Can Majorana Fermions correctly describe the ordered state of an antiferromagnetic Heisenberg chain?

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To check the reliability of the Majorana representation of quantum spin systems, we use it to compute the ground state energy of an antiferromagnetic spin 1/2 chain to one loop order. We find a very small one loop correction of the mean field energy and a discrepancy of >100% compared to the Bethe Ansatz result. We conclude that a careful handling of the gauge degrees of freedom of this representation is crucial to get correct results.

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I. INTRODUCTION

The Majorana representation is a promising tool for describing frustrated quantum spin 1/2 antiferromagnets and heavy fermion systems \[1, 2\]. It provides a description of spin operators in terms of bilinears of real fermions without any constraints. It is useful to consider the representation of spin operators of the group $O(N)$ and take $N = 3$ only at the end:

\[
O(N) : s_{x}^{k} = -\frac{i}{2} (\eta_{x}^{k} \eta_{x}^{l} - \eta_{x}^{l} \eta_{x}^{k}) , \quad k, l = 1, 2, \ldots, N, \quad [\eta_{x}^{k}, \eta_{y}^{l}]_{+} = \delta_{kl} \delta_{xy}, \quad \eta_{x}^{k+} = \eta_{x}^{k}
\]

\[
O(3) : \vec{s}_{x} = -\frac{i}{2} \vec{\eta}_{x} \times \vec{\eta}_{x}
\]

A mean field treatment of spin systems in this representation gives rise to $O(N)$ invariant bond variables in a natural way and, therefore, this representation seems suited for a description of the disordered or "liquid" phases of quantum spin systems. Indeed it is not difficult to see, by using the Majorana representation, that most $O(N)$ spin systems (in the lowest representation that generalizes spin $\frac{1}{2}$) reduce to RVB like spin liquids at $N = \infty$ \[3\]. However, for the Majorana representation to be really useful, it must also be able to describe the competition between ordered and liquid spin systems as a function of the amount of frustration and for $N = 3$.

Recently, it was pointed out that a simple Hartree Fock treatment of the spin 1/2 Heisenberg antiferromagnetic chain gives qualitatively correct results \[3\]. The purpose of the present note is to show that in a more systematic approach the one loop correction to the mean field energy is small and that the ground state energy still differs from the exact Bethe Ansatz result by more than 100%.

It is very likely that the local $Z_{2}$ invariance of the Majorana representation is responsible for this discrepancy and that it must be dealt with correctly in order to obtain reliable results. The situation is reminiscent of the Yang Mills theory of strong interactions in which a correct treatment of the local invariance is crucial.

Although the local $Z_{2}$ invariance of the Majorana representation was previously dealt with in the context of the two channel Kondo problem \[2\] a more systematic treatment of this invariance using standard gauge theory techniques is needed.

II. MEAN FIELD

The Hamiltonian of the $O(N)$ antiferromagnet is

\[
O(N) : H = \sum_{<x,y>,k,l} \frac{1}{2} s_{x}^{kl} s_{y}^{kl} - \frac{N}{8} = \frac{1}{2} \sum_{<x,y>} \left(\eta_{x\mu} \eta_{y\mu}\right)^{2}
\]

\[
O(3) : H = \sum_{<x,y>} \vec{s}_{x} \cdot \vec{s}_{y} - \frac{3}{8} = \frac{1}{2} \sum_{<x,y>} \left(\vec{\eta}_{x} \cdot \vec{\eta}_{y}\right)^{2}
\]

with $<x,y>$ denoting neighboring points, $J = 1$ and we will suppress the internal symmetry indices in the following. To allow for a systematic treatment of fluctuations the mean field must be introduced by a Hubbard-Stratonovich transformation:
\[ Z = \text{Tr} e^{-\beta H} = \int D\eta e^{-\int_0^\beta dt \left( \dot{\eta}_p \partial_t \eta_p + H(\eta) \right)} \]

\[ = \int DB D\eta e^{-\int_0^\beta dt \left( \dot{\eta}_p \partial_t \eta_p + H(B,\eta) \right)}, \quad H(B, \eta) = \frac{1}{4} \sum_{x,y} \frac{B_{xy}^2}{J_{xy}} + \frac{i}{2} \sum_{x,y} B_{xy} \eta_x \eta_y \]

\[ \rightarrow Z = \int DB e^{-\beta F(B)}, \quad F(B) = -\frac{1}{2\beta} \log \det (\partial_t + iB) \quad (3) \]

For a \( d = 1 \) chain and with a uniform auxiliary field

\[ B_{xy} = \frac{M}{2} (\delta_{x,y+1} - \delta_{y,x+1}) \quad (4) \]

we find

\[ H(B, \eta) = \frac{L}{8} M^2 - \frac{M}{2} \sum_{p > 0} (\eta_{pp} \eta_{-pp} - \eta_{-pp} \eta_{pp}) \sin p \]

\[ [\eta_p, \eta_q]_+ = \delta_{p+q,0} \quad (5) \]

where \( L \) denotes the length of the chain. The mean field saddle point is \( M = \frac{2N}{\pi} \) and gives a quasiparticle dispersion and ground state energy (for the original Heisenberg Hamiltonian) of

\[ E(p) = \frac{2N}{\pi} \sin p \quad (\text{Bethe Ansatz: } \frac{\pi}{2} \sin p) \]

\[ \frac{< H(B, \eta) >}{L} + \frac{N}{8} = - \frac{N^2}{2\pi^2} + \frac{N}{8} \approx -0.08 \quad (\text{Bethe Ansatz: } -0.44) \quad (6) \]

It is known that the optimal mean field in the Majorana representation is completely dimerized for a large class of Heisenberg antiferromagnets in any dimension \( \mathbb{Z} \) and we could check whether the fluctuations about the mean field restore the uniform mean field configuration in \( d = 1 \). However, for our purpose of demonstrating a bug in an uncritical use of the Majorana representation this is unnecessary since:

- the exact Bethe Ansatz solution does not break translations -
- as we will see the fluctuations about the uniform mean field in the Majorana representation give only a small correction to the mean field energy, with the one loop corrected ground state energy still differing from the exact result by more than 100%.

**III. ONE LOOP CORRECTION**

The self consistent Gaussian approximation is a very reasonable approximation that gives the first 3 terms of the Stirling series of \( \Gamma(n) = \int_0^\infty dx x^{n-1} e^{-x} \) at one stroke and which should, a priori, give good results also for the spin chain in the Majorana representation. In this approximation, the partition function reduces to

\[ Z \sim \frac{e^{-\beta F(B)}}{\sqrt{\det \delta^2 F/\delta B^2}} = e^{-\beta \tilde{F}(B)}, \quad \tilde{F}(B) = F(B) + \frac{1}{2\beta} \log \det \frac{\delta^2 F}{\delta B^2} \quad (7) \]

To identify the quadratic form \( \delta^2 F/\delta B^2 \) one must expand the free energy \( F(B) \) about the saddle point

\[ F(B + \delta B) = F(B) + \frac{1}{2} \frac{\delta^2 F}{\delta B^2} \delta B \delta B + O(\delta B, \delta B^3) \]

\[ \frac{1}{2} \frac{\delta^2 F}{\delta B^2} \delta B \delta B = \frac{1}{4\beta} \int_0^\beta dt \sum_{x,y} \delta B_{xy}^2 + \frac{1}{4\beta} \text{tr} \left( \frac{1}{\partial_t + iB} \right) \delta B \left( \frac{1}{\partial_t + iB} \right) \delta B \quad (8) \]

After some simplifications the total quadratic form turns out to be
\[
\delta^2 F \delta B \delta B = \sum \delta b^* (q) F(q) \delta b(q)
\]
\[
F(q) = 1 + \frac{1}{L} \sum_{p+r-q=0} \left( 1 - e^{i(r-p)} \right) g(p) g(r), \quad q = (q_0, q_1)
\]
\[
\delta B = \frac{1}{\sqrt{L} \beta} \sum \delta b(q) e^{iqx},
\]
\[
\frac{1}{\partial_q + iB} = \frac{1}{\sqrt{L} \beta} \sum g(p) e^{ipx}, \quad g(p) = -\frac{1}{i p_0 + M \sin p_1}
\]

At zero temperature, the sum over Matsubara frequencies turns into an integral and one obtains:

\[
\delta E_{\text{fluctuations}} = \frac{1}{2\beta} \log \det \left( \frac{\delta^2 F}{\delta B \delta B} \right)_{\mathbb{T}=0} = \frac{1}{8\pi^2} \int_{-\infty}^{\infty} dq_0 \int_{-\pi}^{\pi} dq_1 \log F(q_0, q_1)
\]

\[
F(q_0, q_1) = 1 - \frac{1}{L} \sum_p (1 - e^{2ip}) \frac{n_F(M \sin(p - \frac{q_1}{2})) - n_F(M \sin(p + \frac{q_1}{2}))}{M \sin(p - \frac{q_1}{2}) - M \sin(p + \frac{q_1}{2}) - i q_0}
\]

\[
= 1 + \frac{1}{\pi M \sin(\frac{q_1}{2})} \int_0^\frac{\pi}{2} dp \sin^2 p \cos p \left( \frac{\cos \left( \frac{q_0}{M \sin(\frac{q_1}{2})} \right)}{2 \sin^2(p + \frac{q_1}{2})} \right)
\]

\[
= 1 + \frac{1}{\pi M} \left( -1 + \frac{\sqrt{1 + x^2}}{\sin(\frac{q_1}{2})} \tanh^{-1} \left( \frac{\sin q_1/2}{\sqrt{1 + x^2}} \right) \right), \quad x = \frac{q_0}{2M \sin \frac{q_1}{2}}
\]

The total energy that includes the fluctuations about the un dimerized saddle point is, therefore,

\[
E_N = \frac{M^2}{8} - \frac{NM}{2\pi} + \frac{\delta E_{\text{fluctuations}}}{2}\pi
\]

\[
\delta E_{\text{fluctuations}}(M) = \frac{M}{\pi^2} \int_0^\pi dq \int_0^{\infty} dx \log F \sin \frac{q}{2} dxdq
\]

Setting \( N = 3 \) and \( M = \frac{6}{\pi} \) we find \( \delta E_{\text{fluctuations}} = 0.036 \) and since the correction is so small, it is not necessary to do the Gaussian approximation self consistently. The total energy differs from the exact Bethe Ansatz result still by much more than 100%. So the loop expansion converges very well, but...to the wrong result.

**IV. THE PROBLEM OF GAUGE INVARIANCE**

In the Majorana representation of eq(1), there is an infinity of operators that commute with the Hamiltonian \[2\]

\[
Q(\eta_x) = i \prod_{\mu=1}^{N} \eta_{x\mu}
\]

\[
[Q(\eta_x), H] = 0
\]

N even : \( [Q(\eta_x), Q_y(\eta_y)]_- = 0 \)

N odd : \( [Q(\eta_x), Q_y(\eta_y)]_+ = \left( \frac{1}{2} \right)^{N-1} \delta_{x,y} \)

The oscillation in statistics of \( Q(\eta_x) \) as a function of \( N \) may be considered to be responsible for the even/odd oscillation in the energy of a small cluster as a function of \( N \) that was observed in [4]. The \( \eta_x \) are gauge transformed by commuting (anticommuting) them with the operators \( Q(\eta_x) \). The theory of quantising gauge invariant systems is highly developed [2], but a caricature of existing methods runs as follows:

- some redundant parameter is eliminated and the system, now without gauge invariance, is treated in terms of the remaining variables by conventional methods -
• or, alternatively, one refrains from eliminating redundant variables. Instead, one imposes a constraint on the space of variables and provides a correction factor in a way that essentially extracts the volume of the gauge group from the partition function. This is done by inserting unity in the form of

\[ 1 = \Delta_{FP}(\eta) \int D\varepsilon \delta(f(\eta)) \]

into the partition function, where \( f(\eta) \) is a function of \( \eta \) that breaks the symmetry, and where \( D\varepsilon \) integrates over the group. \[\Box\]. \( \Delta_{FP}(\eta) \) is the determinant of the operator \( \frac{\delta F}{\delta \varepsilon} \) and is represented by auxiliary or "ghost" particles.

To apply the first method, one notices that the constant multiplicity \( 2^{L/2} \) of extra spurious states in a system of \( L \) spins can be understood in the representation \[\Box\]:

\[ \eta_{x\mu} = \sigma_{x\mu} f_x \]

where \( f_x \) are Majorana fermions and \( \sigma_{x\mu} \) are Pauli matrices of the group \( O(N) \). It can be shown that the extra fermions \( f_x \) get eliminated by imposing a positive spectrum, \( i\eta_x \eta_y > 0 \), on a non-overlapping covering by dimers \((x, y)\) or on dimers between points on the original system and an extra copy of it. In the second approach, because the symmetry group is fermionic, \( \Delta_{FP}(\eta) \) is actually the inverse of the determinant of \( \frac{\delta F}{\delta \varepsilon} \) and will be represented by bosonic auxiliary or "ghost" particles. The details of this gauge approach to the Majorana representation still remain to be worked out, however.

In conclusion, we have seen that ground state energy of a spin 1/2 antiferromagnetic chain treated by Majorana representation and mean field plus Gaussian fluctuations comes out incorrectly, although the loop correction is small. This strongly suggests that a proper treatment of the Majorana representation of spin systems must address the problem of local \( Z_2 \) invariance or the local supersymmetry of the system.

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