_{\uparrow i} - a^\dagger_{\downarrow i} a_{\downarrow i}\right). \end{cases} \tag{2}$$
Are they verified ?

2. What is the number of possible states on a site for the spin model of Eq (1) ? What is it for the bosonic model ? Show that to make these two models equivalent, we must impose the following constraint:
$$a^\dagger_{\uparrow i} a_{\uparrow i} + a^\dagger_{\downarrow i} a_{\downarrow i} = 1. \tag{3}$$

3. We define the operator $\hat{A}_{ij}$, defined on the (oriented) link $i - j$ of the lattice by:
$$\hat{A}_{ij} = \frac{1}{2}\left(a_{\uparrow i} a_{\downarrow j} - a_{\downarrow i} a_{\uparrow j}\right). \tag{4}$$
such that
$$\mathbf{S}_i \cdot \mathbf{S}_j = \frac{1}{4} - 2\hat{A}^\dagger_{ij}\hat{A}_{ij}. \tag{5}$$
Show that this theory possesses a local $U(1)$ gauge symmetry. What is its effect on the $\hat{A}_{ij}$ operators ? What are the gauge invariant operators (how to construct them, what is their meaning) ?

4. What do you think about the complexity of the Hamiltonian expressed in terms of bosons ? Can we solve it ?

2 The mean-field approximation

5. By generalizing this model to N spins 1/2 per site ($\sum_{\alpha=1}^{N} a_{\uparrow i}^{\alpha\,\dagger} a_{\uparrow i}^{\alpha} + a_{\downarrow i}^{\alpha\,\dagger} a_{\downarrow i}^{\alpha} = N$):

$$\hat{A}_{ij} = \frac{1}{2}\sum_{\alpha=1}^{N}\left(a_{\uparrow i}^{\alpha} a_{\downarrow j}^{\alpha} - a_{\downarrow i}^{\alpha} a_{\uparrow j}^{\alpha}\right), \qquad \hat{H} = \frac{1}{N}\sum_{\langle i,j\rangle}\left(\frac{N}{4} - 2\hat{A}_{ij}^{\dagger}\hat{A}_{ij}\right) \tag{6}$$

show that the following mean-field approximation becomes exact for $N \to \infty$:

$$\hat{A}_{ij}^{\dagger}\hat{A}_{ij} \simeq \hat{A}_{ij}^{\dagger}\langle\hat{A}_{ij}\rangle + \langle\hat{A}_{ij}^{\dagger}\rangle\hat{A}_{ij} - \langle\hat{A}_{ij}^{\dagger}\rangle\langle\hat{A}_{ij}\rangle. \tag{7}$$

6. In the following, we consider only the case $N = 1$. We include a Lagrange multiplier λ_i and consider the mean-field Hamiltonian at zero temperature:

$$H_{MF} = \sum_{\langle i,j\rangle}\left(\frac{1}{4} - 2\alpha_{ij}\hat{A}_{ij}^{\dagger} - 2\alpha_{ij}^{*}\hat{A}_{ij} + 2|\alpha_{ij}|^2\right) + \sum_i \lambda_i(1 - \hat{n}_i). \tag{8}$$

Show that H_{MF} can be written under the form of:

$$H_{MF} = v^{\dagger}Mv + \epsilon_0, \tag{9}$$

with $v^{\dagger} = (a_{\uparrow 1}^{\dagger}, \ldots, a_{\uparrow N_s}^{\dagger}, a_{\downarrow 1}, \ldots, a_{\downarrow N_s})$, M a $2N_s \times 2N_s$ matrix and ϵ_0 a constant.

7. Can we solve the mean-field Hamiltonian ?

8. We would like to put the Hamiltonian in the diagonal form

$$\hat{H}_{MF} = \sum_{j\sigma}\epsilon_j \tilde{a}_{\sigma j}^{\dagger}\tilde{a}_{\sigma j} + \tilde{\epsilon}_0. \tag{10}$$

Let $\tilde{M}$ be the diagonal matrix with coefficients ϵ_i and J the following matrix

$$J = \begin{pmatrix} 1_{N_s} & 0 \\ 0 & -1_{N_s} \end{pmatrix}. \tag{11}$$

We define $\tilde{v}^{\dagger} = (\tilde{a}_{\uparrow 1}^{\dagger}, \ldots, \tilde{a}_{\uparrow N_s}^{\dagger}, \tilde{a}_{\downarrow 1}, \ldots, \tilde{a}_{\downarrow N_s})$ and the $\tilde{a}_{\sigma j}$ are bosonic operators, linear combinations of the original ones (j no longer stands for a lattice site). They are characterized by a matrix P such that $v = P\tilde{v}$. Show that the operators $\tilde{a}_{\sigma j}$ have bosonic commutation relations as long as the matrix P enjoys the matrix P must obey

$$PJP^{\dagger} = J$$

Moreover the matrix P must be such that $P^{\dagger}MP = \tilde{M}$[1].

[1] One could wonder about the existence of such a P matrix. A sufficient condition for this existence is that the matrix M is positive-definite. In this case the matrix M can be decomposed as $M = K^{\dagger}K$ with K upper triangular (Cholesky decomposition). The hermitian matrix $KJK^{\dagger}$ can be diagonalized with a unitary matrix U, namely $KJK^{\dagger} = UDU^{\dagger}$, and we can always choose U such that the positive eigenvalues come first, and the negative ones last. Since J has N_s positive eigenvalues, and N_s negative ones, so does $KJK^{\dagger}$, which means that the matrix $\tilde{M} = JD$ is diagonal with strictly positive eigenvalues. It is then straightforward to check that the following matrix P does the job :

$$P = K^{-1}U\tilde{M}^{\frac{1}{2}}$$

If M is not positive-definite, for instance if it has some zero eigenvalues, then the existence of P is no longer guaranteed.

9. Show that the energies ϵ_j are the eigenvalues of JM, times ± 1.

10. What are the condition on ϵ_j to have a well defined ground state for the Hamiltonian of Eq. (10) ? What is the ground state in terms of the tilde operators ? What is the ground state energy E_0 in terms of ϵ_0 and ϵ_j ? In terms of $\tilde{\epsilon}_0$?

11. We did a mean-field approximation. What are the self-consistency conditions on λ_i and α_{ij} ? Show that the condition on α_{ij} is equivalent to $\frac{\partial E_0(\{\lambda_i\},\{\alpha_{ij}\})}{\partial \Re \alpha_{ij}} = 0$ and $\frac{\partial E_0(\{\lambda_i\},\{\alpha_{ij}\})}{\partial \Im \alpha_{ij}} = 0$.

12. Beside the mean-field approximation, we also use the approximation of using a chemical potential λ_i (or Lagrange multiplier) on each site to adjust the number of bosons per site. But this is not enough to impose the constraint of Eq. (3). This constraint is only verified in average. We now try to quantify this error. What is $\langle \hat{n}_i \rangle$ in the exact model ? And in the mean-field approximation ? Same questions for $\langle \hat{n}_i^2 \rangle - \langle \hat{n}_i \rangle^2$.

3 Resolution of the two sites problem

At this point, we have one mean-field parameter α_{ij} per link and one chemical potential λ_i per site. Using lattice symmetry consideration, we suppose that $\lambda_i = \lambda$ is site independent and that the α_{ij} are related by symmetry relations discussed in the next section.

13. Write M for the mean-field Hamiltonian on two sites (a simple link). What are the ϵ_i ?

14. Write and solve the self-consistent equations. What is the ground state energy ? Compare it to the non approximated ground state energy.

4 Resolution on a frustrated Bravais lattice: the triangular lattice

15. We chose a triangular lattice. What is exactly the ground state in the classical limit (where the spin becomes a classical vector of length S, true in the $S \to \infty$ limit) ? What is the energy on a link ? The link energy is not its minimal value (equal to $-S^2$): the model is said to be frustrated.

16. The lattice symmetries are generated by two translations, a rotation and a reflexion. Any link (i, j) can be sent on any other one (k, l) by some symmetry operation. However this does not imply that all α_{ij} are equal. Why ?

17. As a consequence of the previous question, a non zero Ansatz cannot be invariant with respect to all the lattice symmetries. Still, such an Ansatz can possess physical (spin) quantities that respect the lattice symmetries. Explain why it is so. Use the fact that the α_{ij} are not gauge invariant, whereas physical operators are. Show that the lattice symmetry operator X must have the same effect as a gauge transformation G on the Ansatz.

18. The implications of the symmetries on the Ansatz is a difficult task. We chose the following Ansatz and admit that it leads to a symmetric physical (i.e. respecting the constraint) state: $\alpha_{ii+x} = \alpha_{ii+y} = \alpha_{ii-x-y} = \alpha$ with α a real positive number. Using the Fourier transform:

$$a_{\sigma \mathbf{q}} = \frac{1}{\sqrt{N_s}} \sum_i a_{\sigma i} e^{-i\mathbf{q}\cdot\mathbf{r}_i}, \tag{12}$$

where $\mathbf{r}_i$ the position of the i'th site, show that we can put H_{MF} under the form

$$\sum_{\mathbf{q}} \phi_{\mathbf{q}}^\dagger M_{\mathbf{q}}(\alpha, \lambda) \phi_{\mathbf{q}} + \ N_s \epsilon_0(\alpha, \lambda), \qquad \phi_{\mathbf{q}} = \begin{pmatrix} a_{\uparrow \mathbf{q}} \\ (a_{\downarrow -\mathbf{q}})^\dagger \end{pmatrix}, \tag{13}$$

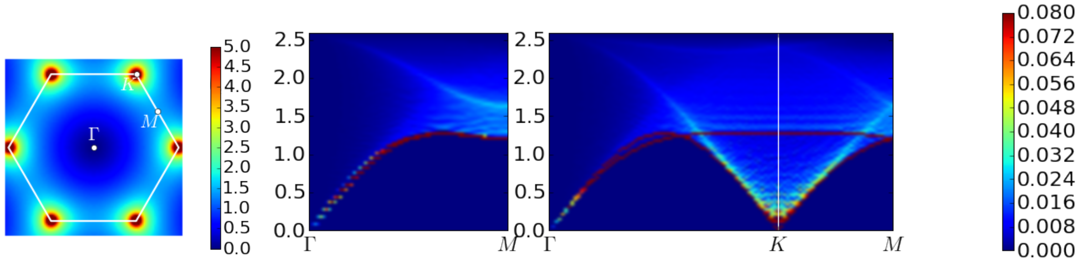


Figure 1: Static and dynamic structure factors on the triangular lattice, obtained by SBMFT. The color scale is truncated.

where $M_{\mathbf{q}}(\alpha,\lambda)$ is a 2×2 matrix.

19. We give

$$\epsilon_0(\alpha,\lambda) = N_s\left(\frac{3}{4}+6\alpha^2+2\lambda\right) \tag{14}$$

$$M_{\mathbf{q}}(\alpha,\lambda) = \begin{pmatrix} -\lambda & -\alpha f_{\mathbf{q}} \\ -\alpha f^*_{\mathbf{q}} & -\lambda \end{pmatrix} \tag{15}$$

$$f^{\triangle}_{\mathbf{q}} = 2i(\sin(\mathbf{q}\cdot\mathbf{e}_x)+\sin(\mathbf{q}\cdot\mathbf{e}_y)-\sin(\mathbf{q}\cdot(\mathbf{e}_y+\mathbf{e}_x))) \tag{16}$$

The linear transformation such that $\tilde{M}_{\mathbf{q}}$ is diagonal:

$$\phi_{\mathbf{q}} = P_{\mathbf{q}}\tilde{\phi}_{\mathbf{q}} \tag{17}$$

$$\tilde{M}_{\mathbf{q}} = {P_{\mathbf{q}}}^{\dagger}M_{\mathbf{q}}P_{\mathbf{q}} \tag{18}$$

and preserves the commutation relations is called the Bogoliubov transformation and defines new operators $\tilde{a}_{\uparrow\mathbf{q}}$ and $\tilde{a}_{\downarrow\mathbf{q}}$. What is the condition on $P_{\mathbf{q}}$ to preserve the commutation relations ? What should be the sign of the diagonal coefficients of $\tilde{M}_{\mathbf{q}}$? What is the ground state in terms of the $\tilde{a}_{\mathbf{q}}$ operators ?

20. Find the dispersion relation (the eigenenergies $\epsilon_{\uparrow k}$ and $\epsilon_{\downarrow k}$) as a function of λ and α. Express the ground state energy as an average over the Brillouin zone.

21. Write the self-consistency equations.

22. We give the (numerical) result here: $\lambda = -1.282$ and $\alpha = 0.4936$. In this frame, we can calculate the dynamical structure factor $S(\mathbf{q},\omega)$ which is the space-time Fourier transform of spin-spin correlation functions $\langle \mathbf{S}(i,t)\cdot\mathbf{S}(i=0,t=0)\rangle$ and the static (equal time) structure factor $S(\mathbf{q}) = \int_0^\infty \frac{d\omega}{2\pi}S(\mathbf{q},\omega)$. Such figures are obtained by inelastic neutron scattering.

    What is the static structure factor of the classical ground state (where the spin is a classical vector) ? Compare it to the SBMFT result.