For the Quantum Heisenberg Ferromagnet, Some Conjectured Approximations

Paul Federbush  
Department of Mathematics  
University of Michigan  
Ann Arbor, MI 48109-1109  
(pfed@math.lsa.umich.edu)

Abstract

We present some conjectured approximations for spin expectations in a Quantum Heisenberg system. The conjectures are based on numerical experimentation, some theoretical insights and underpinning, and aesthetic value. We hope theoretical developments will follow from these ideas, even leading to a proof of the phase transition (in three dimensions).
We organize this paper into three sections. The first presents preliminary definitions and the conjectures. The second contains a rigorous theoretical development of a useful framework for the system. The final section introduces an “average-field” structure that may lead to an understanding, and hopefully a proof, of the conjectures.

I) THE CONJECTURES.

We consider a lattice, $\Lambda$, and the associated Quantum Heisenberg Hamiltonian

$$H = - \sum_{i \sim j} (I_{ij} - 1)$$

where $I_{ij}$ interchanges the spins of the two neighboring sites $i$ and $j$ in the lattice $\Lambda$. We let $p_i$ be the projection onto spin up at site $i$.

$$p_i = \frac{1}{2} (\sigma_{zi} + 1).$$

We consider a state $\psi_0$ with spin up at sites in $S_0$, and spin down at the complementary sites.

$$p_i \psi_0 = \begin{cases} 
\psi_0, & i \in S_0 \\
0, & i \notin S_0
\end{cases}$$

We assume there are $N$ spin ups,

$$\# \{S_0\} = N.$$  

We let $\phi_{\mu}(i)$ be a solution of the lattice heat equation

$$\frac{\partial}{\partial \mu} \phi_{\mu}(i) = (\Delta \phi_{\mu})(i)$$

with initial conditions

$$\phi_0(i) = \begin{cases} 
1, & i \in S_0 \\
0, & i \notin S_0
\end{cases}$$

We define

$$\rho_{\mu}(i) = \frac{\phi_{\mu}^2(i)}{\phi_{\mu}^2(i) + (1 - \phi_{\mu}(i))^2}$$
and

\[ < p_i >_\mu = \frac{\langle e^{-\mu H} \psi_0, p_i e^{-\mu H} \psi_0 \rangle}{\langle e^{-\mu H} \psi_0, e^{-\mu H} \psi_0 \rangle} \].

(8)

**Conjecture 1.**

\[ | < p_i >_\mu - \rho_\mu(i) | < c_d < 1. \]

(9)

**Conjecture 2.**

\[ | < p_i >_\mu - \phi_\mu(i) | < c_d < 1. \]

(10)

In one-dimension the corresponding \( c_1 \) may be picked to be \( \frac{1}{2} \), according to our numerical studies.

**Conjecture 3.**

\[ \lim_{\mu \to 0} \frac{1}{\mu} | < p_i >_\mu - \rho_\mu(i) | = 0 \]

(11)

the limit taken in \( \ell^\infty(\Lambda) \), and convergence independent of \( S_0 \) and \( N \). In one-dimension the \( \mu \) in (11) may be replaced by \( \mu^{2-\varepsilon} \).

Contrary to our earlier expectations (as presented in a previous version of this note) the behavior of \( < p_i >_\mu \) as \( \mu \) becomes large is not simple. A better approximation than \( \rho_\mu(i) \) or \( \phi_\mu(i) \) when \( \mu \) is large is realized in \( \phi_{\frac{\mu}{2}}(i) \). We present in our next conjecture the result of our numeric study:

**Conjecture 4.**

For \( \mu \geq 4 \) one has

\[ | < p_i >_\mu - \phi_{\frac{\mu}{2}}(i) | < .1. \]

(12)
We have been specific with numbers in (12) to give the flavor of the estimate’s quality.
We have some theoretical understanding of the reason $\phi_\mu(i)$ is a good approximation to
$<p_i>\mu$, but we do not discuss it in this note, restricting our attention to $\rho_\mu(i)$ and $\phi_\mu(i)$
in later sections.

Implicit in all these estimates is a locality property of $<p_i>\mu$. We state a very weak form
of this in the following conjecture.

**Conjecture 5.**

For any $\varepsilon > 0$, there is an $L_{\varepsilon,\mu}$, such that $<p_i>\mu$ is determined within $\varepsilon$ by knowledge
of the spin configuration (as specified in (3)) in a region within distance $L_{\varepsilon,\mu}$ of site $i$, i.e.
changing spins outside this distance cannot effect $<p_i>\mu$ by more than $\varepsilon$

Conjecture 5 is the most basic of our assertions, and should fit into some very general
theoretical framework.

*Cave Adfirmationes:* Most of the numerical investigation was on a one-dimensional lattice. (But also in periodic two-dimensional sets and three-dimensional sets.)

**II) SOME SIMPLE THEORY.**

The Hilbert space of the system is naturally viewed as a direct sum

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots \oplus \mathcal{H}_{|\Lambda|}$$

where in $\mathcal{H}_N$ there are $N$ spin ups. We write $H_N$ for $H$ restricted to $\mathcal{H}_N$. The space $\mathcal{H}_N$
is an invariant subspace of $H$, the set of $N$ spin waves.

We let $Q$ be an operator interchanging spin up and spin down, $Q$ a unitary operator commuting with $H$. $Q$ interchanges $H_N$ and $H_{|\Lambda|−N}$ as follows

$$Q \left( \bigotimes_{i \in S} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \bigotimes_{j \not\in S} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right) = \bigotimes_{i \in S} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \bigotimes_{j \not\in S} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

(13)
Vectors in $\mathcal{H}_N$ are described by symmetric functions on $N$ distinct lattice sites. $f = f(\ldots)$ is associated to vectors in $\mathcal{H}_N$ as follows

$$f \leftrightarrow \sum_{i_1 \ldots i_N} f(i_1, \ldots, i_N) \bigotimes_{i \in \{i_1, \ldots, i_N\}} \left( \begin{array}{c} 1 \\ 0 \end{array} \right) \bigotimes_{i \not\in \{i_1, \ldots, i_N\}} \left( \begin{array}{c} 0 \\ 1 \end{array} \right). \tag{14}$$

The sum in (14) is over distinct indices.

For $N > M$ there is a linear map from $\mathcal{H}_N$ to $\mathcal{H}_M$ called $P_{N,M}$. Let $f$ be in $\mathcal{H}_N$, then we define $P_{N,M}f$ in $\mathcal{H}_M$ by

$$(P_{N,M}f)(i_1, \ldots, i_M) = \sum_{i_{M+1}, \ldots, i_N} f(i_1, \ldots, i_M, i_{M+1}, \ldots, i_N) \tag{15}$$

$P_{N,M}$ commutes with $H$ and interlaces $H_N$ and $H_M$

$$P_{N,M}H_N = H_M P_{N,M}. \tag{16}$$

If $2N \leq |\Lambda|$ then it is easy to show $P_{N,M}$ is onto. The preceding structure is related to the invariance of the system under global rotations.

For $f$ in any $\mathcal{H}_N$ we define

$$f_\mu \equiv e^{-\mu H} f . \tag{17}$$

Of course

$$e^{-\mu H} P_{N,M} = P_{N,M} e^{-\mu H_N}. \tag{18}$$

In $\mathcal{H}_1$, $f_\mu$ satisfies the heat equation

$$\frac{\partial}{\partial \mu} f_\mu = -H_1 f_\mu = \Delta f_\mu . \tag{19}$$

So for $f$ in $\mathcal{H}_N$ we note the amusing fact that $P_{N,1}f_\mu$ satisfies the heat equation.

**III) AN AVERAGE-FIELD APPROXIMATION.**

Let $\psi_0$ be a state in $\mathcal{H}_N$, sharp in the spins, with spin up at $i$ if $i \in S_0$, spin down if $i \not\in S_0$, $S_0$ a set of $N$ sites.

$$\psi_0 \leftrightarrow \bigotimes_{i \in S_0} \left( \begin{array}{c} 1 \\ 0 \end{array} \right) \bigotimes_{i \not\in S_0} \left( \begin{array}{c} 0 \\ 1 \end{array} \right). \tag{20}$$
and
\[ \psi_{\mu} = e^{-\mu H_N} \psi_0. \]  

(21)

We define
\[ \phi_{\mu} = N \, P_{N,1} \, \psi_{\mu} \]

(22)

\( \phi_{\mu} \) in \( H_1 \), satisfies the heat equation and
\[ \phi_0(i) = \begin{cases} 
1, & i \in S_0 \\
0, & i \notin S_0 
\end{cases} \]

(23)

We introduce an “average-field”-like “approximation” to \( \psi_{\mu} \).

\[ \psi_{\mu}^{AP} = \bigotimes_i \left( \begin{array}{c}
\phi_{\mu}(i) \\
1 - \phi_{\mu}(i)
\end{array} \right). \]

(24)

This approximation has two nice features.

1) The approximation is “invariant and \( Q \)”. That is, it is \( Q \) of the approximation obtained starting with \( Q \psi_0 \) instead of \( \psi_0 \).

2) The approximation is not sharp in spin wave number. (It does not lie in a single \( H_N \).) But in a reasonable sense it projects using \( \{P_{N,1}\} \) onto \( \phi_{\mu}(i) \) in \( H_1 \), that does satisfy the heat equation.

We note that \( \rho_{\mu}(i) \), from equation (7), is given by
\[ \rho_{\mu}(i) = \frac{\langle \psi_{\mu}^{AP} : P_{\mu} \psi_{\mu}^{AP} \rangle}{\langle \psi_{\mu}^{AP} : \psi_{\mu}^{AP} \rangle}. \]

(25)

Thus our approximate wave function, the “average-field” function (24) yields the spin up probabilities of approximation 1, equation (9'). The “average-field” wavefunction satisfies the equation
\[ \frac{d}{d\mu} \psi_{\mu}^{AP} = -H \psi_{\mu}^{AP}. \]

(26)
in the limit of nearly constant $\phi_\mu(i)$. We expect there is some truth to the average field wavefunction; perhaps enough, so that its study (objective genitive) leads towards a proof of the phase transition for magnetization. We note that $\phi_\mu(i)$ and $\rho_\mu(i)$ differ by less than .16. Both $\phi_\mu(i)$ and $\rho_\mu(i)$ are “invariant under $Q$” as approximations.