



Application of Jastrow Wave Functions to Quantum Lattice Spin Theories

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ABSTRACT

The use of variational wave functions which are products of overlapping locally correlated functions for studying the ground state of lattice spin theories is described. It is found that very accurate results can be obtained for very simple trial functions. The method is superior for determining the energy, to methods based on blocks.

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I. INTRODUCTION

The Raleigh-Ritz variational method works well for problems with a small number of degrees of freedom (d.o.f.), but if the number of d.o.f. is large one must make some further approximation. A simple one is to choose as a trial wave function a product of functions each of which depends on a single or a distinct set or block of d.o.f. This is the Hartree or mean field approximation. Systematic improvements can be obtained by doing perturbation theory on the mean field ground state, or including a larger number of d.o.f. within each block. The first is sometimes inappropriate because the perturbation theory is poorly behaved while the latter may converge slowly as the size of the blocks increases. The block method may be further improved by using iterative renormalization group-like methods,¹ but still remains sensitive to finite size effects. An alternative to considering blocks of disjoint sets of d.o.f. is to allow the blocks to overlap. This approximation is used for quantum gasses under the name Jastrow wave functions.^{2,3}

In this paper we wish to study the application of Jastrow type functions to quantum spin systems and by means of several simple examples bring out the advantages of this method. All of these examples will involve collections of Pauli spins at the vertices of a regular lattice. We will consider the class of wave functions which may be written in the form

$$\psi = Z^{-1/2} \prod_C (1 + \omega_C S^C)^{1/2} \quad (1.1)$$

where the product extends over all spin clusters C . S^C is given by

$$S^C = \prod_{i \in C} S^i \quad (1.2)$$

and $S^i = \pm 1$. ω_C is a number less than one in magnitude. The normalization factor

$$Z = \sum_{(S)=\pm 1} \prod_C (1 + \omega_C S^C) \quad (1.3)$$

is the partition function for a generalized Ising model. This is the central observation of this paper for it allows us to relate a quantum mechanical system to an equivalent statistical mechanical problem. The couplings (or temperature) of the statistical mechanical system will be variational parameters.

For the ground state if the Hamiltonian of the system is homogeneous it is clear that $\omega_C = \omega_{C'}$ if C and C' are related to each other by a rotation or translation. The S^i are the eigenvalues of σ_z^i but we are free to choose any direction we wish for this Z axis, and we will use this direction as a variational parameter in one example. Matrix elements of the Pauli spins can be computed in terms of thermodynamic averages in the Ising model (1.3) from the action of the spins on ψ

$$\begin{aligned} \sigma_z^i \psi &= S^i \psi \\ \sigma_x^i \psi &= \prod_{CC'} \left[\frac{1 - \omega_C S^C}{1 + \omega_C S^C} \right]^{1/2} \psi \\ \sigma_y^i \psi &= i S^i \sigma_x^i \psi \\ \langle \psi | O(\sigma) | \psi \rangle &= \langle \tilde{O}(S) \rangle_{\text{Ising}} \end{aligned} \quad (1.4)$$

If we restrict all the ω_C to zero except for a restricted class then these may be used as variational parameters. If we include only those C 's which correspond to

single spins or pairs of spins then an approximation in terms of the usual Ising model results. If only single spin clusters remain then we have mean field theory. When this is a reasonable starting point the method of high temperature series may be effectively used to treat the dependence on the other ω_C .

II. EXAMPLE I-ONE DIMENSIONAL PLANAR MODEL

As a first example we consider the planar model

$$H = -\frac{1}{2} \sum_i \left(\sigma_x^i \sigma_x^{i+1} + g \sigma_z^i \sigma_z^{i+1} \right) \quad (2.1)$$

This system has an energy density per spin

$$\epsilon = -(1+g) \frac{1}{\pi} E(4g/(1+g)^2) \quad (2.2)$$

in the ground state, where E is the complete elliptic integral. For small g ϵ has the expansion

$$\begin{aligned} \epsilon(g) &= -\frac{1}{2} - \frac{1}{2} \sum_{k=1}^{\infty} (2k-3)!! / (2k)!! \ 2^k g^{2k} \\ &= -\frac{1}{2} - \frac{g^2}{8} - \frac{g^4}{128} - \frac{g^6}{512} - \frac{25g^8}{32708} - \dots \end{aligned} \quad (2.3)$$

For $|g| < 1$ the best single site mean field estimate is obtained by polarizing the spins along x which gives $\epsilon \leq -\frac{1}{2}$ while the best mean field estimate formed from adjacent blocks of L spins gives for small g

$$\epsilon \leq -\frac{1}{2} - \left(1 - \frac{1}{L}\right) \frac{g^2}{8} - \dots \quad (2.4)$$

Now consider a trial wave function of the form (1.1) with only the ω for nearest neighbors nonzero. Then the corresponding Ising model is the usual one. The necessary matrix elements are

$$\begin{aligned} \langle \psi | \sigma_z^i \sigma_z^{i+1} | \psi \rangle &= \langle S^i S^{i+1} \rangle = \omega \\ \langle \psi | \sigma_x^i \sigma_x^{i+1} | \psi \rangle &= \left\langle \left(\frac{1 - \omega S^{i-1} S^i}{1 + \omega S^{i-1} S^i} \right)^{\frac{1}{2}} \left(\frac{1 - \omega S^{i+1} S^{i+2}}{1 + \omega S^{i+1} S^{i+2}} \right)^{\frac{1}{2}} \right\rangle \\ &= (1 - \omega^2) \end{aligned} \quad (2.5)$$

So we obtain

$$\epsilon(g) \leq -\frac{1}{2}(1 - \omega^2) - \frac{g\omega}{2} \leq -\frac{1}{2} - \frac{g^2}{8} \quad (2.6)$$

The largest error occurs for $g = 1$ (for $g > 1$ we would interchange the z and x directions) where the exact answer, $2/\pi$, is given to within 1.83%. The comparable Block mean field result--in the complexity of the correlations treated by ψ and the difficulty of the calculation--is for $L = 2$ which gives an error of 11.64% when $g = 1$. To achieve a comparable accuracy would require $L \geq 16$.

If we want to improve the estimate (2.6) more of the ω 's must be allowed to vary. The next term in ψ to make an important contribution for small g is the four spin term $(1 + \omega_4 S^i S^{i+1} S^{i+2} S^{i+3})$. Rather than attempt the difficult approach of solving an Ising model with a four spin operator we resort to the method of high temperature series. The series for the two point function $\langle S^i S^j \rangle$ is standard while the series for $\langle \psi | \sigma_x^i \sigma_x^j | \psi \rangle$ is most easily computed by noting that

$$\langle \psi | \sigma_x^i \sigma_x^j | \psi \rangle = \frac{\prod_{C_1} (1 - \omega_C^2)^{1/2}}{\prod_{C_2} (1 + \omega_C S^C)} \langle \prod_C (1 + \omega_C S^C) \rangle / \langle \prod_C (1 + \omega_C S^C) \rangle \quad (2.7)$$

where C_1 consists of clusters which contain i or j but not both, and C_2 all others. The ratio of expectation values is given by the sum of volume independent coefficients of free energy graphs which do not contain any of the C_1 interactions. Specifically we obtain

$$\begin{aligned} \langle \psi | \sigma_z^i \sigma_z^{i+1} | \psi \rangle &= \omega + \omega_4 (2\omega(1 - \omega^2)) + \omega_4^2 (2\omega(1 - \omega^2)(1 - 3\omega^2)) \\ &\quad + \omega_4^3 (2\omega(1 - \omega^2)(1 - \dots)) + \dots \\ \langle \psi | \sigma_x^i \sigma_x^{i+1} | \psi \rangle &= (1 - \omega^2)(1 - \omega_4^2) \left[1 - \omega_4(3\omega^2) \right. \\ &\quad \left. - \omega_4^2(4\omega^2 - 10\omega^4) - \omega_4^3(5\omega^2 - \dots) \right] \end{aligned} \quad (2.8)$$

With $g^2 \sim \omega^2 \sim \omega_4$ the expansions in (2.8) will be valid through g^8 so for small g with ω and ω_4 nonzero we obtain

$$\epsilon \leq -\frac{1}{2} - \frac{g^2}{8} - \frac{g^4}{128} + 0g^6 + \frac{g^8}{4096} + \dots \quad (2.9)$$

with

$$\begin{aligned} \omega &= g/2 - g^3/16 + 0g^5 - g^7/512 + \dots \\ \omega_4 &= g^2/8 + g^4/32 + 3g^6/512 + \dots \end{aligned} \quad (2.10)$$

for general values of g the energy obtained from (2.8) does not represent an upper bound since we do not know the sign of the remainder of the series, but since the expansion in ω_4 certainly converges it represents a useful approximation to the true energy. In this case it agrees to within .62% of the exact answer in the range $|g| \leq 1$ while the error in truncating the series in (2.8) causes an error which is of the order of .05%.

We do not emphasize the power series expansion (2.9) because this is a good method for computing the coefficients (perturbation theory is more direct), but because it holds out the hope that for fixed g successive approximations may converge very rapidly compared to the $1/L$ behavior of mean field theory on blocks. The requirement for this to happen is that only a finite number of new operators need be added to agree with each order in perturbation theory. Naively there are many operators which could have contributed at order g^4 --namely the next nearest neighbor two spin interaction and all four spin operators of the form $S^i S^{i+1} S^j S^{j+1}$ --but all except the one kept vanish. We do not know if this persists in general.

Consider the two dimensional version (2.1) on a square lattice, and specialize to $g = 1$. This problem is not exactly solvable but by various methods the ground state energy is known to be approximately $\epsilon = -1.099 \pm .004$.⁴ Keeping only the nearest neighbor interaction as in (2.6) we obtain an approximation in terms of the standard 2D Ising model with

$$\begin{aligned} \langle \sigma_z^i \sigma_z^j \rangle_{n.n.} &= \omega + 2\omega^3 + 4\omega^5 + 12\omega^7 + 42\omega^9 + 164\omega^{11} + \dots \\ \langle \sigma_x^i \sigma_x^j \rangle_{n.n.} &= (1 - \omega^2)^3 (1 - 6\omega^4 - 17\omega^6 - 40\omega^8 - \dots) \end{aligned} \quad (2.11)$$

and

$$\epsilon \leq \min_{\omega} - \langle \sigma_z^i \sigma_z^j \rangle_{n.n.} - \langle \sigma_x^i \sigma_x^j \rangle_{n.n.} \leq -1.092685 \pm \frac{0}{10} \quad (2.12)$$

at

$$\omega \approx .1958 \quad (2.13)$$

Thus the simplest possible bound of this type gives (to 5 figures) $\epsilon \leq -1.0927$ which compares very favorably with the best available bound⁴ for this quantity $\epsilon \leq -1.0944$. Inclusion of the diagonal nearest neighbor term gives $\epsilon \leq -1.0936 \pm .0001$.

EXAMPLE 2: 1D ISING MODEL IN A TRANSVERSE FIELD

Consider

$$H = - \sum_i \left(\sigma_z^i \sigma_z^{i+1} + J \sigma_x^i \right) \quad (3.1)$$

This system exhibits a ground state phase transition at $J = 1$ from a degenerate state with $S_z = \langle \sigma_z \rangle \neq 0$ to a nondegenerate state with $S_z = 0$ for $J \geq 1$. We will study (3.1) with the trial function

$$\psi = Z^{-1/2} \prod_i e^{i \theta \sigma_y^i} (1 + \omega S^i S^{i+1})^{1/2} (1 + \nu S^i)^{1/2} \quad (3.2)$$

So

$$Z = \sum_{\{S\}} \prod_i (1 + \omega S_i S_{i+1})(1 + \nu S_i) \quad (3.3)$$

which is the partition function for a 1D Ising model with a field. The operators $e^{i\theta \sigma_y}$ if implemented on ψ would produce a very complicated wave function, but acting on H only rotate the Pauli spin matrices in the x-z plane. The necessary matrix elements are

$$S_z = \langle \sigma_z \rangle = (\alpha^2 - \beta^2)/(\alpha^2 + \beta^2)$$

$$S_x = 2(1 - \omega^2)(1 - \nu^2)^{1/2} (1 + \nu S_z + 2\alpha\beta(1 - \nu^2)^{1/2}/(\alpha^2 + \beta^2))/\lambda^2$$

$$D_z = \langle \sigma_z^0 \sigma_z^1 \rangle = ((1 + \omega)(1 + \nu S_z) - 2\alpha\beta(1 - \nu^2)^{1/2}(1 - \omega)/(\alpha^2 + \beta^2))/\lambda$$

$$D_x = 2(1 - \nu^2)^{1/2} S_x/\lambda$$

$$D_{xz} = 2(1 - \omega^2)(1 - \nu^2)^{1/2}(\nu + S_z)/\lambda^2 \quad (3.4)$$

where the components of the eigenvector and eigenvalue of the transfer matrix are

$$\alpha = (1 - \omega)(1 - \nu^2)^{1/2}$$

$$\beta = \lambda - (1 + \omega)(1 + \nu)$$

$$\lambda = (1 + \omega) + ((1 - \omega)^2 + 4\nu^2\omega)^{1/2} \quad (3.5)$$

The energy density is bounded by

$$\epsilon \leq - \left[(1 - \mu^2) D_z + \mu^2 D_x - 2\mu(1 - \mu^2)^{1/2} D_{xz} + J(\mu S_x + (1 - \mu^2)^{1/2} S_z) \right]$$

$$\mu = \cos \theta \quad . \quad (3.6)$$

The results of varying over ω, ν , and μ give remarkable agreement with the exact result for the energy density

$$\epsilon = \frac{2}{\pi} (1 + J) E \left(\frac{4J}{(1 + J)^2} \right) \quad . \quad (3.7)$$

(Note this is just twice the energy (2.2).) For $J \lesssim 1$ this bound is significantly better than any bound based on disjoint blocks of spins, even when improved using renormalization group methods.¹ For example, when J is small one has the expansions

$$\epsilon = -1 - J^2/4 - J^4/64 - J^6/256 - \dots \quad (\text{exact})$$

$$\epsilon = -1 - J^2/4 - J^4/64 - J^6/256 - \dots \quad (\text{this bound})$$

$$\epsilon = -1 - J^2/4 - J^4/128 + \dots \quad (2 \text{ spin manifold})$$

$$\epsilon = -1 - J^2/4 - J^4/96 + \dots \quad (\text{variational R-G on 2 spin block}) \quad (3.8)$$

For J large this bound gives the result

$$\epsilon = -J(1 + 1/4J^2) \quad (\text{this bound})$$

$$\epsilon = -J(1 + 1/4J^2 + 1/64J^4 + \dots) \quad (\text{exact}) \quad (3.9)$$

This calculation gives a transition at $J = 1.206$ with mean field indices. The transition point is improved over the mean field point, $J = 2$. In order to improve the exponents one would need to apply RG methods but we do not know how to do this.

IV. CONCLUSIONS

By means of simple one and two dimensional examples with known solutions I have demonstrated the simplicity and efficacy of a variational scheme based on a correlated product wave function. The potential range of applications to lattice Hamiltonian systems is large. Because of its ability to fit the first few terms of the weak coupling limit of a theory this method provides a natural continuation in coupling which preserves a bound. The method can be generalized to nonclassical statistical mechanics systems via the generalization of the Raleigh-Ritz bound

$$E \leq \text{tr}(O^\dagger H O) / \text{tr}(O^\dagger O) \quad . \quad (4.1)$$

Other areas where improvements may be possible are, to apply this method to lattice field theories, and to study the connection of real space RG transformations on ψ to RG transformations of H .

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