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A polymer expansion for the quantum Heisenberg ferromagnet wave function

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A polymer expansion is given for the quantum Heisenberg ferromagnet wave function. Working on a finite lattice, one is dealing entirely with algebraic identities; there is no question of convergence. The conjecture to be pursued in further work is that effects of large polymers are small. This is relevant to the question of the utility of the expansion and its possible extension to the infinite volume. In themselves the constructions of the present paper are neat and elegant and have surprising simplicity. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1627958]

This paper assumes the fundamentals of the Heisenberg model but is basically self-contained; it arises from the work in Refs. 1 and 2, but these references need not be referred to. We intend to continue the work in the present paper, to obtain bounds on polymer contributions enabling extension to the infinite lattice.

Unpublished preprints (Refs. 1 and 2) are the previous works by the author, directly related to the current paper. Reference 1 is an experimental study of a number of approximations for certain spin expectations. Incidentally, one of the formal constructs studied below was introduced, with some properties there stated without proof, which are in the present paper. This is detailed below. We do hope that the present cluster expansion can be used to justify some of the approximations of Ref. 1; this is a line of theoretical interest for future work. In Ref. 2 there is an alternate construction of a cluster expansion to our present one. Therein there is also proof of convergence in the t small region. Our present construction is much simpler. Whether patent or latent, underlying all our work on the Heisenberg model is the hope that it eventually leads to a proof of the phase transition.

Equation (16) is the representation of the Heisenberg wave function we devote this paper towards developing. It is in the form commonly called a ''polymer expansion'' or ''cluster expansion'' in statistical mechanics nomenclature. At the end of the paper we give a brief physical discussion addressing usual interpretations of such expansions.

We work with a finite rectangular lattice, V, in d-dimensions, $\mathcal{V}$ the set of its vertices. The Hamiltonian is taken as

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

where I_{ij} interchanges the spins at nearest neighbor sites i and j. The Hilbert space $\mathcal{H}$ is constructed from basis elements $\mathbf{i}_{\mathcal{S}}$, basis elements in 1–1 correspondence with subsets $\mathcal{S}$ of $\mathcal{V}$, used for their labeling. In a spin-up spin-down representation

$$\mathbf{i}_{\mathcal{S}}=\bigotimes_{i\in\mathcal{S}}\begin{pmatrix}1\\0\end{pmatrix}_i\bigotimes_{j\notin\mathcal{S}}\begin{pmatrix}0\\1\end{pmatrix}_j. \tag{2}$$

A vector $\mathbf{f}$ in $\mathcal{H}$ may be expanded as

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$$\mathbf{f}=\sum_{\mathcal{S}} f(\mathcal{S})\mathbf{i}_{\mathcal{S}}. \tag{3}$$

For two sets $\mathcal{S}$ and $\mathcal{S}'$ we write $\mathcal{S}\sim\mathcal{S}'$ if $\mathcal{S}'$ is constructed from $\mathcal{S}$ by replacing some single element of $\mathcal{S}$ by one of its nearest neighbors. That is, $\mathcal{S}\sim\mathcal{S}'$ if there is a set $\mathcal{F}$ and elements of $\mathcal{V}$, i and j, so that

$$\begin{aligned}\mathcal{S}&=\mathcal{F}\cup i,\\ \mathcal{S}'&=\mathcal{F}\cup j,\end{aligned} \tag{4}$$

where $i\sim j$ and the unions in (4) are disjoint. If we write

$$\mathbf{f}(t)=e^{-Ht}\mathbf{f}=\sum_{\mathcal{S}} f(\mathcal{S},t)\mathbf{i}_{\mathcal{S}}, \tag{5}$$

it is easy to see that the $f(\mathcal{S},t)$ satisfy the differential equations

$$\frac{\partial}{\partial t}f(\mathcal{S},t)=\sum_{\mathcal{S}'\sim\mathcal{S}}(f(\mathcal{S}',t)-f(\mathcal{S},t)). \tag{6}$$

This is the graph heat equation, corresponding to a graph with vertices the subsets of $\mathcal{V}$, and with an edge connecting vertices $\mathcal{S}_1$ and $\mathcal{S}_2$ if and only if $\mathcal{S}_1\sim\mathcal{S}_2$. Physically, Eq. (6) is the imaginary time Schrödinger equation corresponding to the quantum Heisenberg Hamiltonian given in (1). (In Ref. 1 as in many other places the Heisenberg model has been experimentally studied by solving the coupled differential equations of (6) numerically.)

We now write $\mathcal{H}$ as direct sum

$$\mathcal{H}=\bigoplus_{n=0}^{\#(\mathcal{V})}\mathcal{H}^n, \tag{7}$$

where as indicated n ranges from 0 to $\#(\mathcal{V})$. $\mathcal{H}^n$ is spanned by the basis elements $\mathbf{i}_{\mathcal{S}}$, where $\#(\mathcal{S})=n$. $\mathcal{H}^n$ is the n spin-wave vector of the Hilbert space $\mathcal{H}$. The $\mathcal{H}^n$ are invariant subspaces of H. We write H^n for H restricted to $\mathcal{H}^n$.

We introduce operators $T^{r,s}$, where $T^{r,s}$ is a linear mapping from $\mathcal{H}^r$ to $\mathcal{H}^s$. They are defined as follows:

(1) $T^{r,r}$ is the identity on $\mathcal{H}^r$;
(2) If $s>r$,

$$T^{r,s}=0;$$

(3) If $s<r$ let $\mathbf{g}$ be in $\mathcal{H}^r$,

$$\mathbf{g}=\sum_{\mathcal{S}} g(\mathcal{S})\mathbf{i}_{\mathcal{S}}, \tag{8}$$

where $g(\mathcal{S})$ is nonzero only if $\#(\mathcal{S})=r$. Let

$$\mathbf{h}=T^{r,s}\mathbf{g}=\sum_{\mathcal{S}} h(\mathcal{S})\mathbf{i}_{\mathcal{S}}. \tag{9}$$

Then $h(\mathcal{S})=0$ unless $\#(\mathcal{S})=s$, and

$$h(\mathcal{S}) = \sum_{\mathcal{S}' \supset \mathcal{S}} g(\mathcal{S}') \quad \text{if} \quad \#(\mathcal{S}) = s. \tag{10}$$

We note that if $r > s > k$, then

$$T^{s,k} T^{r,s} = \frac{(r-k)!}{(s-k)!(r-s)!} T^{r,k}. \tag{11}$$

This is easy counting.

A nice result is that $T^{r,s}$ intertwines H^r and H^s. That is

$$T^{r,s} H^r = H^s T^{r,s}, \tag{12}$$

where both sides of (12) are viewed as mappings from $\mathcal{H}^r$ to $\mathcal{H}^s$. This is treated in Appendix A. The formalism of the mappings $T^{r,s}$ was introduced in Sec. II of Ref. 1, without proofs therein. We know of no earlier references to these operators. They may also be studied as a direct consequence of the global rotation invariance of the Heisenberg model, a viewpoint we do not pursue here. From any view, upon familiarlity the $T^{r,s}$ and their properties soon become trivial. A similar more complex parallel theory is given in Ref. 3 for random walks on the permutation group, instead of subspaces of a lattice.

We start presenting the polymer expansion for $\mathbf{f}(t)$ of Eq. (5). We assume $\mathbf{f}(t)$ is normalized so that

$$\sum_{\mathcal{S}} f(\mathcal{S}, t) = 1. \tag{13}$$

We note that if at any time this equation holds, the heat equation, Eq. (6), preserves the identity. We do not consider the possibility that the sum on the left-hand side of (13) be zero, so no such normalization is possible.

We let $\mathcal{P}$ be a partition of $\mathcal{V}$. We write $\mathcal{S}_\alpha < \mathcal{P}$ for a subset $\mathcal{S}_\alpha$ of the partition $\mathcal{P}$. One has

$$S_\alpha \cap S_\beta = \varnothing, \quad \alpha \neq \beta, \tag{14}$$

$$\bigcup_{\alpha \in I^{\mathcal{P}}} \mathcal{S}_\alpha = \mathcal{V}. \tag{15}$$

We will have (summing over all such partitions)

$$\mathbf{f}(t) = \sum_{\mathcal{P}} \bigotimes_{\mathcal{S}\alpha < \mathcal{P}} \mathbf{u}(\mathcal{S}_\alpha, t), \tag{16}$$

where

$$\mathbf{u}(\mathcal{S}_\alpha, t) = \begin{pmatrix} \phi_i(t) \\ 1 - \phi_i(t) \end{pmatrix}_i \tag{17}$$

if $\mathcal{S}_\alpha = \{i\}$.

If $\#(\mathcal{S}_\alpha) = r > 1$,

$$\mathbf{u}(\mathcal{S}_\alpha, t) = u^r(\mathcal{S}_\alpha, t) \bigotimes_{i \in \mathcal{S}\alpha} \begin{pmatrix} 1 \\ -1 \end{pmatrix}_i. \tag{18}$$

We also write

$$u(\mathcal{S},t)=u^r(\mathcal{S},t) \quad \text{if} \quad \#(\mathcal{S})=r \tag{19}$$

and, for the special case $r=1$,

$$u(\mathcal{S},t)=u^1(\mathcal{S},t)=\phi_i(t) \quad \text{if} \quad \mathcal{S}=\{i\}. \tag{20}$$

We write $\mathbf{f}(t)$ as a sum of its different spin-wave number components

$$\mathbf{f}(t)=\sum_{n=0}^{\#(\mathcal{V})} \mathbf{f}_n(t), \tag{21}$$

$$\mathbf{f}_n(t)\in\mathcal{H}^n. \tag{22}$$

We set

$$\mathbf{c}_r(t)=\sum_{n=0}^{\#(\mathcal{V})} T^{n,r}\mathbf{f}_n(t) \tag{23}$$

and

$$\mathbf{c}_r(t)=\sum_{\mathcal{S}} c^r(\mathcal{S},t)\mathbf{i}_{\mathcal{S}}. \tag{24}$$

(Notice that the c^r satisfy the graph heat equation, (6).) Then we find that Eq. (16) is satisfied if the $u(\mathcal{S},t)$ are chosen to satisfy:

$$c^r(\mathcal{S},t)=u^r(\mathcal{S},t)+\sum_{\mathcal{P}} \prod_{\mathcal{S}_\beta<\mathcal{P}} u(\mathcal{S}_\beta,t), \tag{25}$$

where here the $\mathcal{P}$ are all **proper** partitions of $\mathcal{S}$ and $\#(\mathcal{S})=r$. r will range from 1 to $\#(\mathcal{V})$. Equations (16) and (25) are prototype cluster-expansion/polymer-expansion equations. But the form of Eq. (18) is perhaps surprising. Appendix B treats the consistency of the formalism; that there is a unique solution for the u's from (25), and they yield Eq. (16).

We present in bold strokes the conventional ways of thinking about cluster expansions like Eq. (16). In the second term in Eq. (5) as one expands the exponent in powers of H, each I_{ij} that appears represents a ''collision'' and interchanges spins at i and j. We can neglect interchanges when both spins are the same. Then we have a picture where spins ''collide'' and change places. The evolution yields a sequence of collisions and corresponding motions of the spins. This naturally leads to a ''random-walk'' picture of spins moving and colliding. $u^r(\mathcal{S},t)$ is related to a process where the spins at the sites in $\mathcal{S}$ at time t have had a history in which they have all mutually collided, and where spins in no smaller subset of $\mathcal{S}$ has not collided with spins in the complementary portion of $\mathcal{S}$.

Reference 4 is a standard general treatment of cluster expansions, and Ref. 5 a treatment of the random walk picture sketched above. However knowledge of these detailed technical directions will not simplify our derivation above; and further, starting from Refs. 4 and 5, I think it unlikely that many researchers would find our ''simple'' result. However to get the estimates on the u^r needed for applications, these references will be useful.

The proof of convergence in the infinite volume, commonly referred to simply as ''convergence of the cluster expansion,'' depends on obtaining appropriate bounds on the u^r. Convergence in the ''small t'' region was proven in Ref. 2 for a different construction of a cluster expansion. A proof for the ''small t'' region can certainly be greatly simplified over that in Ref. 2. The author believes that the expansion converges also in the ''large t'' region, i.e., for $t>T_0$ for some T_0 (possibly even for all t). This will be difficult to prove. It seems that the proof for large t will depend on incorporating unusual probabilistic estimates, exhibiting probabilistic cancellations in

certain sums involving many terms. One may hope that the compact form of the present construction of the cluster expansion may simplify some details of a proof, still a substantial theoretical challenge.

APPENDIX A: INTERTWINING RESULT

In virtue of Eq. (11) it is enough to show $T^{r,r-1}$ intertwines. We choose to show equivalently that $T^{r,r-1}$ carries a solution of the heat equation into a solution of the heat equation. Let $f(\mathcal{S},t)$ satisfy the heat equation, and be zero unless $\#(\mathcal{S})=r$. We define

$$g(s,t)=\sum_j f(s\cup j,t),\quad \#(s)=r-1. \tag{A1}$$

We wish to show g satisfies the heat equation. Writing the heat equation for f:

$$\frac{\partial f}{\partial t}(s\cup i,t)=\sum_{\mathcal{S}'\sim(s\cup i)}(f(\mathcal{S}',t)-f(s\cup i,t)). \tag{A2}$$

We sum the two sides of (A2) over i,

$$\frac{\partial}{\partial t}g(s,t)=\sum_i\sum_{\mathcal{S}'\sim(s\cup i)}(f(\mathcal{S}',t)-f(s\cup i,t)). \tag{A3}$$

The right-hand side splits into two terms I_1 and I_2,

$$I_1=\sum_i\sum_{s'\sim s}(f(s'\cup i,t)-f(s\cup i,t)) \tag{A4}$$

and

$$I_2=\sum_i\sum_{j\sim i}(f(s\cup j,t)-f(s\cup i,t)). \tag{A5}$$

It is easy to see

$$I_1=\sum_{s'\sim s}(g(s',t)-g(s,t)) \tag{A6}$$

and just a little harder to see

$$I_2=0$$

and the result is proved.

APPENDIX B: IN THREE PARTS

We divide the demonstration of consistency into three parts:

(i) We first note that Eq. (25) has a unique solution for the u^r (these are the unknowns). One solves inductively over r, the rth equation uniquely determining u^r.

(ii) Once the u's are determined from Eq. (25), we substitute them in the right-hand side of Eq. (16) which we call $\mathbf{X}(t)$, so Eq. (16) becomes

$$\mathbf{f}(t)=\mathbf{X}(t). \tag{B1}$$

(Of course we do not know whether (B1) is true, that is what we are trying to show.) We decompose $\mathbf{X}(t)$,

$$\mathbf{X}(t)=\sum_{n=0}^{\#(\mathcal{V})}\mathbf{X}_n(t), \tag{B2}$$

$$\mathbf{X}_n(t)\in\mathcal{H}^n, \tag{B3}$$

and define

$$\mathbf{d}_r(t)=\sum_{n=0}^{\#(\mathcal{V})}T^{n,r}\mathbf{X}_n(t), \tag{B4}$$

$$\mathbf{d}_r(t)=\sum_{\mathcal{S}}d^r(\mathcal{S},t)\mathbf{i}_{\mathcal{S}}. \tag{B5}$$

The result we seek to now show is the following: If $d^r(\mathcal{S},t)=c^r(\mathcal{S},t)$ all $\mathcal{S},r$, then $\mathbf{f}(t)=\mathbf{X}(t)$.

This we also show by induction over r, but in the opposite direction, from $r=\#(\mathcal{V})$ down to $r=0$. At the step $r=r$ we clearly get

$$\mathbf{f}_r(t)=\mathbf{X}_r(t). \tag{B6}$$

(One only needs $T^{r,r}=I$, and $T^{r,s}=0$ if $s>r$.)

(iii) We are left with the task of showing

$$d^r(\mathcal{S},t)=c^r(\mathcal{S},t). \tag{B7}$$

We first do a preliminary investigation.

Let

$$\mathbf{h}(t)=\sum h(\mathcal{S},t)\mathbf{i}_{\mathcal{S}} \tag{B8}$$

$$=\sum_{n=0}^{\#(\mathcal{V})}\mathbf{h}_n(t), \tag{B9}$$

$$\mathbf{h}_n(t)\in\mathcal{H}^n \tag{B10}$$

and define

$$\mathbf{g}_r(t)=\sum_n T^{n,r}\mathbf{h}_n(t) \tag{B11}$$

$$=\sum_{\mathcal{S}}g^r(\mathcal{S},t)\mathbf{i}_{\mathcal{S}}. \tag{B12}$$

We then find the following expression for $g^r(\mathcal{S},t)$:

$$g^r(\mathcal{S},t)=\sum_{\substack{\mathcal{S}'\\ \mathcal{S}'\cap\mathcal{S}=\phi}}h(\mathcal{S}\cup\mathcal{S}',t), \tag{B13}$$

where $\#(\mathcal{S})=r$.

Now when we compute $d^r(\mathcal{S},t)$ using expression (B13) with X replacing h ($\mathbf{X}(t)=\Sigma_{\mathcal{S}}X(\mathcal{S},t)\mathbf{i}_{\mathcal{S}}$), the only terms in the expression for $\mathbf{X}(t)$ from (16) which will contribute are of the form

$$\left(\mathbf{u}^r(\mathcal{S},t)+\sum_{\mathcal{P}}\bigotimes_{\mathcal{S}_\beta<\mathcal{P}}\mathbf{u}(\mathcal{S}_\beta,t)\right)\bigotimes_{i\notin\mathcal{S}}\begin{pmatrix}\phi_i(t)\\ 1-\phi_i(t)\end{pmatrix}_i \tag{B14}$$

using the notation from Eq. (25). That is because the sum over $\mathcal{S}'$ in (B13) may be written as an iterated sum, summing for each vertex not in $\mathcal{S}$, whether the vertex is in $\mathcal{S}'$ or not. This amounts to summing over spin-up and spin-down at that vertex. At vertex k this sum applied to the term in the tensor product

$$\begin{pmatrix} \phi_k(t) \\ 1-\phi_k(t) \end{pmatrix}_k$$

yields 1, and applied to

$$\begin{pmatrix} 1 \\ -1 \end{pmatrix}_k$$

yields 0. We get from the terms in $\mathbf{X}(t)$ in (B14) that

$$d^r(\mathcal{S},t)=c^r(\mathcal{S},t). \tag{B15}$$

Q.E.D.

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