For the Quantum Heisenberg Ferromagnet, Some Conjectured Approximations

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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, Λ, and the associated Quantum Heisenberg Hamiltonian

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

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

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

We consider a state ψ_0 with spin up at sites in $\mathcal{S}_0$, and spin down at the complementary sites.

$$p_i\, \psi_0 = \begin{cases} \psi_0\ , & i \in \mathcal{S}_0 \\ 0\ , & i \notin \mathcal{S}_0 \end{cases} \tag{3}$$

We assume there are N spin ups,

$$\#\, \{\mathcal{S}_0\} = N. \tag{4}$$

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

$$\frac{\partial}{\partial \mu}\, \phi_\mu(i) = (\Delta \phi_\mu)(i) \tag{5}$$

with initial conditions

$$\phi_0(i) = \begin{cases} 1\ , & i \in \mathcal{S}_0 \\ 0\ , & i \notin \mathcal{S}_0 \end{cases} \tag{6}$$

We define

$$\rho_\mu(i) = \frac{\phi_\mu^2(i)}{\phi_\mu^2(i) + (1 - \phi_\mu(i))^2} \tag{7}$$

and

$$< p_i >_\mu = \frac{\left\langle e^{-\mu H}\psi_0,\ p_i\, e^{-\mu H}\psi_0\right\rangle}{\left\langle e^{-\mu H}\psi_0,\ e^{-\mu H}\psi_0\right\rangle} \quad . \tag{8}$$

Conjecture 1.

$$| < p_i >_\mu - \rho_\mu(i) | < c_d < 1. \tag{9}$$

Conjecture 2.

$$| < p_i >_\mu - \phi_\mu(i) | < c_d < 1. \tag{10}$$

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

Conjecture 3.

$$\lim_{\mu \to 0} \frac{1}{\mu} | < p_i >_\mu - \rho_\mu(i) | = 0 \tag{11}$$

the limit taken in $\ell^\infty(\Lambda)$, and convergence independent of $\mathcal{S}_0$ and N. In one-dimension the μ 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 μ becomes large is not simple. A better approximation than $\rho_\mu(i)$ or $\phi_\mu(i)$ when μ 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

$$| < p_i >_\mu - \phi_{\frac{\mu}{2}}(i) | < .1 \ . \tag{12}$$

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 $\phi_{\frac{\mu}{2}}(i)$ 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 ε 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 ε

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

$$Q\left(\bigotimes_{i\in\mathcal{S}}\begin{pmatrix}1\\0\end{pmatrix}_i\bigotimes_{j\notin\mathcal{S}}\begin{pmatrix}0\\1\end{pmatrix}_j\right) = \bigotimes_{i\in\mathcal{S}}\begin{pmatrix}0\\1\end{pmatrix}_i\bigotimes_{j\notin\mathcal{S}}\begin{pmatrix}1\\0\end{pmatrix}_j . \tag{13}$$

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

$$f \longleftrightarrow \sum_{i_1,\dots,i_N} f(i_1,\dots,i_N) \bigotimes_{i\in\{i_i,\dots,i_N\}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}_i \bigotimes_{j\notin\{i_i,\dots,i_N\}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}_j . \tag{14}$$

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

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

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

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

If $2N \le |\Lambda|$ 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

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

In $\mathcal{H}_1$, f_μ 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 ψ_0 be a state in $\mathcal{H}_N$, sharp in the spins, with spin up at i if $i \in \mathcal{S}_0$, spin down if $i \notin \mathcal{S}_0$, $\mathcal{S}_0$ a set of N sites.

$$\psi_0 \longleftrightarrow \bigotimes_{i\in\mathcal{S}_0} \begin{pmatrix} 1 \\ 0 \end{pmatrix}_i \bigotimes_{j\notin\mathcal{S}_0} \begin{pmatrix} 0 \\ 1 \end{pmatrix}_j \tag{20}$$

and

$$\psi_\mu = e^{-\mu H_N} \psi_0 \ . \tag{21}$$

We define

$$\phi_\mu = N \ P_{N,1} \ \psi_\mu \tag{22}$$

ϕ_μ in H_1, satisfies the heat equation and

$$\phi_0(i) = \begin{cases} 1 \ , & i \in \mathcal{S}_0 \\ \\ 0 \ , & i \notin \mathcal{S}_0 \end{cases} \tag{23}$$

We introduce an "average-field"-like "approximation" to ψ_μ.

$$\psi_\mu^{AP} \equiv \bigotimes_i \begin{pmatrix} \phi_\mu(i) \\ \\ 1 - \phi_\mu(i) \end{pmatrix}_i \ . \tag{24}$$

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 ψ_0.

2) The approximation is not sharp in spin wave number. (It does not lie in a single $\mathcal{H}_N$.) But in a reasonable sense it projects using $\{P_{N,1}\}$ onto $\phi_\mu(i)$ in $\mathcal{H}_1$, that does satisfy the heat equation.

We note that $\rho_\mu(i)$, from equation (7), is given by

$$\rho_\mu(i) = \frac{\left\langle \psi_\mu^{AP}, p_i \psi_\mu^{AP} \right\rangle}{\left\langle \psi_\mu^{AP}, \psi_\mu^{AP} \right\rangle}. \tag{25}$$

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

$$\frac{d}{d\mu} \ \psi_\mu^{AP} = -H \ \psi_\mu^{AP} \tag{26}$$

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.