Single Site Spin Expectation for the Imaginary Time Heisenberg Ferromagnet Wave Function, Numerical Approximation and Theoretical Argument

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Abstract

Certain approximations for the spin expectations have been studied both numerically and theoretically. Approximations are constructed using solutions of the lattice heat equation. The most interesting idea is a certain randomness assumption for a theoretically derived quantity, that leads directly to a given approximation. We are betting the randomness assumption is rigorously correct.

The model is constructed on a rectangular lattice, V. The Hamiltonian is taken as

$$H = -\sum_{i\sim j} \frac{1}{2}\Big(\vec{\sigma}_i \cdot \vec{\sigma}_j - 1\Big) = -\sum_{i\sim j} \Big(I_{ij} - 1\Big) \tag{1}$$

where I_{ij} interchanges the spins at nearest neighbor sites i and j. The wave function, $\vec{\psi}(t)$,

$$\vec{\psi}(t) = e^{-Ht}\vec{\psi}(0) \tag{2}$$

is chosen so that at $t = 0$ the σ_{zi} are diagonalized at each site

$$\vec{\psi}(0) = \left(\underset{i\in\mathcal{S}_0}{\otimes} \begin{pmatrix} 1 \\ 0 \end{pmatrix}_i \right) \bigotimes \left(\underset{j\notin\mathcal{S}_0}{\otimes} \begin{pmatrix} 0 \\ 1 \end{pmatrix}_j \right) \tag{3}$$

where $\mathcal{S}_0$ is the set of vertices where the spin is "up" at $t = 0$. Instead of working with σ_{zi} as basic variables, we work with

$$p_i = \frac{1}{2}\,(\sigma_{zi} + 1). \tag{4}$$

The basic quantity we want to study is

$$\Big\langle p_i \Big\rangle_t = \frac{\Big\langle \vec{\psi}(t), p_i\,\vec{\psi}(t) \Big\rangle}{\Big\langle \vec{\psi}(t),\ \vec{\psi}(t) \Big\rangle} \tag{5}$$

The approximations we consider for the $< p_i >_t$ of (5) involve $\phi_t(i)$ the solution of the lattice heat equation:

$$\frac{\partial}{\partial t}\,\phi_t(i) \;=\; (\Delta\phi_t)(i) \tag{6}$$

$$\phi_0(i) \;=\; \begin{cases} 1, & i \in \mathcal{S}_0 \\ 0, & i \notin \mathcal{S}_0 \end{cases} \tag{7}$$

If $|V|$ is the number of vertices in V, then solving the differential equations (6)-(7) involves solving $|V|$ coupled differential equations. By contrast solving for $\vec{\psi}(t)$ involves solving $2^{|V|}$ coupled differential equations. (True, the decoupling of sectors of fixed spin wave number simplifies the equations slightly). Thus estimating $\left\langle p_i \right\rangle_t$ by some function of the ϕ_t is a great simplification over direct computation.

In [1] three approximations for $\left\langle p_i \right\rangle_t$ in terms of the $\phi_t(i)$ were considered.

<u>Approximation 1</u>

$$\left\langle p_i \right\rangle_t \cong \phi_t(i) \tag{8}$$

<u>Approximation 2</u>

$$\left\langle p_i \right\rangle_t \cong \rho_t(i) \equiv \frac{\phi_t^2(i)}{\phi_t^2(i) + \Big(1 - \phi_t(i)\Big)^2} \tag{9}$$

<u>Approximation 3</u>

$$\left\langle p_i \right\rangle_t \cong \phi_{t/2}(i) \tag{10}$$

These approximations were studied numerically solving the $|V| + 2^{|V|}$ differential equations using MAPLE. Work was primarily restricted to one dimensional lattices, say five initial spin ups on a periodic chain of length twelve. These approximations are not as different as one might think. The right and left sides of (8), (9), (10) all lie between all lie between 0 and 1. And for example

$$|\phi_t(i) - \rho_t(i)| < .16 \tag{11}$$

The numerical study reported in [1] can only be thought of as suggestive, due to the limitations of lattice size considered. We here consider only the first two of the approximations.

Equation (13) of [3] yields an exact expression for $\vec{\psi}(t)$ with "leading term"

$$\bigotimes_i \begin{pmatrix} \phi_i(t) \\ \\ 1 - \phi_i(t) \end{pmatrix}_i \tag{12}$$

If we compute $\left\langle p_i \right\rangle_t$ using this approximate wave function, equation (12), instead of $\vec{\psi}(t)$, we find exactly the expression $\rho_t(i)$! This leading term expression becomes exact as

$t \to 0$. An overblown study of this is given in [2]. Thus Approximation 2 is the right expression in the small t limit.

In this paper we argue for Approximation 1 as the correct choice for large t. It is easiest to state a clean conjecture for the infinite lattices.

<u>Asymptotic Behavior Conjecture</u>

Let V be an infinite lattice. Then

$$\lim_{t\to\infty} |\phi_i(t) - \left\langle p_i \right\rangle_t| = 0. \tag{13}$$

We have chosen to state a result for the infinite lattice so there are no time (length^2) units. For a finite lattice the limit in (13) is clearly zero (on some preternatural scale). Like lots of the theorems in probability books this result, (13), would be useless even if true till one could predict at which rate zero is approached.

Approximation 1 has two nice properties

1) The approximation is invariant under the symmetry spin up $\leftrightarrow$ spin down, $\phi \leftrightarrow 1-\phi$. All three approximations share this feature.
2) The approximation conserves the conserved quantity

$$\sum_i \sigma_{zi} \tag{14}$$

That is

$$\sum_i \left\langle p_i \right\rangle_t = \sum_i \phi_i(t) \tag{15}$$

Approximation 3 shares this virtue.

We conclude with a simple theoretical argument that leads to our Asymptotic Behavior Conjecture. At the heart of our discussion will be a certain randomness assumption.

We proceed with our certainly esthetic computation. From equation (13) of [3] (a rigorous paper) we may write

$$\vec{\psi}(t) = \begin{pmatrix} \phi_i(t) \\ \\ 1-\phi_i(t) \end{pmatrix}_i \bigotimes \vec{v}(t) + \begin{pmatrix} 1 \\ -1 \end{pmatrix}_i \bigotimes \vec{w}(t) \tag{16}$$

where $\vec{v}(t)$ and $\vec{w}(t)$ are vectors in the tensor product space built up from all the two dimensional Hilbert spaces from all sites but site i. Thus they live in a $2^{|V|-1}$ dimensional space. We make the following single assumption in our procedure, which we will discuss later.

<u>Vector Randomness Assumption.</u> We assume

$$\lim_{t\to\infty} \left(\frac{\vec{v}(t)\cdot\vec{w}(t)}{|\vec{v}(t)|\cdot|\vec{w}(t)|} \right) = 0. \tag{17}$$

So in what follows we merely set

$$\vec{v}(t)\cdot\vec{w}(t) = 0. \tag{18}$$

We note that (17) is certainly true for finite lattices on a time scale $\sim L^2$, L the lattice length. The conjecture is that it is in fact true on a time scale ~ 1. Using (16) under assumption (18) we compute several quantities:

$$\begin{aligned} \left\langle \vec{\psi}(t), \vec{\psi}(t) \right\rangle &= \vec{v}(t)\cdot\vec{v}(t)\left(\phi_i^2(t) + (1-\phi_i(t))^2\right) + 2\vec{w}(t)\cdot\vec{w}(t) && (19) \\ \left\langle \vec{\psi}(t),\ \sigma_{xi}\, \vec{\psi}(t) \right\rangle &= 2\vec{v}(t)\cdot\vec{v}(t)\phi_i(t)(1-\phi_i(t)) - 2\vec{w}(t)\cdot\vec{w}(t) && (20) \\ \left\langle \vec{\psi}(t),\ \sigma_{zi}\, \vec{\psi}(t) \right\rangle &= \vec{v}(t)\cdot\vec{v}(t)\left(\phi_i^2(t) - (1-\phi_i(t))^2\right) && (21) \end{aligned}$$

But the expectation of σ_{xi}, equation (20), must be zero by invariance of the interaction under global rotation of spins and the rotation properties of $\vec{\psi}(0)$ under rotation about the z axis! Setting equation (20) to zero, trivially leads to the computation

$$\left\langle p_i \right\rangle_t = \phi_i(t)\ . \tag{22}$$

We conclude with a discussion of the Vector Randomness Assumption. We compare the current computation to an ergodic theory. Equation (20) being zero is parallel to conservation of energy in ergodic theory...there is to be randomness except for a single conserved quantity. As we stated before $\vec{v}(t)$ and $\vec{w}(t)$ live in $2^{|V|-1}$ dimensional spaces. But by propagation of effects with $x^2 \sim t$ it is better to think that they live in subspaces of dimension

$$\sim 2^{ct^{d/2}} \ . \tag{23}$$

This is the dimension of space in which the vectors' components are "chosen at random". This is why the dot product $\vec{v} \cdot \vec{w}$ goes to zero with $t \to \infty$. A slight study led the author to believe that within this high dimensional space (23) there are no obvious favored directions in which components of the vector are large.

The Vector Randomness Assumption may be true, deep, hard, and "obvious" like the ergodic hypothesis for a classical gas. Or we may be dealing here with an entirely specious argument, Federbush's (latest) Folly. Indeed there was some weak evidence pointed out in [1] that Approximation 3 is better than Approximation 1 as $t \to \infty$. Probably the authors of [4] would also opt against our Approximation 1. We hope the present paper at least serves to stimulate interest in numerically and theoretically clarifying the situation.

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References

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