A Perturbative/Variational Approach to Quantum Lattice Hamiltonians

José G. Esteve\textsuperscript{a} and Germán Sierra\textsuperscript{b}
\textsuperscript{a} Departamento de Física Teórica, Facultad de Ciencias, Univ. de Zaragoza. Zaragoza, Spain.
\textsuperscript{b} Instituto de Matemáticas y Física Fundamental, CSIC, Madrid, Spain.

Abstract

We propose a method to construct the ground state $\psi(\lambda)$ of local lattice hamiltonians with the generic form $H_0 + \lambda H_1$, where $\lambda$ is a coupling constant and $H_0$ is a hamiltonian with a non degenerate ground state $\psi_0$. The method is based on the choice of an exponential ansatz $\psi(\lambda) = \exp(U(\lambda))\psi_0$, which is a sort of generalized lattice version of a Jastrow wave function. We combine perturbative and variational techniques to get succesive approximations of the operator $U(\lambda)$. Perturbation theory is used to set up a variational method which in turn produces non perturbative results. The computation with this kind of ansatzs leads to associate to the original quantum mechanical problem a statistical mechanical system defined in the same spatial dimension. In some cases these statistical mechanical systems turn out to be integrable, which allow us to obtain exact upper bounds to the energy. The general ideas of our method are illustrated in the example of the Ising model in a transverse field.
1 Introduction

In Statistical Mechanics and Quantum Field Theory there is a large class of two-dimen-
sional models whose basic magnitudes can be computed exactly\(^1\). The mathematics and
physics of these integrable models are very rich, constituing areas of intensive investiga-
tion. There are in contrast very few integrable models in higher dimensions\(^2, 3\), where
almost all the models which are interesting from a physical point of view are believed to
be non integrable. These facts represent a major conceptual and technical gap between
the 2d and the higher dimensional worlds, which would be desirable to fill in.

The lack of exact techniques has always motivated the construction of approximative
methods which very often give good quantitative and qualitative results. These methods
can be roughly classified according to four main categories, namely: perturbative, vari-
tational, numerical and renormalization group, every one having advantages and limitations.
The perturbative methods can be developed in a systematic way but are restricted to small
values of the coupling constants. The variational ones give in general non perturbative
results but rely on aprioristic or intuitive conjectures. The numerical approaches are in
general unbiased but limited to small lattices. Finally, the RG techniques when combined
with one of the previous ones are very powerful for the study of critical phenomena.

In this paper we shall restrict ourselves to the first two methods. Our aim is to combine
perturbative and variational techniques choosing the best of each and by passing some of
their limitations. The problem we cope with is the construction of the ground state of
a local lattice hamiltonian of the form \( H_0 + \lambda H_1 \), where \( \lambda \) is a coupling constant. Our
strategy is to use perturbation theory to set up a variational approach to the computation
of the ground state wave function. The starting point is the choice of an exponential ansatz
for the exact ground state of the hamiltonian \( H_0 + \lambda H_1 \). The peculiarity of this ansatz is
that, under certain assumptions about the ground state of the unperturbed hamiltonian
\( H_0 \), the whole hierarchy of perturbative equations can be solved systematically in terms
of a collection of irreducible local operators \( V_I \), which are characterized by the order \( \nu_I \) at
which the operator \( V_I \) first appears in perturbation theory. Each operator \( V_I \) comes in the
ansatz multiplied by a weight \( \alpha_I(\lambda) = \lambda^{\nu_I} + \) higher powers. The data \( \{V_I, \alpha_I(\lambda)\} \) contain
all the information required to built up the ground state. For small lattices it is easy to
construct this set and therefore obtain the exact ground state, but for large lattices we
have to resort to some kind of approximation. The natural thing to do is to truncate the
ansatz considering only those operators \( V_I \) with a level equal or less that a given number
\( \nu \), which is the order in perturbation theory where one is working at. The problem is then to find the weights \( \alpha_I(\lambda) \) for \( \nu_1 \leq \nu \). At this point one can follow two different paths: i) use the truncated ansatz as a trial state in a standard variational fashion or ii) take the truncated ansatz as the exact ground state of a Hamiltonian which should be sufficiently close to the original one. In this paper we shall develop the approach i) and leave the approach ii) for another publication. We have so far outlined the main ideas and techniques which will be exemplified in the case of the Ising model in a transverse magnetic field (ITF), but it should be clear from the exposition that they apply to more complicated models as for example the chiral Potts model, the XXZ-model, etc.

Trial wave functions with an exponential or, more generally, product structure are known as Jastrow wave functions and has been applied to a wide variety of problems in different areas as for example, liquid \(^4\)He \([4]\), nuclear matter \([4]\), solid state physics \([4, 6]\) and more recently in the fractional quantum Hall effect \([8]\). In quantum mechanics a Jastrow wave function is simply the exponential of the potential energy, \( \psi(x) = \exp(-\alpha V(x)) \) and becomes exact for the simple harmonic oscillator. In a many body problem one replaces \( V(x) \) in the exponential by \( \sum_{i,j} f(x_i - x_j) \) where \( f \) is some two body effective potential. In this paper we shall consider discrete versions of generalized Jastrow states in contrast of the continuous versions described above. To our knowledge there is not in the literature a general and systematic study of this type of wave functions except for some interesting observations and discussions confined to particular models \([9]\). Among these observations is the fact that the norm of the Jastrow wave functions coincides, in certain cases, with the partition function of an associated classical statistical mechanical model defined in the same dimension, with the variational parameter playing the role of inverse temperature. Indeed, in the example of the ITF we find that the norm of the exponential ansatz is given by the partition function of a classical Ising model with couplings among the spins dictated by the family of operators \( V_I \) and as many coupling constants as weights \( \alpha_I \). Working with these generalized Jastrow wave functions requires the knowledge of thermodynamic quantities such as internal energies, susceptibilities, etc. The calculation of these quantities is in general a difficult task and this imposes limitations to the variational approach i) mentioned above. However in certain occasions the computation can be carried out exactly. This happens when the associated statistical system which underlies a particular ansatz is integrable. If the quantum Hamiltonian is one dimensional then the statistical system is also one dimensional and the corresponding partition function can be easily computed. Things are more interesting in two dimensions
where, as we said in the introduction, most of the hamiltonians are not exactly solvable. The approximation method that we propose bring us to statistical systems in the same dimension, and therefore in two dimensions we may some times make contact with 2d integrable models. This opens the possibility of using the huge amount of information known in integrable 2d systems in the study of 2d quantum systems.

The paper is organized as follows. In section 2 we introduce the P/V method. In section 3 we apply the general ideas presented in section 2 to the Ising model in a transverse magnetic field, making special emphasis in the 1d and 2d cases. In section 4 we present our conclusions and future prospects. All the technical details and computations are included in four appendices.

2 The Perturbative/Variational Method

Let \( H(\lambda) = H_0 + \lambda H_1 \) be a local lattice hamiltonian where \( H_0 \) is a Hamiltonian whose ground state \( \psi_0 \) is non degenerate. We suppose that \( \psi_0 \) and its energy \( E_0 \) are known exactly. If \( \lambda \) is sufficiently small one can use standard perturbation theory to expand the ground state wave function \( \psi(\lambda) \) and energy \( E(\lambda) \) of \( H(\lambda) = H_0 + \lambda H_1 \) as follows,

\[
\psi(\lambda) = \sum_{n=0}^{\infty} \lambda^n \psi_n
\]

\[
E(\lambda) = \sum_{n=0}^{\infty} \lambda^n E^{(n)}
\]

where \( \{\psi_n\} \) and \( \{E^{(n)}\} \) are subjected to satisfy a set of equations linking quantities of the same order \([10]\). In order to write this set of equations we shall assume that \( \psi(\lambda) \) can be reached from \( \psi_0 \) with the action of an operator of exponential type,

\[
\psi(\lambda) = e^{U(\lambda)} \psi_0
\]

\[
U(\lambda) = \sum_{n=1}^{\infty} \lambda^n U_n
\]

The relation between the perturbative expansion \([10]\) and the operators \( U_n \) is given by a non-abelian version of the Schur polynomials,

\[
\psi_1 = U_1 \psi_0
\]

\[
\psi_2 = \left( \frac{1}{2} U_1^2 + U_2 \right) \psi_0
\]
\[ \psi_n = \sum_{p=1}^{n} \frac{1}{p!} \sum_{n_1 + \cdots + n_p = n} U_{n_1} \cdots U_{n_p} \psi_0 \]

If the operators \( U_n \) commute among themselves then the above expressions coincide with the Schur polynomials \( S_1, S_2, \cdots, S_n \) as functions of the variables \( U_n \). The equations satisfied by \( \psi_n \) and \( E^{(n)} \) translate now into a set of equations for \( U_n \) and \( E^{(n)} \) which we pass to derive.

Introducing (3) into the eigenvalue equation,

\[ H(\lambda) \psi(\lambda) = E(\lambda) \psi(\lambda) \]  \hspace{1cm} (5)

and multiplying on the left hand side by the inverse of the exponential one gets,

\[ \exp \left( - \sum_{n=1}^{\infty} \lambda^n U_n \right) H(\lambda) \exp \left( \sum_{n=1}^{\infty} \lambda^n U_n \right) \psi_0 = E(\lambda) \psi_0 \]  \hspace{1cm} (6)

To simplify (6) we use the identity \[11\],

\[ e^{-A} B e^A = e^{L_A(B)} = \sum_{n=0}^{\infty} \frac{1}{n!} L^n_A(B) \]  \hspace{1cm} (7)

where

\[ L_A(B) = [B, A], \quad L^2_A = [[B, A], A], \ldots \]  \hspace{1cm} (8)

which yields,

\[ \exp \left( \sum_{n=1}^{\infty} \lambda^n L_{U_n} \right) H(\lambda) \psi_0 = E(\lambda) \psi_0 \]  \hspace{1cm} (9)

The equations for the operators \( U_n \) are finally obtained expanding the exponential in (9) and collecting all the terms of the same power in \( \lambda \),

\[ H_0 \psi_0 = E_0 \psi_0 \]

\[ ([H_0, U_1] + H_1) \psi_0 = E^{(1)} \psi_0 \]

\[ ([H_0, U_2] + \frac{1}{2}[[H_0, U_1], U_1] + [H_1, U_1]) \psi_0 = E^{(2)} \psi_0 \]

\[ \vdots \]

\[ \left[ \sum_{p=1}^{n} \sum_{n_1 + \cdots + n_p = n} \frac{1}{p!} L_{U_{n_1}} \cdots L_{U_{n_p}}(H_0) \right] \psi_0 = E^{(n)} \psi_0 \]

\text{for } n \geq 2
The solution of these equations is by no means unique. In particular the hermiticity properties of \( U(\lambda) \) are not fixed a priori. There are two main choices that can be made in terms of hermitean or antihermitean operators. If \( U(\lambda) \) is choosen to be antihermitean, then eq.(3) becomes a unitary transformation which preserves obviously the norm of the state, i.e. \( <\psi(\lambda)|\psi(\lambda)> = <\psi_0|\psi_0> = 1 \). Moreover if that \( H_1 \) has an off diagonal form, then \( E^{(1)} \) vanishes. When this happens it is customary to perform a unitary transformation,

\[
H_0 + \lambda H_1 \rightarrow e^{-i\lambda S}(H_0 + \lambda H_1)e^{i\lambda S} = H_{\text{eff}}
\]

where \( S = S^\dagger \) is obliged to satisfy,

\[
i[H_0, S] + H_1 = 0
\]

in order to cancel the terms proportial to \( \lambda \) in \( H_{\text{eff}} \). This equation coincides with the first order equation in (10) but expressed in a matrix form, i.e. the dependence on the state \( \psi_0 \) has been dropped. Finally the ”effective hamiltonian” \( H_{\text{eff}} \) has the expansion,

\[
H_{\text{eff}} = H_0 + \frac{i\lambda^2}{2}[H_1, S] + O(\lambda^3)
\]

These kind of unitary transformations are extensively used in Statistical Mechanics and Condensed Matter Physics[12], and have also been considered from a more mathematical point of view [13].

In this paper we are interested in the study of those solutions to equations (10) which are hermitean. An immediate consequence of this choice is that the norm of the state \( \psi(\lambda) \) is no longer the unity and in fact it will be an important quantity to compute,

\[
Z(\lambda) = <\psi(\lambda)|\psi(\lambda)> = <\psi_0|e^{2U(\lambda)}|\psi_0>
\]

A peculiarity of equations (10) is that all the operators \( U_n \) appear always involved in nested commutators. Let us suppose that \( H_0 \) and \( H_1 \) are local operators defined on a lattice, i.e. operators involving a finite number of lattice variables located within a neighbourhood, whose size is independent of the size of the whole lattice. This kind of operators go, in the thermodynamic limit, to local operators in the continuum. We shall also assume that the number of degrees of freedom per site is finite. We want to investigate under which conditions the solution of the equations (10) can be given by a family of local operators. That this kind of solutions may exist is suggested by
the property mentioned above about the nested structure of equations (10). The reason is that the commutator of local operators is again a local operator and therefore each equation (10) reduces to a sum of local operators acting on the unperturbed ground state. The other ingredient we shall require to achieve a local solution is an unperturbed ground state $\psi_0$ with an ordered structure, which can be ferromagnetic, antiferromagnetic, or of some more general type. This is sufficient to guarantee that the operators $H_0, H_1$ and $U_n$ should produce local disturbances acting on $\psi_0$. There are many physical systems where these conditions are fulfilled. The reason for requiring an ordered ground state is that in this case equations (10) become a system of linear equations with a number of unknowns depending on the dimension of the lattice but not on its size. It will also depend on the order of perturbation theory and the number of lattice variables at each point. The aim of the above considerations is to make plausible the existence of solutions of the perturbative equations in terms of local operators $U_n$, but of course it does not constitute a proof. Later on we shall go through particular examples to show that this kind of solutions do indeed exist. In the case of the Ising model, and we suspect it is a general feature, every operator $U_n$ is given by a sum of irreducible local operators which we denote by $V_I$.

$$U_n = \sum_I p_{I,n} V_I$$

(15)

where the coefficients $p_{I,n}$ are obtained by solving equations (10), and where each operator $V_I$ is a product of Pauli matrices located at different points of the lattice. The sum over $I$ in (15) is finite and contains in general operators that have already appeared in the solution of equations of lower order. It is convenient to define the level $\nu_I$ of $V_I$ as the order in perturbation theory at which this operator appears for the first time in the solution of equations (10),

$$\nu_I = \text{minimum} \{ n/ p_{I,n} \neq 0 \}$$

(16)

Introducing (15) into (3) and interchanging the order of the sums $\sum_n \sum_I = \sum_I \sum_n$, we rewrite the exponential ansatz as follows,

$$\psi(\lambda) = \exp \left( \frac{1}{2} \sum_I \alpha_I(\lambda) V_I \right) \psi_0$$

(17)

where $\alpha_I(\lambda)$ is the "weight" of $V_I$ in the ground state,
\[ \alpha_I(\lambda) = 2 \sum_{n=\nu_I}^{\infty} p_{I,n} \lambda^n \] (18)

The factor 1/2 in eq. (17) has been introduced for later convenience. Definition (18) implies that \( \alpha_I(\lambda) \) has a Taylor expansion starting at \( \lambda^{\nu_I} \), and containing non-vanishing terms of higher powers whenever \( V_I \) appears in the solution of eqs. (10). The knowledge of a single function \( \alpha_I(\lambda) \) will in general require solving the entire hierarchy (10)!. At this stage one may wonder whether there are other alternatives to computing \( \alpha_I(\lambda) \) rather than solving the whole hierarchy (10). To handle this problem it is illustrative to compare equations (3) and (17). They both give two different perturbative approximations to the ground state. While (3) is an expansion in the coupling constant \( \lambda \), eq. (17) is a kind of cluster expansion. In a sense they are conjugated perturbative expansions. Exploiting this analogy we shall propose an alternative way for computing \( \alpha_I(\lambda) \). In standard perturbation theory one truncates the state excluding corrections beyond a given power \( \lambda^n \). The analog of this for (17) will be to truncate the sum over \( I \) to contain only those operators \( V_I \) with a level \( \nu_I \) less or equal than a given order \( \nu \),

\[ \psi(\nu)(\lambda) = \exp \left( \frac{1}{2} \sum_{I, \nu_I \leq \nu} \alpha_I^{(\nu)}(\lambda) V_I \right) \psi_0 \] (19)

In eq. (19) we leave open the possibility that the weights \( \alpha_I^{(\nu)} \) depend on the order of the approximation \( \nu \). The problem now is how to determine \( \alpha_I^{(\nu)} \). In this paper we shall use a variational method which consists in taking (19) as a trial wave function for the ground state of the hamiltonian \( H_0 + \lambda H_1 \). \( \alpha_I^{(\nu)} \) are of course the variational parameters. Minimization of the energy of this state will give the weights \( \alpha_I^{(\nu)} \) as functions of \( \lambda \).

It is clear that this minimization procedure should agree with the result obtained in perturbation theory to the same degree of accuracy, i.e.

\[ \alpha_I^{(\nu)}(\lambda) - \alpha_I(\lambda) = O(\lambda^{\nu+1}), \quad \forall I / \nu_I \leq \nu \] (20)

On the other hand, it is well known that if one takes the perturbative solution to an order \( \nu \) as a trial wave function then the variational energy agrees with the perturbative expansion to order \( 2\nu + 1 \).

\[ E(\text{var,}\nu)(\lambda) - E(\lambda) = O(\lambda^{2\nu+2}) \] (21)
This fact already illustrates at the perturbative level the usefulness of combining both perturbative and variational techniques\textsuperscript{1}. Next we consider the non-perturbative aspects of (19). The question is whether this ansatz can be extended to large values of $\lambda$ remaining close to the exact ground state. In particular in the limit $\lambda \to \infty$ we wish the state $\psi^{(\nu)}$ to flow to the ground state manifold of the Hamiltonian $H_1$, i.e.

$$\lim_{\lambda \to \infty} H_1 \psi^{(\nu)}(\lambda) = E_1 \lim_{\lambda \to \infty} \psi^{(\nu)}(\lambda)$$

(22)

where $E_1$ is the ground state energy of $H_1$. If this equation holds then $\psi^{(\nu)}(\lambda)$ will interpolate in a continuous way the ground state of $H_0$ and those of $H_1$, giving certain validity to the results obtained for the intermediate values of the coupling constant $\lambda$, where a weak or a strong coupling expansion are dubious. A sufficient set of conditions for eq. (22) to hold is the existence, within the family of operators expanded by $\{V_I\}$, of an hermitean operator $\sum_{I,\nu I \leq \nu_0} a^{(\nu_0)}_I V_I$ having a common eigenvector, say $\phi_0$, with the Hamiltonian $H_1$, and such that $\phi_0$ and $\psi_0$ have non-vanishing overlap,

\begin{align*}
&i) \quad \sum_{I,\nu I \leq \nu_0} a^{(\nu_0)}_I V_I \text{ is hermitean} \\
&ii) \quad \phi_0 \text{ is a ground state of } H_1 \text{ and } \sum_{I,\nu I \leq \nu_0} a^{(\nu_0)}_I V_I \\
&iii) \quad <\psi_0|\phi_0> \neq 0
\end{align*}

(23)

Under these conditions it is easy to see that the ansatz $\psi^{(\nu)}(\lambda)$ for $\nu \geq \nu_0$ flows to $\phi_0$ in the limit $\lambda \to \infty$. The interest of conditions (23) is that they strongly restrict the possible solutions of the perturbative equations (10) (see appendix C for concrete examples).

3 The Ising Model in a transverse field

3.1 General Considerations

In this section we shall study in detail the Ising model in a transverse field. Let us introduce our notations and some generalities valid in any dimension.

The model is defined in a hypercubic lattice in $d$ dimensions and $L$ sites with a Hamiltonian given by [13, 16, 17],

\textsuperscript{1}Recall that in perturbation theory the knowledge of the $n^{th}$ order correction of the wave function allows the computation of the energy to order $n+1$ according to the formula $E^{(n+1)} = <\psi_0|H_1|\psi^{(n)}>$. 

8
\[ H_d = -\lambda \sum_n \sigma_n^X - \sum_{n,\mu} \sigma_n^Z \sigma_{n+\mu}^{Z} \]  

(24)

where \( \sigma_n^X \) and \( \sigma_n^Z \) are Pauli matrices acting at the site \( n \), with \( n = (n_1, \ldots, n_d) \), \( n_0 = 1, \ldots, L^{1/d} \) and \( \mu \) is any of the lattice vectors \( \mu_1 = (1, 0, \ldots, 0), \ldots, \mu_d = (0, 0, \ldots, 1) \). The cases \( d = 1 \) and \( 2 \) correspond to a linear chain and a rectangular planar lattice respectively. We shall suppose periodic boundary conditions.

The phase diagram of this Hamiltonian as a function of \( \lambda \) and the temperature is well known [18]. We shall restrict ourselves to zero temperature, whose analysis is interesting because it shows a simple but non trivial example of quantum critical phenomena [19, 20]. In this case there is a critical transverse field \( \lambda_c \) below which there are two ferromagnetic ground states characterized by the non vanishing of \( \langle \sigma_n^Z \rangle \). For \( \lambda > \lambda_c \) the ground state is disordered and \( \langle \sigma_n^Z \rangle = 0 \) but \( \langle \sigma_n^X \rangle \neq 0 \). Near \( \lambda_c \) the critical behaviour of the 1d Ising model with transverse field as a function of \( \lambda \) at \( T = 0 \) is the same as the critical behaviour of the classical Ising model in two dimensions as a function of \( T \) [19]. This can be seen from the fact that the Ising model hamiltonian in 1d is related to the transfer matrix of the 2d Statistical Ising model. The analogy between the quantum critical behaviour of the d-dimensional ITF and the statistical critical behaviour of the Ising model in \( d+1 \) dimensions for \( d=1 \) is believed to hold for \( d \geq 1 \) [19, 21, 22]. This fact is not peculiarity of the ITF but a property which holds more generally [23, 24].

In 1d the model has been solved exactly by many different methods [20, 25, 19]. The ground state energy of a periodic chain of \( L \) sites is,

\[ E_0^{(1d)} = -\frac{L}{2} \sum_{n=-L/2}^{L/2-1} \sqrt{1 + \lambda^2 + 2\lambda \cos \left( \frac{(2n+1)\pi}{L} \right)} \]  

(25)

which gives the following energy density in the thermodynamic limit,

\[ e_0^{(1d)} = \lim_{L \to \infty} \frac{E_0^{(1d)}}{L} = -(1 + \lambda) F \left( -\frac{1}{2}, \frac{1}{2}; 1; \frac{4\lambda}{(1+\lambda)^2} \right) \]  

(26)

Eqs.\( (25) \) and \( (26) \) exhibit the Krammers-Wannier duality,

\[ e_0^{(1d)}(\lambda) = \lambda e_0^{(1d)} \left( \frac{1}{\lambda} \right) \]  

(27)

in agreement with the fact that \( \lambda_c = 1 \) is the selfdual critical transverse field. The density energy at the critical field is,
\[ e_0^{(1d)} = -\frac{4}{\pi} \]  

For dimensions higher than one the exact solution is not known and only approximations are available \(^{20}\). In the next subsections we shall obtain variational upper bounds for the exact energy. It is also possible to obtain a lower bound for the ground state energy of the Hamiltonian (24),

\[ e_0^{(d)}(\lambda) \geq d e_0^{(1d)} \left( \frac{\lambda}{d} \right) \]  

There are two extreme cases where one can find the exact ground state of the Hamiltonian (24). At \( \lambda = 0 \) there are two ferromagnetic ground states corresponding to \( <\sigma^Z> = \pm 1 \) given by,

\[ |\uparrow> = \bigotimes_n |\uparrow>_n, |\downarrow> = \bigotimes_n |\downarrow>_n \]  

where \( |\uparrow>_n, |\downarrow>_n \) denote the eigenstates of \( \sigma^Z_n \) with eigenvalues 1, -1 respectively. The density energy of these states is,

\[ e_0(\lambda = 0) = -d \]  

At \( \lambda = +\infty \) the ground state is the non degenerate disordered state \( ( <\sigma^Z> = 0 ) \),

\[ |0> = \bigotimes_n |0>_n = \bigotimes_n \frac{1}{\sqrt{2}} (|\uparrow>_n + |\downarrow>_n) \]  

whose energy is given in the limit \( \lambda \to \infty \) by,

\[ e_0(\lambda \to +\infty) \simeq -\lambda \]  

The Hamiltonian (24) commutes with the spin rotation operator,

\[ R = \prod_n \sigma^n_X \]  

and therefore its spectrum can be split into an even \( (R = 1) \) and odd \( (R = -1) \) sectors. The ground state (32) of the disorder phase belongs to the even sector whereas in the ordered phase there is a ground state belonging to each of the two sectors.

We shall study the ordered and disordered phases independently. In the next two subsections we present the results of the computation of the energy and the variational
parameters using the variational method. The details of their derivation will be presented in the appendices. The formulae for the energy and the weights $\alpha_I$ are labelled by the type of approximation used, its order and the spatial dimension of the lattice, namely, $e(\text{app}, \text{order}, d)$, $\alpha_I(\text{app}, \text{order}, d)$, where $\text{app}=\text{per}$ (perturbative), $\text{var}$ (variational).

### 3.2 Ordered Phase

In this phase the ground state is degenerate and therefore we could not in principle apply the techniques of section 2. However in practice this is not an obstacle since for large lattices the state $|\uparrow\rangle$ does not mix with the state $|\downarrow\rangle$ at finite orders in perturbation theory and one can effectively apply non degenerate perturbation theory, say to the state $|\uparrow\rangle$. In the ordered phase $\lambda$ is a small parameter and therefore the hamiltonian (34) split as follows,

$$H = H_0 + \lambda H_1$$

$$H_0 = -\sum_n \sum_{\mu} \sigma_n^Z \sigma_{n+\mu}^Z$$

$$H_1 = -\sum_n \sigma_n^X$$

The unperturbed ground state is taken to be,

$$\psi_0 = |\uparrow\rangle = \prod_n |\uparrow\rangle_n$$

A solution of the perturbative equations (10) which satisfy also conditions (23) is given by,

$$U_1 = \frac{1}{4d} \sum_n \sigma_n^X$$

$$U_2 = \frac{1}{16d^*(2d-1)} \sum_{n,\mu} \sigma_n^X \sigma_{n+\mu}^X$$

In appendix C we consider another solutions to equations (10), which do not satisfy (23), and discuss their significance.

The perturbative energy to third order in $\lambda$ which can be derived from this solution is,

$$e(\text{per}, n = 3, d) = -\left(d + \frac{\lambda^2}{4d}\right)$$
Notice that odd powers in $\lambda$ do not enter into the energy.

We shall now apply the P/V method corresponding to $\nu = 1$ and 2. From eq. (37) the ansatz for $\nu = 1$ is given by,

$$
\psi^{(1)} = \exp \left( \frac{h}{2} \sum_n \sigma_n^X \right) | \uparrow > = \prod_n \left( \cosh \frac{h}{2} | \uparrow >_n + \sinh \frac{h}{2} | \downarrow >_n \right)
$$

which shows that $\psi^{(1)}$ is a mean field state parametrized in terms of hyperbolic functions of the variational parameter $h$. This mean field state is usually written in terms of an angle $\theta$, which describes the deviation of the up pointing spin under the action of the transverse field \cite{15}. These two kinds of parametrizations can be explained from the hermiticity properties of $U_1$, i.e. $h$(non-compact variable) $\leftrightarrow U_1$(hermitean), $\theta$(compact variable) $\leftrightarrow U_1$(antihermitean) (see appendix C).

The minimization of the energy of (40) is achieved for,

$$
e(\text{var}, \nu = 1, d) = \begin{cases} 
-(d + \frac{\lambda^2}{4d}) & \lambda \leq 2d \\
-\lambda & \lambda \geq 2d
\end{cases} \quad (41)
$$

For $\lambda \leq 2d$ the variational energy (41) coincides with the perturbative result (39), in agreement with condition (21). For $\lambda \geq 2d$ this energy coincides with the strong coupling limit (33), in agreement now with eq. (22).

The mean field state (40) illustrates in the simplest possible way the interpolating properties of the variational states constructed out from solutions of the perturbative equations (10) fulfilling conditions (23). Later on we shall see more examples of this.

The dependence of the variational parameter $h$ on $\lambda$ is given by,

$$
h(\text{var}, \nu = 1, d) = \begin{cases} 
\arctanh \left( \frac{\lambda}{2d} \right) & \lambda \leq 2d \\
\infty & \lambda \geq 2d
\end{cases} \quad (42)
$$

The value $h = \infty$ for $\lambda \geq 2d$ implies that $\psi^{(1)}$ can be identified with the state $| 0 >$, which is precisely the eigenstate of the Hamiltonian $H_1$.

The magnetization of (40) is,

$$
< \sigma^Z > = \begin{cases} 
\left[ 1 - \left( \frac{\lambda}{2d} \right)^2 \right]^{1/2} & \lambda \leq 2d \\
0 & \lambda \geq 2d
\end{cases} \quad (43)
$$

which shows that $\lambda_c = 2d$ and the exponent $\beta$, defined by $< \sigma^Z > \sim (\lambda_c - \lambda)^\beta$, takes the mean field value $\beta = 1/2$. The exact result in 1d is given by,
\[
< \sigma^Z > = \begin{cases} 
(1 - \lambda^2)^{1/8} & \lambda \leq 1 \\
0 & \lambda \geq 1 
\end{cases} 
\] (44)

To go beyond the mean field approximation we shall consider the second order ansatz \( \nu = 2 \), which according to (38) reads

\[
\psi^{(2)} = \exp \left( \frac{h}{2} \sum_n \sigma^X_n + \frac{\alpha}{2} \sum_{n,\mu} \sigma^X_n \sigma^X_{n+\mu} \right) | \uparrow \rangle 
\] (45)

The term in the exponential of (45) proportional to \( \alpha \) introduces in \( \psi^{(2)} \) correlations which were absent in \( \psi^{(1)} \). Hence \( \psi^{(2)} \) is no longer a mean field state. The norm of \( \psi^{(2)} \) coincides with the partition function of a d-dimensional classical Ising model with inverse temperature \( \alpha \) and magnetic field \( h \). In 1d the computations can be done exactly (see appendix A). The results for the energy and magnetization are shown in figure 1 and 2. The variational estimation of the energy for \( \nu = 2 \) considerably improves the mean field value result. The magnetization is also improved, but the singular mean field behaviour is lost obtaining instead a smooth curve (see table 1). This implies that in order to obtain an estimation of the exponent \( \beta \) we should resort to another techniques as for example Padé approximants. The study of these questions, though interesting, is beyond the scope of this paper.

In \( d \geq 1 \) the norm of the state (44) cannot be computed exactly hence we have to use some kind of approximation. For small values of \( \lambda \) we expect both \( h \) and \( \alpha \) to be also small, in which case this norm can be computed through a ”high temperature” expansion. Doing this computation we obtain,

\[
e(\text{var}, \nu = 2, d) = - \left( d + \frac{\lambda^2}{4d} + \frac{\lambda^4}{64d^3(2d-1)} + O(\lambda^6) \right) 
\] (46)

The fourth order term in \( \lambda \) agrees with the perturbative result in accordance with (21).

For large values of \( \lambda \) we expect that \( h, \alpha \) or both become also very large in which case the norm of the variational state can be computed by means of a ”low temperature” expansion. Of course if the model is integrable we can compute in the whole range of couplings including the intermediate ones, obtaining rigorous upper bounds for the exact energy.
3.3 Disordered Phase

In this phase the ground state is non degenerate and hence the techniques explained in section 2 could be automatically applied. The perturbative parameter in the disordered phase is $\frac{1}{\lambda}$, which leads us to write the Hamiltonian (24) as,

$$H = \lambda \left( H_0 + \frac{1}{\lambda} H_1 \right)$$

$$H_0 = - \sum_n \sigma_n^x$$

$$H_1 = - \sum_{n, \mu} \sigma_n^z \sigma_{n+\mu}^z$$

The unperturbed ground state is,

$$\psi_0 = |0> = \prod_n |0>_n$$

A solution of the equations (10) and (23) reads,

$$U_1 = \frac{1}{4} \sum_{n, \mu} \sigma_n^z \sigma_{n+\mu}^z$$

$$U_2 = \frac{1}{16} \left( \sum_{n, \mu} \sigma_n^z \sigma_{n+2\mu}^z + \sum_{n, \mu_1 \neq \mu_2} \sigma_n^z (\sigma_{n+\mu_1+\mu_2}^z + \sigma_{n+\mu_1-\mu_2}^z) \right)$$

The perturbative energy to third order is,

$$e(\text{per}, n = 3, d) = -(\lambda + \frac{d}{4\lambda})$$

In this phase we shall only study the first order ansatz ($\nu = 1$) which according to (49) becomes,

$$\psi^{(1)} = \exp \left( \frac{\theta}{2} \sum_{n, \mu} \sigma_n^z \sigma_{n+\mu}^z \right) |0>$$

The norm of $\psi^{(1)}$ coincides with the partition function of the d-dimensional classical Ising model with inverse temperature $\alpha$. This implies that computations with (52) can only be done exactly in $d = 1$ and 2.

The 1d case is very easy to handle (see appendix B). The energy of (52) is after minimization,

$$e(\text{var}, \nu = 1, d = 1) = \begin{cases} - \left( \lambda + \frac{1}{4\lambda} \right) & \lambda \geq 1/2 \\ -1 & \lambda \leq 1/2 \end{cases}$$
Comparing this result with the corresponding one in the ordered phase \((41)\), we observe that they satisfy the duality relation \((27)\), which means that we have incorporated the KW duality in our ansatzs. We have now two kinds of variational results at order \(\nu = 1\), which can be combined in order to optimize the upper bound to the energy,

\[
e(\text{var}, \nu = 1, d = 1) = \text{Minimum} \left(e^{\text{(order)}}(\text{var}, \nu = 1, d = 1), e^{\text{(disorder)}}(\text{var}, \nu = 1, d = 1)\right)
\]

\[
= \begin{cases} 
- \left(1 + \frac{\lambda^2}{4}\right) & \lambda \leq 1 \\
- \left(\lambda + \frac{1}{4}\right) & \lambda \geq 1
\end{cases}
\]

(55)

Let us define \(\lambda_{OD}^{(\nu)}\) as the crossing point between the ordered and disordered variational energies at order \(\nu\). We expect that \(\lambda_{OD}^{(\nu)}\) will approach \(\lambda_c\) as \(\nu \to \infty\). Eq.(55) shows that \(\lambda_{OD}^{(1)} = 1\) in 1d. In fact from KW duality it is clear that \(\lambda_{OD}^{(\nu)} = 1\) for all \(\nu\) in 1d.

Let us turn to the more interesting case of 2d, where the partition function and other related quantities are known exactly. In figure 3 we show our results for the energy. The value of \(\lambda_{OD}^{(1)}\) is 2.7239 which is not far from the critical value computed by other methods which is around 3.08 \([20]\).

3.4 First Excited State: the Gap

A better determination of \(\lambda_c\) will be for example to compute the energy gap \(\Delta\) in the spectrum of the Hamiltonian. For values of \(\lambda\) near and above \(\lambda_c\) the singular behaviour of \(\Delta\) is characterized by an exponent \(s\),

\[
\Delta \sim (\lambda - \lambda_c)^s, \quad \lambda \geq \lambda_c
\]

(56)

which is computed in the disordered region.

Assuming that the first excited state is translationally invariant and that it belongs to the odd sector \((R=-1)\), we propose the following ansatz,

\[
\psi^{(1)}_{exc} = \sum_m \sigma_m^z \exp \left(\frac{\beta}{2} \sum_{n,\mu} \sigma_n^z \sigma_{n+\mu}^z\right) |0\rangle
\]

(57)

where the variational parameter \(\beta\) can in principle be different from the ground state parameter \(\alpha\) appearing in \((52)\). The norm of \((57)\) is essentially given by the susceptibility at zero magnetic field of a classical Ising model (see appendix D). We have only considered
the 1d case where the result that we obtain coincides quite surprisingly with the exact result,

\[ E_1(\text{var}, \nu = 1, d = 1) - E_0(\text{var}, \nu = 1, d = 1) = E_1(\text{exact}, d = 1) - E_0(\text{exact}, d = 1) = 2(\lambda - 1) \] (58)

For \( d > 1 \) the computation of \( \Delta \) could be performed using high-temperature expansions for the susceptibility.

4 Concluding Remarks

We have shown in the study of the ITF that a discrete versions of generalized Jastrow wave functions are very adequate to develop a perturbative/variational approach to local lattice Hamiltonians. The information encoded in the lowest orders of perturbation theory is amplified to all orders by means of a variational method. In this way the ansatzs for the ground state of the hamiltonians become less aprioristic, since they are subjected to satisfy a set of strong constraints which eliminates much of the arbitrariness.

An expected weakness of our method shows up for Hamiltonians near criticality, as for the energy and magnetization do not exhibit the desired singular behaviour. This can be understood from the fact that we do not take into account all the scales involved near the critical point. To make further progress one should fertilize the P/V method with renormalization group ideas, in the spirit of references [27, 28].

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Appendix A: Variational Calculations in the Ordered Phase

The basic matrix elements needed to compute the energy of the trial wave function (40) are the following,

\[ < \psi^{(1)} | \psi^{(1)} > = \cosh L h \]
\[ < \psi^{(1)} | \sum_n \sigma_n^X | \psi^{(1)} > = L \cosh h \tanh h \]
\[ < \psi^{(1)} | \sum_n \sigma_n^Z | \psi^{(1)} > = L \cosh^{L-1} h \]
\[ < \psi^{(1)} | \sum_{n, \mu} \sigma_n^Z \sigma_{n+\mu}^Z | \psi^{(1)} > = L d (\cosh h)^{L-2} \] \hspace{1cm} (59)

We have assumed that \( h \) is real. Using these equations the density energy of \( \psi^{(1)} \) becomes,

\[ e(\text{var, } \nu = 1, d) = - \left( \lambda \tanh h + \frac{d}{\cosh h} \right) \] \hspace{1cm} (60)

The minimum of (60) is obtained for

\[ \lambda = 2 d \tanh h \quad \text{if } \lambda \leq 2d \]
\[ 1 = \tanh h \quad \text{if } \lambda \geq 2d \] \hspace{1cm} (61)

Introducing (61) into (60) we obtain (41).

The relevant matrix elements of the trial wave function \( \psi^{(2)} \) are,

\[ < \psi^{(2)} | \psi^{(2)} > = Z_L(\alpha, h) \]
\[ < \psi^{(2)} | \sum_n \sigma_n^X | \psi^{(2)} > = \frac{\partial}{\partial h} Z_L(\alpha, h) \]
\[ < \psi^{(2)} | \sum_n \sigma_n^Z | \psi^{(2)} > = L Z^{(\text{site})}_{L-1}(\alpha, h) \]
\[ < \psi^{(2)} | \sum_{n, \mu} \sigma_n^Z \sigma_{n+\mu}^Z | \psi^{(2)} > = L d \cosh \alpha Z^{(\text{bond})}_{L-2}(\alpha, h) \] \hspace{1cm} (62)

where \( Z_L(\alpha, h) \) is the partition function of a classical statistical Ising model defined in a d-dimensional hypercubic lattice,

\[ Z_L(\alpha, h) = \frac{1}{2^L} \sum_{\{s_1, \ldots, s_L\}} \exp \left( \alpha \sum_{n, \mu} s_n s_{n+\mu} + h \sum_n s_n \right) \] \hspace{1cm} (63)

where \( s_n = \pm \).

\( Z^{(\text{site})}_{L-1}(\alpha, h) \) is the same as \( Z_L(\alpha, h) \) except for the removal of one lattice variable located at a single site, say \( L \), together with all possible couplings among this variable and the ones in its neighbour,
Finally $Z^{(\text{site})}_{L-1}(\alpha, h) = \frac{1}{2^{L-1}} \sum_{\{s_1, \ldots, s_{L-1}\}} \exp \left( \alpha \sum_{n, n+\mu \neq L} s_n s_{n+\mu} + h \sum_{n \neq L} s_n \right)$ (64)



$$Z^{(\text{bond})}_{L-2}(\alpha, h) = \frac{1}{2^{L-2}} \sum_{\{s_1, \ldots, s_{L-2}\}} \exp \left( \alpha \sum_{n, n+\mu \neq L, L-1} s_n s_{n+\mu} + h \sum_{n \neq L, L-1} s_n \right)$$ (65)

To derive eqs.(62) we use the following general formula which relates matrix elements of Pauli matrices and statistical sums of Ising models,

$$\langle \uparrow | f(\sigma^x_1, \sigma^x_2, \cdots, \sigma^x_M) | \uparrow \rangle = \frac{1}{2^M} \sum_{s_1, \cdots, s_M} f(s_1, s_2, \cdots, s_M)$$ (66)

where $f(x_1, \cdots, x_M)$ is a generic function of $M$ variables.

Using eqs.(62) the energy of $\psi^{(2)}$ becomes,

$$E(\text{var}, \nu = 2, d) = -\lambda \frac{\partial}{\partial h} \ln Z_L(\alpha, h) - d L \frac{Z^{(\text{bond})}_{L-2}(\alpha, h)}{Z_L(\alpha, h)}$$ (67)

and the magnetization reads,

$$\langle \sigma^Z \rangle = \frac{Z^{(\text{site})}_{L-1}(\alpha, h)}{Z_L(\alpha, h)}$$ (68)

In 1d these partition functions can be computed exactly in the limit $L \to \infty$,

$$Z^{(1d)}_L(\alpha, h) = z^L$$

$$Z^{(1d, \text{site})}_{L-1}(\alpha, h) = \frac{1}{2} \left[ \cosh h + \frac{1+e^{2\alpha} \sinh^2 h}{\sqrt{1+e^{4\alpha} \sinh^2 h}} \right] z^{L-2}$$ (69)

$$Z^{(1d, \text{bond})}_{L-2}(\alpha, h) = \frac{1}{2} \left[ \cosh h + \frac{1+e^{2\alpha} \sinh^2 h}{\sqrt{1+e^{4\alpha} \sinh^2 h}} \right] z^{L-3}$$

where

$$z = \frac{1}{2} \left[ e^{\alpha} \cosh h + e^{-\alpha} \sqrt{1+e^{4\alpha} \sinh^2 h} \right]$$ (70)

Introducing these equations into (67) we obtain the energy in 1d,
\[ e(\text{var}, \nu = 2, d = 1) = -2 \left( \frac{\lambda \sqrt{s^2 - 1}}{2s} + \frac{1}{st} - \frac{1}{t^2} + \frac{\sqrt{1 + t^2 - 2st}}{t} \right) \]  \hspace{1cm} (71)

\[ s = \sqrt{1 + e^{4\alpha} \sinh^2 h} \]  \hspace{1cm} (72)

\[ t = s + \sqrt{s^2 + e^{4\alpha} - 1} \]  \hspace{1cm} (73)

Minimization of (71) with respect to \( t \) and \( s \) gives,

\[ s = \frac{1}{9t} \left[ 3t^2 + 2 + \sqrt{3t^2 + 4} \right] \]  \hspace{1cm} (74)

\[ \lambda = \frac{2\sqrt{s^2 - 1}}{t} \left( 1 + \frac{s^2}{\sqrt{1 + t^2 - 2st}} \right) \]  \hspace{1cm} (75)

The magnetization in 1d is given, using the variables \( s \) and \( t \), by

\[ < \sigma^Z > = \frac{2}{t^2} \left[ t - \frac{1}{s} + \frac{1}{s} \sqrt{1 + t^2 - 2st} \right] \]  \hspace{1cm} (76)

Plots of the energy (71) and the magnetization (76), using (74) and (75), are given in figures 1 and 2 respectively. Some numerical results are shown in table 1, where we have included for comparison the results obtained in reference [29] using a variational renormalization group method. In this particular case the variational energy obtained through the P/V method is better than the one obtained using the RG method. As for the magnetization, in the RG method there is a finite value of \( \lambda \) at which it vanishes, whereas in the P/V method \( \lambda \) has to go to \( \infty \).

| \( \lambda \) | energy (var) | energy (RG) | \( < \sigma^Z > \) (var) | \( < \sigma^Z > \) (RG) |
|--------|-------------|-------------|----------------|----------------|
| 0.2    | -1.010 024 99 [525] | -1.010 000 | 0.994 912 [0] | 0.994 93 |
| 0.4    | -1.040 399 [417] | -1.040 306 | 0.978 56 [44] | 0.978 83 |
| 0.9    | -1.212 4 [60] | -1.210 8 | 0.859 3 [125] | 0.860 4 |
| 1.0    | -1.264 9 [732] | -1.262 9 | 0.8 [0] | non zero |

Table 1: Energy density and magnetization of the 1d ITF obtained by the \( \nu = 2 \) variational method and the RG methods of reference [29]. Numbers in brackets are last digits of the exact results.
Appendix B: Variational Calculations in the Disordered Phase

The matrix elements for the ansatz (52) are,

\[ <\psi^{(1)}|\psi^{(1)}> = Z_L(\alpha) \]
\[ <\psi^{(1)}|\sum_n \sigma_n^X |\psi^{(1)}> = L Z_{L-1}^{\text{site}}(\alpha) \]
\[ <\psi^{(1)}|\sum_n \sigma_n^Y \sigma_{n+\mu}^Y |\psi^{(1)}> = \frac{\partial}{\partial\alpha} Z_L(\alpha) \] (77)

where \( Z_L(\alpha) = Z_L(\alpha, h = 0) \) and \( Z_{L-1}^{\text{site}}(\alpha) = Z_{L-1}^{\text{site}}(\alpha, h = 0) \).

The energy reads,

\[ E(\text{var}, \nu = 1, d) = -\frac{\partial}{\partial\alpha} \ln Z_L(\alpha) - \lambda L \frac{Z_{L-1}^{\text{site}}(\alpha)}{Z_L(\alpha)} \] (78)

In 1d one has,

\[ Z_L^{(1d)}(\alpha) = \cosh L \alpha \] (79)
\[ Z_{L-1}^{(1d,\text{site})}(\alpha) = \cosh L^{-2} \alpha \] (80)

which yields the energy density,

\[ e(\text{var}, \nu = 1, d = 1) = -\left( \tanh \alpha + \frac{\lambda}{\cosh^2 \alpha} \right) \] (81)

The minimum of this expression is obtained for,

\[ \frac{1}{\lambda} = 2 \tanh \alpha \quad \text{if} \quad \lambda \geq 1/2 \]
\[ 1 = \tanh \alpha \quad \text{if} \quad \lambda \leq 1/2 \] (82)

Substituting (82) into (81) one obtains eq.(53).

To study the 2d disordered case we need the well known results obtained by Onsager in his study on the 2d Ising model [26]. Calling \( f_{2d} = -\lim_{L \to \infty} \frac{1}{L} \log Z_L(\alpha) \) the free energy per site, \( u_{2d} = \partial f_{2d}/\partial\alpha \) the internal energy and \( c_{2d} = -\alpha^2 \partial^2 u_{2d}/\partial\alpha^2 \) the specific heat we have,

\[ f_{2d} = -\ln \cosh(2\alpha) - \frac{1}{\pi} \int_0^{\pi/2} d\phi \ln \frac{1+\sqrt{1-q^2 \sin^2 \phi}}{2} \]

20
\[ u_{2d} = -\coth(2\alpha) \left\{ 1 + \frac{2}{\pi} q' K(q) \right\} \] (83)

\[ c_{2d} = \frac{4\alpha^2}{\pi} \coth^2(2\alpha) \left\{ K(q) - E(q) + \frac{1}{2} (q' - 1) \left( \frac{\pi}{2} + qK(q) \right) \right\} \]

where

\[ q = \frac{2 \sinh 2\alpha}{\cosh^2(2\alpha)} \]
\[ q' = 2 \tanh^2(2\alpha) - 1 \] (84)

and \( K(q) \) and \( E(q) \) are the elliptic integrals,

\[ K(q) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - q^2 \sin^2 \phi}} , \quad E(q) = \int_0^{\pi/2} d\phi \sqrt{1 - q^2 \sin^2 \phi} \] (85)

The computation of \( Z_{L-1}^{(2d,\text{site})} \) is a bit more complicated but it can be related to the original partition function through two point correlation functions as follows,

\[ \frac{Z_{L-1}^{(2d,\text{site})}}{Z_{L-1}^{(2d)}} = \frac{1}{2} \left[ 2 + x^2 - x(5 + x^2) < s_0 s_{\mu_1} > + x^2 ( < s_0 s_{2\mu_1} > + 2 < s_0 s_{\mu_1+\mu_2} > ) \right] \] (86)

where \( x = \tanh\alpha \) and \( s_0, s_{\mu_1}, s_{2\mu_1}, s_{\mu_1+\mu_2} \) are classical Ising variables located at the points \( 0, \mu_1, 2\mu_1, \mu_1 + \mu_2 \) respectively. The correlators entering eq.(86) has been computed in reference [30],

\[ \begin{align*}
< s_0 s_{\mu_1} > &= \frac{1}{2} \cotanh(2\alpha) \left[ 1 + \frac{2}{\pi} q' K(q) \right] \\
< s_0 s_{\mu_1+\mu_2} > &= \frac{1}{2} \cotanh^2(2\alpha) [E(q) + q' K(q)] \\
< s_0 s_{2\mu_1} > &= \frac{1}{2} \cotanh^2(2\alpha) - \left( \frac{2}{\pi q} \right)^2 [E^2(q) - 2q' K(q) E(q) + (q')^3 K^2(q)]
\end{align*} \] (87)

Introducing equations (83),(86) and (87) into (78) and minimizing this energy numerically we obtain figure 3, where we have also include the mean field result (41) for 2d and the lower bound given by eq.(29).

21
Appendix C: Other P/V solutions

We mentioned in section 2 the non uniqueness of the solution of the perturbative equations (10). This in turn lead us to look for solutions which in the limit $\lambda \to \infty$ will flow to the ground state of $H_1$. This is the reason to impose conditions (23). To get further motivation for the need of these conditions it is illustrative to investigate another solutions to equations (10) than those given in section 3. This will be done only at the lowest order $\nu = 1$.

In the ordered phase an antihermitean solution of eq. (10) is given by,

$$U_1 = \frac{-i}{4d} \sum_n \sigma_n^Y$$

which leads to the following ansatz,

$$\psi^{(1)} = \exp \left( -\frac{i\theta}{2} \sum_n \sigma_n^Y \right) | \uparrow > = \Pi_n \left( \cos \frac{\theta}{2} | \uparrow > + \sin \frac{\theta}{2} | \downarrow > \right)$$

where $\theta$ is a real parameter. The variational energy of this state can be computed as in appendix A obtaining,

$$e(\text{var}, \nu = 1, d) = - \left( \lambda \sin \theta + d \cos^2 \theta \right)$$

Whose mimimum is achieved at $\theta$ given by,

$$\sin \theta_0 = \begin{cases} \frac{\lambda}{2d} & \lambda \leq 2d \\ 1 & \lambda \geq 2d \end{cases}$$

Substituting this result in (90) we get the same energy as the one given by eq.(41), which was obtained with the hermitean solution (40). Indeed if we compare eqs.(40) and (89) we see that the trigonometric variable $\theta$ can be related to the hyperbolic variable $h$ by means of the Gudermannian function,

$$\theta = gd(h) = 2 \text{arctanh}(e^h) - \frac{\pi}{2}$$

The mean field value computation of reference [15] is performed in terms of the variable $\theta$ whose physical meaning is the semiclassical rotation suffered by the spin under the action of the external field $\lambda$,
\[ < \sigma^Z > = \cos \theta \] (93)

Let us move on to the disordered case. We shall make the following choice of the operator \( U_1 \),

\[
U_1 = \epsilon \sum_{n,\mu} (\vec{r} \cdot \sigma_n) (\vec{r} \cdot \sigma_{n+\mu})
\]
\[ U_1^\dagger = \epsilon^2 U_1 \] (94)

where \( \vec{r} = (0,y,z) \) is a vector with real components and \( \epsilon^4 = 1 \). There are 4 possible solutions of the first order perturbative equation (10) which we display in table 2 together with the corresponding variational energies in the 1d case.

| Solutions | \( \epsilon \) | \( \vec{r} \) | \( e(var, \nu = 1, d = 1) \) |
|-----------|---------------|---------------|------------------|
| I         | 1             | \((0,0,\frac{1}{2})\) | \[
\begin{cases}
-\left(\lambda + \frac{1}{4\lambda}\right) & \lambda \geq \frac{1}{2} \\
-1 & \lambda \leq \frac{1}{2}
\end{cases}
\]
| II        | -1            | \((\frac{1}{2},0)\) | \[-\frac{2}{27} \lambda (9 - \lambda^2) + (\lambda^2 + 3)^{3/2}\] |
| III       | i             | \((0,\frac{1}{2\sqrt{2}},\frac{1}{2\sqrt{2}})\) | \[-\frac{1}{2} \lambda + \sqrt{1 + \lambda^2}\] |
| IV        | -i            | \((0,-\frac{1}{2\sqrt{2}},\frac{1}{2\sqrt{2}})\) | \[-\frac{1}{2} \lambda + \sqrt{1 + \lambda^2}\] |

Table 2: Variational states and energies for the \( \nu = 1, d = 1 \) disordered case

We observe that only solution I, which is the one used in section 3, goes in the limit \( \lambda \to 0 \) to the correct value of the energy of the ordered region. Indeed this solution satisfies conditions (23) while the others do not. Table 2 shows that for the ansatz (94) there exists no equivalence between hermitean and antihermitean solutions as it happens in the mean field case.

Appendix D: Calculation of the Mass Gap

The relevant matrix elements for this state are,

\[
\begin{align*}
< \psi^{(1)}_{exc} | \psi^{(1)}_{exc} > &= \tilde{Z}_L(\beta) \\
< \psi^{(1)}_{exc} | \sum_n \sigma_n^X | \psi^{(1)}_{exc} > &= L \left( \tilde{Z}^{(site)}_{L-1}(\beta) - \tilde{Z}^{(site)}_{L}(\beta) \right) \\
< \psi^{(1)}_{exc} | \sum_{n,\mu} \sigma_n^Z \sigma_{n+\mu}^Z | \psi^{(1)}_{exc} > &= \frac{\partial}{\partial \beta} \tilde{Z}_L(\beta)
\end{align*}
\] (95)
where
\[ \tilde{Z}_L(\beta) = \frac{\partial^2}{\partial h^2} Z_L(\beta, h) |_{h=0} \] (96)
and similarly for \( \tilde{Z}_L^{\text{site}}(\beta) \). The expression of the energy of the state (57) is,
\[ E_1(\text{var}, \nu = 1, d) = - \left( \frac{\partial}{\partial \beta} \ln \tilde{Z}_L(\beta) + \frac{L \lambda}{Z_L(\beta)} (\tilde{Z}_L^{\text{site}} - Z_L^{\text{site}}) \right) \] (97)

A long but straightforward calculation using eqs (69) yields,
\[ E_1(\text{var}, \nu = 1, d = 1) = - L \left( \tanh \beta + \frac{\lambda}{\cosh^2 \beta} \right) + 2(\lambda - 1) \] (98)
whose minimization gives (58). The value of \( \beta \) coincides with that of \( \alpha \) given by eq.(82).
Figure Captions

Fig.1.- Energy versus $\lambda$ in 1d: exact (continuous line), mean field (+++) and $\nu = 2$ variational in the ordered regime (...).

Fig.2.- Magnetization $\langle \sigma^z \rangle$ versus $\lambda$ in 1d: exact (continuous line), mean field (+++) and $\nu = 2$ variational in the ordered regime (...).

Fig.3.- Energy versus $\lambda$ in 2d: lower bound (29) (continuous line), $\nu = 1$ ordered phase (+++) and $\nu = 1$ disordered phase (...).
Fig. 1
Fig. 2
$E/(1+\lambda)$

$\lambda/(1+\lambda)$
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