Quantum mechanical ground states, nonlinear Schrodinger equations and linked cluster expansions

1981 J. Phys. A: Math. Gen. 14 1291

(http://iopscience.iop.org/0305-4470/14/6/009)

J. Phys. A: Math. Gen. **14** (1981) 1291–1305. Printed in Great Britain

Quantum mechanical ground states, nonlinear Schrödinger equations and linked cluster expansions†

Leo P Kadanoff and Mahito Kohmoto‡

The James Franck Institute and the Department of Physics, The University of Chicago, Chicago, IL 60637, USA

Received 25 September 1980

Abstract. The ground state wavefunction of an infinitely large, spatially homogeneous system is evaluated in terms of wavefunctions for linked clusters of points within the system. The linked cluster wavefunction is shown to obey a nonlinear form of the Schrödinger equation, with the unlinked pieces providing the nonlinearity. A variational principle for the ground state energy is derived.

1. Introduction

In this paper we study lattice problems with a Hamiltonian which consists of kinetic terms and interaction terms. The kinetic terms act on each lattice site individually and the interaction terms, on the other hand, give interactions between different lattice sites. The unperturbative ground state of the total system, $|\rangle$, is simply the product of unperturbative ground states at each lattice point which gives the lowest kinetic energy. The true ground state is expressed in terms of excitations superposed upon the unperturbed ground state, $|\rangle$. These excitations include unlinked terms, i.e. several individual excitations separated by large distances in which the wavefunction for the composite state is a product of wavefunctions for the individual regions of the lattice. In order to achieve a smooth transition to the infinite lattice, it is helpful to eliminate these unlinked terms from the wavefunction. When this is done, one can write the resulting problem in terms of a set of wavefunctions ψ_g, in which the graph g describes a linked excitation, i.e. a set of relatively closely neighbouring lattice sites with a quantum number associated with each lattice site. (Since we focus upon translationally invariant systems, two graphs g_1 and g_2 which differ by a lattice translation are considered to be the same graph.) Then ψ_g obeys a simple nonlinear type of Schrödinger equation, namely an equation of the form

$$W_g[\psi] = t(g)\psi_g + v_g[\psi]. \tag{1.1}$$

Here $t(g)$ is the kinetic energy associated with a graph g and $v_g[\psi]$ is a function with terms of order ψ to the powers 0 through 4. One important property of this expression for the wavefunction is that all coefficients in it are independent of the size of the system.

† Work supported by NSF Grant DMR77-12637.

‡ Present address: Department of Physics, FM-15, University of Washington, Seattle, Washington 98195 USA.

0305-4470/81/061291+15$01.50

In a similar fashion, the ground state energy per site is given by

$$\varepsilon_0 = E_0/N = v_0[\psi], \tag{1.2}$$

where v_0 has in it linear and quadratic terms in the ψ_g's.

The final major result of this paper is a variational principle based upon the functional

$$U[\psi] = v_0[\psi] + \tfrac{1}{2}\sum_g W_g[\psi]\frac{\partial}{\partial\psi_g} D[\psi], \tag{1.3}$$

where $D[\psi]$ is a specified, potential independent, functional of the ψ_g's. This functional reaches an extremal value for the correct choice of ψ_g's, with that extremum being ε_0.

These results are obtained formally and quite generally. However, they can be easily sharpened to give useful results for practical problems. For example, they can be used to calculate series expansions of ground state energy for lattice field theories in the time continuum Hamiltonian formulation, as in Hamer *et al* (1979). In § 5, the two-dimensional Ising model is treated in this formulation. The ground state energy is calculated in a high-temperature series expansion and the procedure is explained in detail.

The results of this paper may also prove to be of interest in more analytical studies of many-body ground state problems.

2. Formulation

2.1. Statement of problem

Given a lattice with translational invariance in which the individual sites are labelled by the index, r, at each site there is a 'momentum' variable P_r and a coordinate variable Q_r which do not commute. All variables at different sites commute with one another. A rather general Hamiltonian for this type of problem is a sum of a kinetic energy

$$T = \sum_r t(P_r) \tag{2.1}$$

and a two-body potential energy. The potential energy is expressed as a sum of terms in which sites separated by a distance $\boldsymbol{R}$ interact:

$$V = \sum_{\boldsymbol{R}} V_{\boldsymbol{R}} \tag{2.2}$$

with each interaction term being translationally invariant,

$$V_{\boldsymbol{R}} = \sum_r v_{\boldsymbol{R}}(Q_r, Q_{r+\boldsymbol{R}}). \tag{2.3}$$

We assume that each momentum variable has eigenvalues

$$P_r' = 0, P_1, P_2, \ldots, P_\alpha, \ldots \tag{2.4}$$

and that the ground state of T is $|\,\rangle$, a state with all momenta equal to zero. If we assume periodic boundary conditions and short-range forces, the ground state of the system will have an energy which is linear in the number of sites in the system, at least in the case studied here in which the true ground state may be obtained perturbatively from $|\,\rangle$.

Thus we wish to solve

$$(T+V)|\psi\rangle = N\varepsilon_0|\psi\rangle \tag{2.5}$$

for the ground state $|\psi\rangle$ and the energy per site ε_0.

Before we set out to calculate, we make some additional assumptions which are not really restrictive but rather are of a notational character. We choose T to vanish in the unperturbed ground state, i.e.

$$t(0) = 0, \tag{2.6a}$$

and also V to have zero diagonal matrix element in this state:

$$\langle\,|V|\,\rangle = 0. \tag{2.6b}$$

One can then construct a complete and orthogonal set of basis states by using the operators $a^+(\boldsymbol{r})$ which, when they act upon $|\,\rangle$, convert $P'_{\boldsymbol{r}}$ from zero to the value P_α. A graph of order n is specified by a set of n non-zero momenta $P_{\alpha_1}, P_{\alpha_2}, \ldots, P_{\alpha_n}$ and n distinct lattice sites $\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_n$ at which the momenta lie. The graph g is specified by these data, except that translations $\boldsymbol{r}_j \to \boldsymbol{r}_j + \boldsymbol{r}$ (for all $j = 1, 2, \ldots, n$) produce exactly the same graph. We define a creation operator for the graph via

$$A_g^+(\boldsymbol{r}) = a^+_{\alpha_1}(\boldsymbol{r}_1+\boldsymbol{r})a^+_{\alpha_2}(\boldsymbol{r}_2+\boldsymbol{r}) \ldots a^+_{\alpha_n}(\boldsymbol{r}_n+\boldsymbol{r}) \tag{2.7a}$$

so that the creation operator is

$$A_g^+ = \sum_{\boldsymbol{r}} A_g^+(\boldsymbol{r}) \tag{2.7b}$$

and the state associated with it is

$$|g\rangle = A_g^+|\,\rangle. \tag{2.7c}$$

To calculate the properties of a translationally invariant state, like the ground state, note that the $|g\rangle$'s form a complete set with the normalisation

$$\langle g|h\rangle = N\delta_{g,h}. \tag{2.8}$$

One can expand the ground state wavefunction in terms of these states as

$$|\psi\rangle = |\,\rangle + \sum_g \phi_g|g\rangle \tag{2.9}$$

and then find an expression for the eigenvalue equation

$$(t(g) - N\varepsilon_0)\phi_g + \sum_h \frac{\langle g|V|h\rangle}{N}\phi_h + v_{g_0} = 0 \tag{2.10}$$

with v_{g_0} being the N-independent quantity

$$v_{g_0} = \langle g|V|\,\rangle/N = v^*_{0g} \tag{2.11}$$

and $t(g)$ being the total kinetic energy of the excitation g, i.e. in terms of the definition (2.7)

$$t(g) = \sum_{l=1}^{n} t(P_{\alpha_l}). \tag{2.12}$$

Equation (2.10) is supplemented by an equation for the ground state energy per site

$$\varepsilon_0 = \sum_g v_{0g}\phi_g. \tag{2.13}$$

2.2. Disconnected and connected

Equation (2.10) forms a perfectly linear Schrödinger equation. However, it has two related defects. First, N appears in the equation and we know that the eventual answer, ε_0, is independent of N. Second, even in low orders of perturbation theory in V disconnected configurations appear, namely ones with momenta on very widely separated sites so that the distance between them is irrelevant. To avoid these difficulties, we reach for another basis, one which is not orthogonal. We still use the states g, as defined by equation (2.27), but now we restrict this set to include only those states in which the non-zero momenta are separated by distances much smaller than the dimension of the system. In fact, in mth-order perturbation theory the largest separation in these states is the force range (the maximum value of $\boldsymbol{R}$ in equation (2.3)) times m.

To take into account the disconnected clusters, we introduce new types of basis states which are not orthogonal. For example, we construct a state with two disconnected clusters of types g_1 and g_2 as

$$|g_1, g_2\rangle = \sum_{rr'}{}' A^+_{g_1}(\boldsymbol{r}) A^+_{g_2}(\boldsymbol{r}')|\,\rangle.$$

Here the cluster creation operators, $A^+_g(r)$, are the quantities defined in equation (2.7). The prime on the summation indicates that as r and r' go through their possible values (i.e. the set of all lattice points), all terms in which the two clusters overlap are omitted. Thus it is never possible for an a^+_α from one cluster to find itself at the same point in space as an $a^+_{\alpha'}$ from the other cluster. This is the only restriction on the sum. The clusters may get to within one lattice spacing of each other. One may find itself totally surrounded by the other. These configurations are possible in $|g_1, g_2\rangle$. But one cluster may not be on top of the other. Similarly, disconnected states with larger numbers of clusters are defined so that

$$|g_1, g_2, \ldots, g_m\rangle = \sum_{r_1,\ldots,r_m}{}' A^+_{g_1}(\boldsymbol{r}_1) \ldots A^+_{g_m}(\boldsymbol{r}_m)|\,\rangle \tag{2.14}$$

with the restriction on the sums that no two clusters overlap.

Now, we use this new set of basis states to rewrite the ground state wavefunction for the problem in the form

$$|\psi\rangle = |\,\rangle + \sum_g \psi_g |g\rangle + \sum_{g_1 g_2} \frac{1}{2!} \psi_{g_1 g_2} |g_1, g_2\rangle + \ldots + \sum_{g_1 \ldots g_m} \frac{1}{m!} \psi_{g_1 g_2 \ldots g_m} |g_1, g_2, \ldots, g_m\rangle + \ldots . \tag{2.15}$$

In this basis, the state $|g_1, g_2, \ldots, g_m\rangle$ includes every configuration of g_i's which do not overlap among themselves. Each configuration gives the same contribution, $\psi_{g_1,\ldots,g_m}$, to the true ground state $|\psi\rangle$.

This means the coefficient $\psi_{g_1,\ldots,g_m}$ is independent of the separations between graphs and consequently can be written as a product of the weights for the linked states $g_1, \ldots, g_m$:

$$\psi_{g_1 \ldots g_m} = \psi_{g_1} \psi_{g_2} \ldots \psi_{g_m}. \tag{2.16}$$

The contribution from the parts which depend on the relative distance between the graphs has been already taken into account as a linked contribution.

For any translationally invariant system, the states $|\,\rangle$ and $|g\rangle$ form a set. Hence equation (2.15) with equation (2.16) is not an assertion but merely a redefinition of

basis. This redefinition is useful precisely because ψ_g will, in a given order of perturbation theory, be given an N-independent value if the system is larger than the order of perturbation theory times the force range. Hence for large enough N the rewriting (2.15) permits the definition of an N-independent Schrödinger equation.

The reason that equation (2.15) will be successful lies precisely in the fact that it correctly takes into account the disconnected effects of the potential acting upon different regions of the lattice. Then ψ_g, as distinct from ϕ_g, will be non-zero only for the case in which all arguments in the cluster are close to one another.

The relationship between ϕ_g and ψ_g is easily stated. Let $m(g; g_1 g_2)$ be the number of ways one can partition the lattice sites in the cluster g to form two groups, one of which makes up the cluster g_1 and the other the cluster g_2. Then

$$\phi_g = \psi_g + \sum_{g_1 \leqslant g_2} m(g; g_1 g_2) \phi_{g_1} \phi_{g_2}. \tag{2.17}$$

Thus ψ_g forms the fully linked part of ϕ_g and the second term represents the disconnected contribution which is independent of the separation between graphs g_1 and g_2.

To derive a nonlinear Schrödinger equation, we take the wavefunction (2.15) and apply $(T + V - N\varepsilon_0)$. We then prove that the resulting expression takes the form

$$(T + V - N\varepsilon_0)|\psi\rangle = NW_0|\ \rangle + \sum_g W_g \frac{\partial}{\partial \psi_g}|\psi\rangle. \tag{2.18}$$

Here W_0 and W_g are functionals of ψ_h. We then simply adjust ε_0 to set W_0 to zero and ψ_g to set W_g to zero. In the process one notices that ψ_g is completely connected in low orders of perturbation theory, i.e. the only non-vanishing ψ_g's are those which contain closely neighbouring points.

2.3. Expression for ground state energy

To obtain an expression for the ground state energy, simply multiply equation (2.18) on the left by $\langle\ |$. We then have

$$W_0 = -\varepsilon_0 + \langle\ |V|\psi\rangle / N. \tag{2.19}$$

When V acts upon $|\psi\rangle$ it can give the ground state in two possible ways. Either V acts entirely within one excitation and reduces the momenta in that excitation to zero via

$$\langle 0|V|g\rangle = Nv_{0g} \tag{2.20a}$$

(of course this can only happen if g is an excitation of order two, since V can change at most two momenta to zero at the same time), or alternatively, V can act upon a disconnected state $|g_1, g_2\rangle$ in which both pieces contain just one non-zero momentum. A part of this state has these pieces within a force range of each other. When this happens one can get a contribution to the ground state energy arising from the matrix element

$$v_{0;g_1 g_2} = \langle 0|V|g_1, g_2\rangle / N. \tag{2.20b}$$

Thus, by putting together equations (2.15), (2.18), (2.19) and (2.20), one finds an expression for the ground state energy

$$0 = W_0 = -\varepsilon_0 + \sum_g v_{0g}\psi_g + \tfrac{1}{2} \sum_{g_1 g_2} v_{0;g_1,g_2}\psi_{g_1}\psi_{g_2}. \tag{2.21}$$

For the purposes of later analysis, it is important to decompose the effect of V into the components caused by the different separations $\boldsymbol{R}$ in equations (2.2) and (2.3). Here $\boldsymbol{R}$ represents the relative coordinate of the two sites at which the potential acts. We can then write equations (2.20a) and (2.20b) in terms of $V_{\boldsymbol{R}}$ as

$$V_{0g}(\boldsymbol{R}) = (1/N)\langle 0|V_{\boldsymbol{R}}|g\rangle, \tag{2.22a}$$

$$V_{0;g_1,g_2}(\boldsymbol{R}) = (1/N)\langle 0|V_{\boldsymbol{R}}|g_1, g_2\rangle, \tag{2.22b}$$

and then rewrite equation (2.21) in a form which will later prove useful:

$$\varepsilon_0 = \sum_{\boldsymbol{R}} \varepsilon_0(\boldsymbol{R}), \tag{2.23}$$

$$\varepsilon_0(\boldsymbol{R}) = \sum_g v_{0g}(R)\psi_g + \tfrac{1}{2}\sum_{g_1 g_2} v_{0;g_1 g_2}(R)\psi_{g_1}\psi_{g_2}. \tag{2.24}$$

3. Derivation of nonlinear Schrödinger equation

We now proceed to our major task, the derivation of a nonlinear Schrödinger equation, i.e. the evaluation of W_g. To achieve this we require some notation for disconnected states containing many connected components. An mth-order disconnected state $|g_1, g_2, \ldots, g_m\rangle$ is written simply as $|\boldsymbol{G}\rangle$, where $\boldsymbol{G}$ is an abbreviation for the list $g_1, g_2, \ldots, g_m$. If we eliminate the μ element from the list the result is written $\boldsymbol{G}/g_\mu$, while if we add a new element, g, to the list the result is $\boldsymbol{G}, g$.

3.1. Effect of kinetic energy and V

The kinetic energy term produces an essentially trivial effect upon the disconnected states. Since they are disconnected, the kinetic energy is simply the sum of the kinetic energies of the individual pieces,

$$T|\boldsymbol{G}\rangle = \sum_{\mu=1}^{m} t(g_\mu)|\boldsymbol{G}\rangle. \tag{3.1}$$

Therefore the effect of multiplying a state of the form (2.15) by the operator T is very simple, namely

$$T|\psi\rangle = \sum_g t(g)\psi_g \frac{\partial}{\partial \psi_g}|\psi\rangle. \tag{3.2}$$

Here $\psi_g\, \partial/\partial g$ picks out the terms in the ground state $|\psi\rangle$ which contain the graph g. We have therefore formed a piece of the functional $W_g[\psi]$ mentioned in equations (1.1) and (2.18), namely the piece corresponding to the kinetic energy

$$W_g^t = \psi_g t(g). \tag{3.3}$$

The potential energy term, V, has a much more complicated structure. Acting to the right upon an mth-order cluster $|\boldsymbol{G}\rangle$, it may:

(1) affect the momenta in one cluster, say g_μ;
(2) affect the momenta in two different clusters, say g_μ and g_ν;
(3) act upon two points in space where there are no clusters at all.

We can further subdivide the cases (1) and (2) in the following way.

(1a) The cluster g_μ is changed into the new state g'.

(1b) This cluster is destroyed by setting all its momenta to zero.

For case (2), we have two subcases.

(2a) After the action of the potential some of the momenta in one or both clusters remain different from zero. Then we interpret the results as the single new cluster g'.

(2b) All momenta in both clusters become zero. Both clusters are then destroyed.

This classification exhausts the possible effects of V and permits us to list systematically the possible terms in $V|\psi\rangle$.

3.2. Effects of V: linked diagrams

The simplest effect of V is number (3). This action of V inserts into the old mth-order unlinked state $|\boldsymbol{G}\rangle$ a new unlinked cluster g according to

$$V|\boldsymbol{G}\rangle = \sum_g v_{g0}|\boldsymbol{G}, g\rangle.$$

Thus an $(m+1)$-order cluster is constructed from one of order m. This effect can be taken into account by adding to the W_g of equation (2.18) a term

$$W_g^0 = v_{g0}. \tag{3.4}$$

In the effect of number (1a), V acts within one cluster, g, and produces a new cluster, g', by changing the momenta in g. It is possible for both the Q_r in V to lie in the cluster, or for one to lie in the cluster and the other to fall upon a neighbouring site with zero momentum. Thus the new cluster may have the same size as g, or have a size which is one larger, or one or two smaller than g. In any case, one represents the effect of V upon a single cluster by writing

$$V|g\rangle = Nv_{0g}|\,\rangle + \sum_h v_{h0}|g, h\rangle + \sum_{g'} v_{g';g}|g'\rangle. \tag{3.5}$$

The first term is effect (1b), the second effect (3) and the third represents effect (1a). By multiplying equation (3.5) on the left by $\langle g'|$, the intracluster matrix element $v_{g';g}$ is defined as

$$v_{g';g} = \frac{1}{N}\langle g'|V|g\rangle - \frac{1}{N}\sum_h \langle g'|g, h\rangle v_{0h}. \tag{3.6}$$

Notice that this matrix element is not Hermitian,

$$v_{g';g} \neq (v_{g;g'})^*,$$

since we subtract off the case in which V, acting to the right, adds an entirely new cluster. This effect of V is seen on our composite state as a modification of the individual clusters one by one:

$$V|\boldsymbol{G}\rangle_m = \sum_\mu \sum_{g'_\mu} v_{g'_\mu;g_\mu}|(\boldsymbol{G}/g_\mu), g'_\mu\rangle + \ldots.$$

However, this expression does not yet represent that effect of V completely. A correction due to the excluded volume is needed when the action of V makes a graph whose size is smaller than that of the original one. The state $|(\boldsymbol{G}/g_\mu), g'_\mu\rangle$ is all the translations of the graph g'_μ and the graphs g_ν $(\nu \neq \mu)$ contained in G which do not overlap each other. On the other hand, the original state $|\boldsymbol{G}\rangle$ is all the translations of the

graphs g_μ and g_ν $(\nu \neq \mu)$. When the size of g'_μ is smaller than that of g_μ, the state $|\boldsymbol{G}/g_\mu, g'_\mu\rangle$ contains more translations of the graphs than the original state does. In other words, some configurations of graphs $|\boldsymbol{G}/g_\mu, g'_\mu\rangle$ where the graphs g'_μ and g_ν $(\nu \neq \mu)$ are very close cannot be produced by the action of V because in the original state the larger graph g_μ would overlap the graphs g_ν $(\nu \neq \mu)$.

If the required corrections due to the effect mentioned above have been made, the action of V may be written as

$$V|\boldsymbol{G}\rangle_m = \sum_\mu \sum_{g'_\mu} v_{g'_\mu;g_\mu}\Big(|(\boldsymbol{G}/g_\mu), g'_\mu\rangle - \sum_{\nu\neq\mu} n(g; g'_\mu g_\nu; g_\mu)|(\boldsymbol{G}/g_\mu g_\nu), g\rangle\Big).$$

In the second term in the bracket, the graphs g'_μ and g_ν are very close and the relative spatial relation is fixed; accordingly, we regard them as the connected graph g. The coefficient $n(g; g'_\mu g_\nu; g_\mu)$ is 1 when the graph g_μ does overlap with the graph g_ν and is 0 otherwise. Corresponding terms in W are

$$W^1_g[\psi] = \sum_{g'} v_{g;g'}\psi_{g'} - \sum_{g,g'_1g_2} v_{g'_1;g_1} n(g; g'_1g_2; g_1)\psi_{g_1}\psi_{g_2}. \tag{3.7}$$

The term (2a) is rather simple. When V acts upon $|g_1, g_2\rangle$ and it touches both clusters, we can interpret the result as a new single cluster, i.e.

$$V|g_1, g_2\rangle = \sum_g v^{(2)}_{g;g_1g_2}|g\rangle + \ldots. \tag{3.8}$$

The corresponding effect upon a general disconnected state is

$$V|\boldsymbol{G}\rangle = \sum_{g,\mu<\nu} v^{(2)}_{g;g_\mu g_\nu}|(\boldsymbol{G}/g_\mu g_\nu), g\rangle.$$

As a result W gains a new term which is now quadratic in the ψ's, namely

$$W^2_g = \tfrac{1}{2}\sum_{g_1,g_2} v^{(2)}_{g;g_1g_2}\psi_{g_1}\psi_{g_2}. \tag{3.9}$$

The result which we have so far is equivalent to counting linked graphs in a perturbation expansion. It is summarised by giving the value of W to be

$$W_g = t(g)\psi_g + v^{\mathrm{L}}_g[\psi] + v^{\mathrm{U}}_g[\psi], \tag{3.10}$$

where the term we have calculated so far is

$$v^{\mathrm{L}}_g[\psi] = v_{g0} + \sum_{g'} v_{g;g'}\psi_{g'} - \sum_{g'_1g_1g_2} v_{g'_1;g_1} n(g; g'_1g_2; g_1)\psi_{g_1}\psi_{g_2} + \tfrac{1}{2}\sum_{g_1g_2} v^{(2)}_{g;g_1g_2}\psi_{g_1}\psi_{g_2}. \tag{3.11}$$

We next turn to a calculation of the analogues of the unlinked diagrams in a perturbation expansion. These arise from the $-N\varepsilon_0|\psi\rangle$ terms in equation (2.18) and from the effects (1b) and (2b) of V in destroying clusters.

3.3. Unlinked terms

The next part of our calculation involves seeing how V destroys clusters. The basic problem involves counting how many ways V can destroy one or two clusters in the general mth-order disconnected state $|\boldsymbol{G}\rangle$. This, in turn, requires a counting which is equivalent to the construction of the usual lattice constants in perturbation theory,

namely figuring out how many times a given graph g may be inserted into a state $|(\boldsymbol{G}/g_\mu)\rangle$ without overlapping clusters already present.

Consider the effect (1b), in particular the destruction of a cluster by the part of the potential energy which has its two operators separated by a displacement $\boldsymbol{R}$. The resulting expression for effect (1b) is

$$V_R|\boldsymbol{G}\rangle = \sum_g v_{0g}(\boldsymbol{R}) \sum_r \frac{\partial}{\partial A_g^+(\boldsymbol{r})} |\boldsymbol{G}\rangle + \ldots \tag{3.12}$$

with

$$|\boldsymbol{G}\rangle = \sum_{r_1 \ldots r_m}{}' A_{g_1}^+(\boldsymbol{r}_1) A_{g_2}^+(\boldsymbol{r}_2) \ldots A_{g_m}^+(\boldsymbol{r}_m)|\,\rangle. \tag{3.13}$$

Our basic problem is to count how many times A_g^+, a creation operator for a second-order (two-point) cluster with the points separated by a displacement $\boldsymbol{R}$, can appear in the summation (3.13). We focus upon the case in which the first cluster, g_1, is destroyed. Our counting problem, which is equivalent to the calculation of lattice constants in the usual perturbation theory, is to find out how many times a bond with displacement $\boldsymbol{R}$ can be added to the state $|(\boldsymbol{G}/g_1)\rangle$ without overlapping any of the original clusters $g_2, g_3, \ldots, g_m$.

The total count is N, the number of lattice sites, minus the number of overlaps, N_0. The latter can be computed as the sum of the number of times the bond can overlap a cluster g_μ ($\mu = 2, 3, \ldots, m$), minus a term which accounts for the overcounting of the case in which the bond overlaps two pre-existing clusters which happen to be close together. Thus we write equation (3.12) as

$$V_R|\boldsymbol{G}\rangle = \sum_\mu v_{0,g_\mu}(\boldsymbol{R})\Big(N - \sum_{\nu \neq \mu} n_{g_\nu}(\boldsymbol{R})\Big)|\boldsymbol{G}/g_\mu\rangle + \sum_\mu \sum_{\lambda<\nu} v_{0,g_\mu}(\boldsymbol{R}) m^{(2)}_{\lambda,\nu}(\boldsymbol{G}/g_\mu) + \ldots . \tag{3.14}$$

Here $n_{g_\nu}(\boldsymbol{R})$ counts the number of times a bond of length $\boldsymbol{R}$ may overlap a cluster g_ν. The last term in equation (3.14) describes the effect of the correction required when the bond touches both the cluster g_λ and the cluster g_ν. In this term λ and ν are required to be different from μ.

To describe the second term in equation (3.14), consider the case in which clusters g_2 and g_3 lie at some specified relative position close together so that they may together be viewed as the new cluster g. Let $n_{g;g_2g_3}(\boldsymbol{R})$ count the number of times that, for fixed positions of g_2, g_3 and the bond can be placed so that the combined cluster $(g_2 + g_3)$ is g and also the bond touches both g_2 and g_3. Then the second term of equation (3.14) is given by

$$m^{(2)}_{\lambda,\nu}(\boldsymbol{G}/g_\mu) = \sum_g n_{g;g_\lambda g_\nu}(\boldsymbol{R})|(\boldsymbol{G}/g_\mu g_\lambda g_\nu), g\rangle. \tag{3.15}$$

An exactly similar argument evaluates effect (2b), giving

$$V_R|\boldsymbol{G}\rangle = \sum_{\mu<\nu} v_{0,g_\mu g_\nu}(\boldsymbol{R})\Big(N - \sum_{\lambda \neq \mu,\nu} n_{g_\lambda}(\boldsymbol{R})\Big)|(\boldsymbol{G}/g_\mu g_\nu)\rangle + \sum_{\mu<\upsilon} v_{0;g_\mu g_\nu}(\boldsymbol{R}) \sum_{\lambda<\eta} m^{(2)}_{\lambda,\eta}(\boldsymbol{G}/g_\mu g_\nu). \tag{3.16}$$

In the second sum, λ and η are required to be different from μ and ν. The net result for evaluating the effects of the potential in destroying clusters can then be written down. This part of $V|\psi\rangle$ is combined with the term $(-N\varepsilon_0)|\psi\rangle$ which appears in equation

(2.18). We thus wish to calculate contributions (1b) and (2b) in

$$\left(\sum_{\boldsymbol{R}} V_R - N\varepsilon_0\right)|\psi\rangle = \sum_g v_g^{\mathrm{U}} \frac{\partial}{\partial \psi_g}|\psi\rangle. \tag{3.17}$$

The first point of our calculation is to notice that the terms linear in N cancel out of the left-hand side of equation (3.17). The linear terms in N in equations (3.14) and (3.16) exactly cancel $N\varepsilon_0$ as defined by equations (2.23) and (2.24). After that cancellation is achieved, the remainder of the left-hand side of equation (3.17) is N-independent and can be written in the form indicated on the right-hand side of equation (3.17), with

$$v_g^{\mathrm{U}} = \sum_{\boldsymbol{R}} \left(-n_g(\boldsymbol{R})\psi_g + \tfrac{1}{2} \sum_{g_1 g_2} n_{g;g_1 g_2}(\boldsymbol{R})\psi_{g_1}\psi_{g_2} \right) \varepsilon_0(\boldsymbol{R}), \tag{3.18}$$

where $\varepsilon_0(\boldsymbol{R})$ is given by equation (2.24).

This completes our derivation of the nonlinear Schrödinger equation, which is the statement $W_g = 0$, with W_g being given by equations (3.10), (3.11), (3.18) and (2.23). When all this is added up, we have the final result of this section,

$$\begin{aligned} W_g = {} & t(g)\psi_g + v_{g0} + \sum_{g'} v_{g;g'}\psi_{g'} - \sum_{g_1' g_2 g_1} v_{g_1';g_1} n(g; g_1' g_2; g_1)\psi_{g_1}\psi_{g_2} \\ & + \tfrac{1}{2} \sum_{g_1 g_2} v^{(2)}_{g;g_1 g_2}\psi_{g_1}\psi_{g_2} + \sum_{\boldsymbol{R}} \left(-n_g(\boldsymbol{R})\psi_g + \tfrac{1}{2} \sum_{g_1 g_2} n_{g;g_1 g_2}(\boldsymbol{R})\psi_{g_1}\psi_{g_2} \right) \\ & \times \left(\sum_{g'} v_{0g'}(\boldsymbol{R})\psi_{g'} + \tfrac{1}{2} \sum_{g' g''} v_{0g'g''}(\boldsymbol{R})\psi_{g'}\psi_{g''} \right). \end{aligned} \tag{3.19}$$

4. Variational calculation

Let us assume that we have a rather good solution to the Schrödinger equation, i.e. a set of approximate values of the wavefunction ψ_g. Call these approximate values χ_g. Given this wavefunction, which for example might be accurate to some order M in a perturbation expansion in V, how do we get the best estimate for the energy eigenvalue? The classical answer to this question is to form

$$U = \langle\chi|T + V|\chi\rangle / \langle\chi|\chi\rangle. \tag{4.1}$$

If the error in $|\chi\rangle$ is of order $M+1$, U is an estimate of the energy which automatically has its error of order $2M+2$. Furthermore, if $|\chi\rangle = |\psi\rangle$, the right wavefunction, expression (4.1) is automatically stationary with respect to variations in the wavefunction. Finally, the estimate (4.1) automatically forms an upper bound on the correct ground state energy.

Now let us apply equation (4.1) to our form of the wavefunction, namely

$$|\chi\rangle = |\ \rangle + \sum_g \chi_g |g\rangle + \tfrac{1}{2} \sum_{g_1 g_2} \chi_{g_1}\chi_{g_2}|g_1, g_2\rangle + \ldots. \tag{4.2}$$

The error is not in the form of the solution (equation (4.2) has the same structure as equations (2.15) and (2.16)) but in the numerical value of χ_g. Form $U/N = \varepsilon_a$, our approximation to the ground state energy, and rewrite equation (4.1) in the form

$$\varepsilon_a = U/N = \langle\chi|T + V - N\varepsilon_a^0|\chi\rangle / N\langle\chi|\chi\rangle + \varepsilon_a^0. \tag{4.3}$$

Choose ε_a^0 to be the approximation to the ground state energy given by equation (2.24), i.e.

$$\varepsilon_a^0 = \sum_g v_{0g}\chi_g + \tfrac{1}{2}\sum_{g_1 g_2} v_{0;g_1 g_2}\chi_{g_1}\chi_{g_2}. \tag{4.4}$$

Equation (4.4) gives ε_a, which is likely to be a better approximation to the true ground state energy. It is larger than the true answer but by an amount which is proportional to $(\psi_g - \chi_g)^2$.

From equation (2.18) we can evaluate the right-hand side of equation (4.4) and obtain

$$\varepsilon_a = \varepsilon_a^0 + \langle\chi|\sum_g W_g[\chi]\,\partial/\partial\chi_g|\chi\rangle/N\langle\chi|\chi\rangle \tag{4.5a}$$

where the functional $W_g[\chi]$ is defined by equation (3.19). An adjoint version of the same argument gives the adjoint result

$$\varepsilon_a = \varepsilon_a^0 + \Big(\sum_g W_g[\chi]\partial/\partial\chi_g\langle\chi|\Big)|\chi\rangle/N\langle\chi|\chi\rangle. \tag{4.5b}$$

We average these two results and find a final useful form of the variational principle:

$$\varepsilon_a[\chi] = \varepsilon_a^0[\chi] + \frac{1}{2N}\sum_g W_g[\chi]\frac{\partial}{\partial\chi_g}\ln\langle\chi|\chi\rangle. \tag{4.6}$$

The N-dependence in equation (4.6) is only apparent since

$$D[\chi] = (1/N)\ln\langle\chi|\chi\rangle \tag{4.7}$$

is independent of N for large systems, and $|\chi\rangle$ of the form (4.2). Nonetheless this apparent N-dependence is bothersome since the evaluation of $D[\chi]$ is in essence a linked cluster expansion in which a whole variety of lattice constants must be calculated.

5. The Ising model

In this section, the ground state energy of the one-dimensional Ising model in a transverse magnetic field is obtained perturbatively, using the nonlinear Schrödinger equation given in § 3. This model corresponds to the time continuum formulation of the two-dimensional Ising model (Kogut and Susskind 1975, Fradkin and Susskind 1978). The ground state energy of the one-dimensional Hamiltonian corresponds to the free energy of the two-dimensional Ising model. This ground state energy has been obtained exactly by Pfeuty (1970).

The Hamiltonian is

$$H = T - \lambda V, \tag{5.1}$$

where

$$T = \sum_{n=1}^{N}[1-\sigma_3(n)] \tag{5.2}$$

and

$$V = \sum_{n=1}^{N}\sigma_1(n)\sigma_1(n+1). \tag{5.3}$$

Here $\sigma_1(n)$ and $\sigma_3(n)$ are the usual Pauli spin matrices acting on the spin vector at the site labelled by the index n. Periodic boundary conditions are imposed, so the spin at the $(N+1)$ site is the same as that at the first site. This makes the ground state translationally invariant.

The ground state of T, $|\ \rangle$, consists of spins at all the sites pointing up. The action of V is to flip the spins at two adjacent lattice sites. Only one excitation is allowed at each site, namely the spin is down. The nonlinear Schrödinger equation (3.19) may be written in this case as

$$-t(g)\psi_g = v_{g0} + \sum_{g'} v_{g;g'}\psi_{g'} + \sum_{g_1 \leqslant g_2} v^{(2)}_{g;g_1g_2}\psi_{g_1}\psi_{g_2} - n_g\varepsilon_0\psi_g$$
$$+\varepsilon_0 \sum_{g_1 \leqslant g_2} n_{g;g_1g_2}\psi_{g_1}\psi_{g_2} - \sum_{g_1 g_1' g_2} v_{g_1';g_1} n(g; g_1' g_2; g_1)\psi_{g_1}\psi_{g_2}. \tag{5.4}$$

The graphs consist of the spins pointing up at almost all sites except for some spins pointing down. For example, we have a graph like $g = (11011)$, where 1 means the spin at the site is down and 0 means the spin is up. In this example, four spins are down and the spin in the middle of the graph is up.

Let us explain each term in equation (5.4) in detail. On the left-hand side $t(g)$ is the kinetic energy of the graph g. Each down spin contributes to the kinetic energy by the amount two, so

$$t(g) = 2 \times (\text{number of down spins in } g). \tag{5.5}$$

The first term on the right-hand side is the matrix element of the potential between the ground state of T and the state $|g\rangle$. Therefore this term contributes only to the state $g = (11)$. In the second term, $v_{g;g'}$ is non-zero only when a state g is made from a state g' by the action of V. An example is $v_{(101);(11)} = -\lambda$. Special care must be taken in some cases. For example, $v_{(1111);(11)} = 0$ even though the action of V can make the state (1111) from the state (11). This is due to the subtraction term on the right-hand side of equation (3.6). This equation implies that the new state g has to be made by the action of V which affects at least one site of the original state g'. Then it is easy to see that $v_{g;g'}$ is not symmetric, for example, $v_{(11);(1111)} = -\lambda$ while $v_{(1111);(11)} = 0$. The third term comes from the effect of V which connects two graphs g_1 and g_2 and makes the connected graph g. Then, for example, $v^{(2)}_{(1001);(11)(11)} = -\lambda$. The fourth term is the effect of the exclusion of the graph (11) from the graph g when the graph (11) is annihilated. Then the coefficient n_g is the number of overlaps between graphs (11) and g. For example, $n_{(11011)} = 6$. The fifth term is the correction to the fourth term when the two graphs g_1 and g_2 are close enough so that they can be connected by the action of V. Therefore $n_{g;g_1g_2}$ is non-zero only when the graph g is decomposed into two graphs g_1 and g_2 and also they could be connected by the action of V. In particular, $n_{(1111);(11)(11)} = 1$ while $n_{(11011);(11)(11)} = 0$ because in the latter case two graphs (11) are not close enough. The last term arises when the action of V on g_1 makes the graph g_1' whose size is smaller than the original graph g_1. After the action of V on g_1, some configurations of g_1' and other graphs, say g_2, do not occur when the graph g_2 is very close to g_1' so that g_2 overlaps with the old graph g_1. A subtraction term is needed because of this effect, and eventually two graphs g_1' and g_2 are regarded as one connected graph g because spatial relations between the two graphs are specified.

The coefficient $n(g; g_1'g_2; g_1)$ is non-zero and one only when the graph g is decomposed into the graphs g_1' and g_2 and the graph g_1 overlaps with the graph g_2. An

Table 1. List of terms which are required to calculate the ground state energy of the Ising model up to eighth order in the perturbation.

$\psi_{\mathbf{g}}$	$t_{\mathbf{g}}$	$v_{\mathbf{g}_0}$	$\sum_{\mathbf{g}'} v_{\mathbf{g};\mathbf{g}'}\psi_{\mathbf{g}'}$	$\sum_{\mathbf{g}_1\le\mathbf{g}_2} v^{(2)}_{\mathbf{g}:\mathbf{g}_1\mathbf{g}_2}\psi_{\mathbf{g}_1}\psi_{\mathbf{g}_2}$	$-n_{\mathbf{g}}\varepsilon_0\psi_{\mathbf{g}}$	$\varepsilon_0\sum_{\mathbf{g}_1\mathbf{g}_2} n_{\mathbf{g}:\mathbf{g}_1\mathbf{g}_2}\psi_{\mathbf{g}_1}\psi_{\mathbf{g}_2}$	$-\sum_{\mathbf{g}_1\mathbf{g}_1\mathbf{g}_2} v_{\mathbf{g}_1:\mathbf{g}_1} n(\mathbf{g};\mathbf{g}_1'\mathbf{g}_2;\mathbf{g}_1)\psi_{\mathbf{g}_1}\psi_{\mathbf{g}_2}$
$\psi_{(11)}$	4	$-\lambda$	$-\lambda(2\psi_{(101)}+2\psi_{(1111)}+2\psi_{(11011)})$	0	$-3\varepsilon_0\psi_{(11)}$	0	0
$\psi_{(101)}$	4	0	$-\lambda(2\psi_{(11)}+2\psi_{(1001)}+\psi_{(11101)}+\psi_{(10111)})$	0	$-4\varepsilon_0\psi_{(101)}$	0	0
$\psi_{(1001)}$	4	0	$-\lambda(2\psi_{(101)}+2\psi_{(10001)})+\psi_{(1111)}$	$-\lambda\psi_{(11)}\psi_{(11)}$	$-5\varepsilon_0\psi_{(1001)}$	0	0
$\psi_{(1111)}$	8	0	$-\lambda(\psi_{(1001)}+\psi_{(11101)}+\psi_{(10111)})$	0	$-5\varepsilon_0\psi_{(1111)}$	$\varepsilon_0\psi_{(11)}\psi_{(11)}$	$-(-\lambda)(2\psi_{(101)}\psi_{(11)}+2\psi_{(111111)}+2\psi_{(11011)}\psi_{(11)})$
$\psi_{(10001)}$	4	0	$-\lambda(2\psi_{(1001)}+\psi_{(11101)}+\psi_{(10111)})$	$-2\lambda\psi_{(11)}\psi_{(101)}$	$-6\varepsilon_0\psi_{(10001)}$	0	0
$\psi_{(11101)}=\psi_{(10111)}$	8	0	$-\lambda(\psi_{(1111)}+\psi_{(10001)}+\psi_{(11011)})$	0	$-6\varepsilon_0\psi_{(11101)}$	$\varepsilon_0\psi_{(11)}\psi_{(101)}$	$-(-\lambda)(\psi_{(11)}\psi_{(1001)}+\psi_{(11)}\psi_{(1110)}+\psi_{(101)}\psi_{(101)}+\psi_{(1111)}\psi_{(101)}+\psi_{(11011)}\psi_{(101)})$
$\psi_{(11011)}$	8	0	$-\lambda(\psi_{(11101)}+\psi_{(10111)})$	0	$-6\varepsilon_0\psi_{(11011)}$	0	$-(-\lambda)(2\psi_{(1111)}\psi_{(11)}+2\psi_{(11011)}\psi_{(11)})$

example for the non-vanishing of this coefficient is $g_1 = (1111)$, $g_1' = (11)$, $g_2 = (11)$ and $g = (11011)$. In this example, V acts on two adjacent sites on the right (left) side of the graph $g_1 = (1111)$ and makes graph $g_1' = (11)$. The graph $g_2 = (11)$ sits right (left) next to the graph $g_1' = (11)$ but with one site in between, and g_2 and g_1' are regarded as the connected graph $g_0 = (11011)$. The graph g_2 overlaps with the graph g.

In table 1, all the terms in equation (5.4) which are required to calculate the ground state energy up to eighth order in the perturbation theory are listed. Graphs whose lengths are larger than five do not contribute to the calculation and are omitted in the table. In general, graphs whose number of sites is less than $N+1$ are needed to calculate the ground state energy up to $2N$th order.

Now that we have understood every rule in the nonlinear Schrödinger equation (5.4), the wavefunctions ψ_g and the ground state energy can be obtained in the power of λ. If we write ψ_g as

$$\psi_g = \lambda\psi_g^{(1)} + \lambda^2\psi_g^{(2)} + \ldots, \tag{5.6}$$

the wavefunction $\psi_g^{(n)}$ is obtained using equation (5.4) from the lower-order wavefunctions $\psi_{g'}^{(1)}$, $\psi_{g''}^{(2)}$ ... and $\psi_{g'''}^{(n-1)}$ because on the right-hand side v's are $(-\lambda)$ or zero and ε_0 starts from the second order in λ.

From equation (2.20) the ground state energy per site is given by

$$\varepsilon_0 = \sum_g v_{0g}\psi_g = -\lambda\psi_{(11)}. \tag{5.7}$$

If we write ε_0 as

$$\varepsilon_0 = \lambda\varepsilon_0^{(1)} + \lambda^2\varepsilon_0^{(2)} + \ldots, \tag{5.8}$$

then

$$\varepsilon_0^{(n)} = -\psi_{(11)}^{(n-1)}. \tag{5.9}$$

The wavefunctions needed to calculate up to the eighth-order ground state energy are given in table 2 together with the ground state energy. The ground state energy has only even powers of λ, and the values coincide with the exact results of Pfeuty.

Table 2. The ground state energy per site in powers of λ and wavefunctions for the Ising model calculated from the nonlinear Schrödinger equation (5.4). Here $\varepsilon_0^{(n)}$ is the nth-order contribution to the ground state energy and $\psi_g^{(n)}$ is the nth-order contribution to the wavefunction of the type g.

$-\varepsilon_0^{(2)} = \psi_{(11)}^{(1)} = 1/2^2$	$\psi_{(101)}^{(2)} = 1/2^3$	
$-\varepsilon_0^{(4)} = \psi_{(11)}^{(3)} = 1/2^6$	$\psi_{(1001)}^{(3)} = 5/2^6$	
$\psi_{(101)}^{(4)} = 1/2^6$	$\psi_{(1111)}^{(4)} = 1/2^8$	$\psi_{(10001)}^{(4)} = 7/2^7$
$-\varepsilon_0^{(6)} = \psi_{(11)}^{(5)} = 1/2^8$		
$\psi_{(1001)}^{(5)} = 7/2^9$	$\psi_{(10111)}^{(5)} = \psi_{(11101)}^{(5)} = 1/2^8$	
$\psi_{(101)}^{(6)} = 5/2^{10}$	$\psi_{(1111)}^{(6)} = 3/2^{12}$	$\psi_{(11011)}^{(6)} = 3/2^{12}$
$-\varepsilon_0^{(8)} = \psi_{(11)}^{(7)} = 25/2^{14}$		

Acknowledgments

We have had useful discussions with Steven Shenker, Robert Pearson and Leo Marland. Marland very helpfully reported to us the parallel and independent work being conducted by himself and B Nickel. Pearson pointed out an error in our early calculations and gave us Potts model data for checking our algorithm.

References

Fradkin E and Susskind L 1978 *Phys. Rev.* D **17** 2637
Hamer C J, Kogut J B and Susskind L 1979 *Phys. Rev.* D **19** 3091
Kogut J B and Susskind L 1975 *Phys. Rev.* D **11** 395
Pfeuty P 1970 *Ann. Phys., NY* **57** 79