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Citation: The Journal of Chemical Physics **79**, 969 (1983); doi: 10.1063/1.445876
View online: http://dx.doi.org/10.1063/1.445876
View Table of Contents: http://scitation.aip.org/content/aip/journal/jcp/79/2?ver=pdfcov
Published by the AIP Publishing

A new type of cluster expansion and time-dependent adiabatic perturbation theory on finite and infinite lattices[a)]

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(Received 22 November 1982; accepted 8 April 1983)

A new type of cluster expansion is proposed, which is used to calculate the properties of the lower part of the spectrum of a general lattice Hamiltonian. The method does not involve power series in the number of lattice sites. Surface effects are easily incorporated into the theory in a natural way. Application to the 1-d Ising model in a transverse magnetic field demonstrates that good results can be obtained with moderate computational effort.

I. INTRODUCTION

The Hamiltonians of many models in chemical physics can be classified as lattice Hamiltonians. These Hamiltonians consist of a sum of commuting one-particle operators associated with the points of a lattice, and a term which accounts for the interactions between the lattice sites. As examples we mention lattice dynamics Hamiltonians describing the motion of atoms or molecules in a crystal, Ising and Heisenberg Hamiltonians describing magnetic phenomena in crystals, and PPP Hamiltonians[1] describing electronic motion in planar unsaturated molecules. In the last example the lattice is usually finite and not translationally invariant. Apart from being the generators of time evolution, as in the examples above, lattice Hamiltonians sometimes provide a means to calculate partition functions in statistical physics. In fact the partition functions of several classical d-dimensional spin models can be calculated as the ground state energies of appropriate $(d-1)$-dimensional lattice Hamiltonians.[2] Outside the realm of traditional physics, lattice Hamiltonians are, for example, studied in lattice gauge theories.[2]

Several methods have been used to study the lower part of the spectrum of lattice Hamiltonians. Of these, Green's function methods[1,3,4] have been used extensively. In most cases the Green's functions are calculated within the random phase approximation, and it is difficult to go beyond this approximation. Among the methods that concentrate directly on the Hamiltonian are renormalization methods[5–7] and perturbation methods. A serious drawback of the former is the difficulty to estimate the importance of the approximations made in the actual calculations. Provided the calculations can be carried through high enough orders, perturbation theories do not have this drawback and therefore are of great value in the study of lattice Hamiltonians.

Most often, the sum of one-particle operators is taken as the unperturbed Hamiltonian, and the interaction term as the perturbation. The eigenfunctions of the unperturbed Hamiltonian then serve as a basis in the Hilbert space of the lattice. One way to proceed is to do Rayleigh–Schrödinger perturbation theory.[2,8,9] In the end this leads to a combinatorial problem on the lattice, and for all quantities of interest to a power series in N, the number of lattice points. If, on a lattice with periodic boundary conditions, the combinatorics is done well, all terms cancel in the right way, i.e., extensive quantities are proportional to N and intensive quantities are independent of N. According to a second approach[10] it can be argued that the exact ground state of a lattice with periodic boundary conditions, when expanded in the unperturbed basis, depends on a set of coefficients $\{\psi_g\}$, each of which is associated with a connected graph on the lattice and a set of excitations on the vertices of this graph. The coefficients satisfy a set of complicated nonlinear equations which can be solved perturbatively. A nice feature of this method is that any power series in N is avoided.

The Raleigh–Schrödinger version has been successfully applied to several very simple lattice Hamiltonians. If the complexity of the Hamiltonian is increased, however, the combinatorial part of the method will become extremely difficult. The method of Kadanoff and Kohmoto provides no satisfactory alternative because it is restricted to the ground state; a disadvantage of this method, moreover, is that it is based on an explicit calculation of the ground state wave function. We therefore develop a third formulation of perturbation theory for lattice Hamiltonians, which, we may expect, will prove to be superior to both of these methods. In order to arrive at the final formulas we develop a cluster expansion of the ground state energy in which successive corrections to the unperturbed energy are associated with an increasing sequence of clusters on the lattice. On the basis of this expansion we then calculate several other properties of the model, like ground state averages and excited state energies. Our cluster expansion differs from the usual one in lattice statistics[2,11] in that all combinatorial calculations are performed on finite clusters. This fact will eventually make our method simpler than the Rayleigh–Schrödinger method of Kogut *et al.* An additional property of our method is that it can easily be applied to finite systems, which, moreover, need not to be translationally invariant. This makes it possible, for example, to study the influence of the geometry of the boundary on the bulk properties of the model.

[a)] Supported by the Netherlands Foundation for Chemical Research (SON) with financial aid from the Netherlands Organization for the Advancement of Pure Research (ZWO).

 0021-9606/83/140969-07$02.10

The starting point of our formulation is the Gell-Mann–Low or adiabatic theorem.[12,13] In Secs. II and III we briefly review this theorem and set our notation. In Sec. IV we derive our main results. In order to test the premisses of the adiabatic theorem, which has not been used in the present context before, and in order to get an idea of the amount of work involved in the application of our method, we calculate in Sec. V several properties of a model Hamiltonian for which exact results are available.

II. THE ADIABATIC THEOREM

Consider a system whose dynamics is governed by the Hamiltonian

$$H = H_0 + \Phi \ . \tag{2.1}$$

Suppose at $t = -\infty$ the system is in a nondegenerate eigenstate $|\Psi_0\rangle$ of the unperturbed Hamiltonian H_0 with eigenvalue E^0, i.e.,

$$H_0|\Psi_0\rangle = E^0|\Psi_0\rangle \ . \tag{2.2}$$

Next adiabatically switch on the interaction Φ, which means add a time dependent part

$$H_\alpha(t) = e^{-\alpha|t|}\Phi, \quad \alpha > 0 \tag{2.3}$$

to the unperturbed Hamiltonian and let the state $|\Psi_0\rangle$ evolve under the full Hamiltonian $H_0 + H_\alpha(t)$. The adiabatic theorem then states that at $t = 0$ the system will have evolved into an eigenstate of H. In more exact terms, Gell-Mann and Low have proved[12,13] that

$$|\Psi\rangle = \lim_{\alpha \to 0} \frac{U_\alpha^0 |\Psi_0\rangle}{\langle \Psi_0 | U_\alpha^0 | \Psi_0 \rangle} \tag{2.4}$$

is an eigenstate of H provided it exists to all orders in perturbation theory. Here U_α^t is the evolution operator given by

$$U_\alpha^t = 1 + \sum_{n=1} (-i)^n \int_{-\infty}^{t} dt_n \int_{-\infty}^{t_n} dt_{n-1} \cdots \int_{-\infty}^{t_2} dt_1 \, \Phi_\alpha^{t_n} \Phi_\alpha^{t_{n-1}} \cdots \Phi_\alpha^{t_1} \ , \tag{2.5}$$

where

$$\Phi_\alpha^t = e^{-\alpha|t|} e^{iH_0 t} \Phi e^{-iH_0 t} \ . \tag{2.6}$$

The normalization of $|\Psi\rangle$ is such that $\langle \Psi_0 | \Psi \rangle = 1$. It is well known[14,15] in the case of many-boson or many-fermion systems that this normalization is necessary in order to avoid divergence problems in the phase of $|\Psi\rangle$.

Denoting the eigenvalue of $|\Psi\rangle$ by E, i.e.,

$$H|\Psi\rangle = E|\Psi\rangle \ , \tag{2.7}$$

and making use of the special normalization of $|\Psi\rangle$, we find the energy difference

$$\Delta E = E - E^0 = \langle \Psi_0 | \Phi | \Psi \rangle \ . \tag{2.8}$$

If we just interchange the limit process and the process of taking the inner product we easily derive from Eqs. (2.4), (2.5), and (2.8),

$$\Delta E = \lim_{\alpha \to 0} i \frac{\partial}{\partial t} \ln \langle \Psi_0 | U_\alpha^t | \Psi_0 \rangle |_{t=0} \ . \tag{2.9}$$

In fact this equation can rigorously be shown[12,13,15] to hold true.

Once we have Eq. (2.9) it is simple to derive an expression for the expectation value of a general operator $\hat{O}$ in the state $|\Psi\rangle$.[15] In order to do this we introduce the Hamiltonian

$$H(y) = H + y\hat{O} = H_0 + \Phi + y\hat{O} \tag{2.10}$$

with corresponding eigenvalue problem

$$H(y)|\Psi(y)\rangle = E(y)|\Psi(y)\rangle \ . \tag{2.11}$$

From $\langle \Psi | \hat{O} | \Psi(y) \rangle = \{\langle \Psi | H(y) - H | \Psi(y) \rangle\} y^{-1}$ we then find

$$\frac{\langle \Psi | \hat{O} | \Psi(y) \rangle}{\langle \Psi | \Psi(y) \rangle} = \frac{E(y) - E}{y} \ . \tag{2.12}$$

If we let $y \to 0$ in Eq. (2.12) we find the desired expression. This means that we only need to calculate $E(y) - E$ to the first order in y and then take the coefficient of y.

In the following sections we shall calculate, among other things, the ground state properties of a general lattice Hamiltonian from Eqs. (2.9) and (2.12) by assuming that the state $|0\rangle$ which evolves into the ground state of H will also be the ground state of H_0. In the example given in Sec. V this appears to be true although there is no general proof of this. Clearly this remark applies to any perturbation theory.

III. THE LATTICE HAMILTONIAN

In Sec. IV we derive expressions for the properties of models whose Hamiltonian can be written as

$$H(\Lambda) = \sum_{\mathbf{i}} L(\mathbf{i}) + \sum_{\mathbf{r}} \lambda_{\mathbf{r}} \sum_{\mathbf{i}} \Phi_{\mathbf{r}}(\mathbf{i}, \mathbf{i}+\mathbf{r}) = H_0 + \Phi(\Lambda), \tag{3.1}$$

where $\mathbf{i}$ runs over the N points of a d-dimensional lattice. Except when indicated otherwise we impose periodic boundary conditions on the lattice. The Hamiltonian is assumed to act in a space $D^N = \otimes_{\mathbf{i}} D_{\mathbf{i}}$ where, for each lattice point $\mathbf{i}$, $D_{\mathbf{i}}$ is a copy of a Hilbert space D. The one-particle operator $L(\mathbf{i})$ is defined as $L(\mathbf{i}) = 1 \otimes \cdots \otimes L \otimes \cdots \otimes 1$, where L is in the $\mathbf{i}$th place; we express this by saying that $L(\mathbf{i})$ acts only in the space $D_{\mathbf{i}}$. Similarly for each $\mathbf{r}$, the interaction operator $\Phi_{\mathbf{r}}(\mathbf{i}, \mathbf{i}+\mathbf{r})$ acts only in the spaces $D_{\mathbf{i}}$ and $D_{\mathbf{i}+\mathbf{r}}$. In many cases the interaction can be written as

$$\Phi_{\mathbf{r}}(\mathbf{i}, \mathbf{i}+\mathbf{r}) = \sum_{\mu\nu} K_{\mathbf{r}}^{\mu\nu} \phi_\mu(\mathbf{i}) \phi_\nu(\mathbf{i}+\mathbf{r}) \ . \tag{3.2}$$

Here again $\phi_\mu(\mathbf{i})$ acts only in $D_{\mathbf{i}}$. The coefficient $\lambda_{\mathbf{r}}$ determines the strength of the interaction. In the case of a Hamiltonian with only nearest-neighbor interactions $\lambda_{\mathbf{r}}$ differs from zero only when $\mathbf{r}$ equals one of the d primitive translation vectors.

We denote the ground state of the noninteracting Hamiltonian $H_0 = \sum L(\mathbf{i})$ by

$$|0\rangle = \otimes_{\mathbf{i}} |0)_{\mathbf{i}} \ , \tag{3.3}$$

where $|0)$ denotes the ground state of L in the space D and is assumed to be normalized to unity. The translationally invariant first excited state of H_0 can be written as

$$|1\rangle = \frac{1}{\sqrt{N}} \sum_i \psi^\dagger(i)|0\rangle , \tag{3.4}$$

where $\psi^\dagger$ raises the ground state $|0\rangle$ to the first excited state $|1\rangle$, which is also assumed to be normalized to unity.

IV. CLUSTER EXPANSIONS

We next develop a method to calculate the ground state and first excited state properties of the Hamiltonian (3.1). Although our method applies equally well to finite systems we shall restrict ourselves in the first three subsections to infinite systems. This means that we let $N \to \infty$ keeping Ω/N fixed, where Ω denotes the volume of the system. In what follows it becomes clear that this is equivalent to the use of periodic boundary conditions. In subsection D we describe the changes to be made in the case of a finite system.

In subsection B we derive an expression for the ground state energy per particle $\Delta\epsilon = \Delta E_0/N$, where ΔE_0 is given by Eq. (2.9) with $|\Psi_0\rangle = |0\rangle$. Other ground state properties can be calculated from Eq. (2.12). In subsection C we derive, for a certain condition, an expression for the difference between the energy of the excited state and the energy of the ground state $\omega = E_1 - E_0 = \Delta E_1 - \Delta E_0 + E_1^0 - E_0^0$. Before doing so, we derive in subsection A a useful property of the evolution operator on a lattice.

A. The evolution operator on a lattice

In order to derive the desired property we write the evolution operator as

$$U^t = 1 + \sum_{n=1}^{\infty} U_n^t , \tag{4.1}$$

where

$$U_n^t = \frac{(-i)^n}{n!} \int_{-\infty}^{t} dt_n \cdots \int_{-\infty}^{t} dt_1 T\Phi^{t_n}(\Lambda)\cdots\Phi^{t_1}(\Lambda) . \tag{4.2}$$

We have suppressed the subscript α and we shall continue to do so in the rest of this paper. T is the time ordering operator, which places the factors in the product to the right of it in the order of decreasing t_i from left to right. After introducing $\Phi(\Lambda)$ from Eq. (3.1) and expanding the product we find that we can write the evolution operator as

$$U^t = 1 + \sum_{m=1}^{\infty} {\sum_{A_1\cdots A_m}}' V^t(A_1 \cdots A_m) . \tag{4.3}$$

Here A_1 to A_m run through all connected clusters that can be chosen from the lattice. The prime has been added to the summation sign to indicate that the clusters must be chosen such that $A_i \cap A_j = \phi$ if $i \neq j$. $V^t(A_1\cdots A_m)$ is an operator acting only in the spaces D_i for which $i \in A_l$ for some $l = 1, 2, \ldots, m$; moreover $V^t(A_1\cdots A_m)$ is irreducible in the sense that it acts in all these spaces. It is convenient to write

$$V^t(A_1\cdots A_m) = \sum_{n=1} V_n^t(A_1\cdots A_m) , \tag{4.4}$$

where $V_n^t(A_1\cdots A_m)$ is the contribution of U_n^t to $V^t(A_1\cdots A_m)$. $V_n^t(A)$ for example is a sum of integrals over products of n interactions on A, such that each product is an irreducible operator on A. Different ordering of the interactions in the products leads to different terms; moreover repeated use of the same interaction is allowed. The same applies to $V_n^t(A_1\cdots A_m)$, but now we can collect all terms which do not differ in the relative order of the interactions on each cluster A_i separately; each of these collections consists of $n!/\Pi_{i=1}^m n_i!$ terms, where n_i is the number of interactions on A_i. Because operators on different clusters commute we see from Eq. (4.2) that all terms within one class give the same contribution. On summing over all classes we find

$$V_n^t(A_1\cdots A_m) = {\sum_{n_1\cdots n_m}}^{(n)} V_{n_1}^t(A_1)\cdots V_{n_m}^t(A_m) . \tag{4.5}$$

The superscript on the summation sign indicates that the n_i must satisfy $\sum_{i=1}^m n_i = n$. Inserting this into Eq. (4.4) we derive the desired property

$$V^t(A_1\cdots A_m) = V^t(A_1)\cdots V^t(A_m) . \tag{4.6}$$

The important point here is that the factors in the product on the right-hand side only depend on the clusters on which they are defined and not on m.

When considering a finite system, upper summation limits must be introduced into Eq. (4.3).

B. The ground state

We now calculate the ground state energy from Eq. (2.9) with $|\Psi_0\rangle = |0\rangle$. This means that we assume that the state which evolves adiabatically from the unperturbed ground state is the true ground state and that it exists to all orders in perturbation theory. In the next section we give an example for which these assumptions lead to the correct result.

According to the results of the last subsection we can write the expectation value of the evolution operator in the ground state as

$$\langle 0|U^t|0\rangle = 1 + \sum_{m=1}^{\infty} {\sum_{A_1\cdots A_m}}' \langle 0|V^t(A_1)|0\rangle\cdots\langle 0|V^t(A_m)|0\rangle . \tag{4.7}$$

This equation can be factorized by defining $X^t(A)$ for each A, such that

$$\langle 0|U^t|0\rangle = \prod_A [1 + X^t(A)] . \tag{4.8}$$

In fact this definition is made possible by the factorization property derived in the preceding subsection and already used in Eq. (4.7). For if we expand the product in Eq. (4.8) we see that the result can be written as Eq. (4.7) with

$$\langle 0|V^t(A)|0\rangle = \sum_{m=1}^{M(A)} {\sum_{B_1\cdots B_m}}^{(A)} X^t(B_1)\cdots X^t(B_m) . \tag{4.9}$$

The subscript on the summation sign indicates that the clusters B_i must be such that $\cup_{i=1}^m B_i = A$. $M(A)$ is the maximum number of clusters whose union is equal to A. Clearly $X^t(A) = \langle 0|V^t(A)|0\rangle$ for any cluster consisting of only two lattice points. The term with $m = 1$

in Eq. (4.9) simply is $X^t(A)$. All other $X^t(B_i)$ refer to subclusters B_i of A; if we assume that we already know these $X^t(B_i)$ we can solve for $X^t(A)$ from Eq. (4.9). Induction on the size of the clusters then proves that $X^t(A)$ is well defined for every cluster.

Next we notice that $\langle 0|V^t(A)|0\rangle$ is invariant under any translation of A. From the discussion following Eq. (4.9) we then conclude that the same must be true for $X^t(A)$. This means that for every A there are N clusters A_i, including $A_i = A$, for which $X^t(A_i) = X^t(A)$. Therefore we can write

$$\Delta\epsilon = \lim_{\alpha\to 0} i\frac{\partial}{\partial t}\sum_a \ln[1+X^t(a)]\big|_{t=0} . \tag{4.10}$$

Here a runs over all clusters that are not translationally equivalent.

Finally we derive a perturbation expansion for $\Delta\epsilon$. We say that $\langle 0|V_n^t(a)|0\rangle$ is of order n in perturbation theory or simply that it is of the nth order. Similarly we define

$$X^t(a) = \sum_{n=1}^{\infty} X_n^t(a) , \tag{4.11}$$

where $X_n^t(a)$ is of order n in perturbation theory. Equating terms of equal order left and right in Eq. (4.9) we see that $X_n^t(a)$ is well defined. Next we define the cumulants $\tilde{X}_n^t(a)$ by

$$X_n^t(a) = \sum_{\{n_l|n\}}\prod_l \frac{\{\tilde{X}_l^t(a)\}^{n_l}}{n_l!} , \tag{4.12}$$

where the summation runs over all partitions of n, i.e., over all sets $\{n_l\}$ for which $\Sigma_l l n_l = n$. If we introduce Eqs. (4.11) and (4.12) into Eq. (4.10) we easily derive

$$\Delta\epsilon = \sum_{n=1}^{\infty}\Delta\epsilon^{(n)} , \tag{4.13}$$

where

$$\Delta\epsilon^{(n)} = \lim_{\alpha\to 0} i\frac{\partial}{\partial t}\sum_a \tilde{X}_n^t(a)\big|_{t=0} . \tag{4.14}$$

For the convenience of the reader, we give the inversion formula[16] of Eq. (4.12):

$$\tilde{X}_n^t(a) = \sum_{\{n_i|n\}}(-1)^{\sigma(n_i)-1}[\sigma(n_i)-1]!\prod_i\frac{\{X_i(a)\}^{n_i}}{n_i!} , \tag{4.15}$$

where $\sigma(n_i) = \Sigma_i n_i$.

Let us now look at the effects of finiteness. For a finite system the summation in Eq. (4.10) ends when a is equal to the whole lattice L. The contribution of $X^t(L)$ is at least of order $\frac{1}{2}zN$ in λ, where z is the coordination number of the lattice.

C. The excited state

In this subsection we calculate the energy of the first excited translationally invariant state assuming that this state adiabatically evolves from the unperturbed state $|1\rangle$ given by Eq. (3.4).

The expectation value of U^t in the unperturbed state $|1\rangle$ is given by

$$\langle 1|U^t|1\rangle = \frac{1}{N}\sum_{ij}\langle 0|\psi(j)U^t\psi^\dagger(1)|0\rangle$$
$$= \sum_i\langle 0|\psi(0)U^t\psi^\dagger(1)|0\rangle , \tag{4.16}$$

where ψ is the adjoint of $\psi^\dagger$. The second equality results from use of the cyclic boundary conditions.

Because of the summation over i we cannot in general continue as we did in the preceding subsection. However, for a certain condition on $K_{\mathbf{r}}^{\mu\nu}$ in Eq. (3.2) we can. This condition is such that $\langle 0|\psi(0)V^t(A_1\cdots A_m)\psi^\dagger(1)|0\rangle$ may only be nonzero if i = 0 or if 0 and i belong to the same cluster A_l for some $l = 1, 2, \ldots, m$. We do not discuss this condition any further here, but only mention that it holds true for the Ising model in a transverse magnetic field. This model will be studied in the next section.

Now we make use again of Eqs. (4.3) and (4.6) and find:

$$\langle 1|U^t|1\rangle = 1 + \sum_{m=1}^{\infty}{\sum_{A_1\cdots A_m}}' \langle 0|W^t(A_1)|0\rangle\cdots\langle 0|W^t(A_m)|0\rangle, \tag{4.17}$$

where

$$W^t(A) = V^t(A) \quad \text{if } 0\notin A ,$$
$$W^t(A) = \sum_{i\in A}\psi(0)V^t(A)\psi^\dagger(1) \quad \text{if } 0\in A . \tag{4.18}$$

We factorize as in the preceding subsection by defining $Y^t(A)$ for each A such that

$$\langle 1|U^t|1\rangle = \prod_A[1+Y^t(A)] , \tag{4.19}$$

from which it follows that

$$\langle 0|W^t(A)|0\rangle = \sum_{m=1}^{M(A)}{\sum_{B_1\cdots B_m}}' Y^t(B_1)\cdots Y^t(B_m) . \tag{4.20}$$

By analogy with the discussion following Eq. (4.9) we derive that $Y^t(A) = X^t(A)$ if $0\notin A$. Using this we get as out final result

$$\omega = E_1^0 - E_0^0 + \lim_{\alpha\to 0} i\frac{\partial}{\partial t}\sum_{0\in A}\ln\frac{[1+Y^t(A)]}{[1+X^t(A)]}\Big|_{t=0} . \tag{4.21}$$

Here the sum is over all connected clusters for which $0\in A$.

Perturbation theory can be done in the same way as it was done in the preceding section. The result is

$$\omega = E_1^0 - E_0^0 + \sum_{n=1}^{\infty}\omega^{(n)} , \tag{4.22}$$

where

$$\omega^{(n)} = \lim_{\alpha\to 0} i\frac{\partial}{\partial t}\sum_{0\in A}\{\tilde{Y}_n^t(A) - \tilde{X}_n^t(A)\}\big|_{t=0} . \tag{4.23}$$

The definition of $\tilde{Y}_n^t(A)$ is analogous to that of $\tilde{X}_n^t(A)$.

D. Finite systems

In order to derive the correct ground state energy of a finite system we introduce a few definitions. We

embed the finite lattice L in an infinite lattice (of the same Bravais type) and call L^C the complement of L. The boundary of L will be denoted by ∂L and the number of boundary sites by $N_{\partial L}$. We construct a set T of "standard" clusters, which are all translationally inequivalent and which we generically denote by a. This set is chosen big enough to serve all our purposes. Of each standard cluster we mark one vertex. Any cluster of interest can then be obtained by a translation of some standard cluster a, and can be denoted by $a(\mathbf{i})$ where $\mathbf{i}$ is the position vector of the mark after the translation.

The ground state energy can be calculated from Eqs. (2.9), with $|\Psi_0\rangle = |0\rangle$, and (4.8). To the product on the right-hand side of Eq. (4.8) all clusters $a(\mathbf{i})$ contribute for which $a(\mathbf{i}) \subseteq L$. From the definition it follows that $X^t[a(\mathbf{i})] = X^t(a)$ for all $\mathbf{i} \in L$. Denoting by N_a the number of vectors $\mathbf{i}$ for which $a(\mathbf{i}) \subseteq L$, and defining $N_a^C = N - N_a$ we can write

$$N_{\partial L}\sigma = \Delta E_0 - N\Delta\epsilon = -\lim_{\alpha\to 0} i\frac{\partial}{\partial t}\sum_a N_a^C \ln[1+X^t(a)]\big|_{t=0} , \tag{4.24}$$

where $\Delta\epsilon$ is given by Eq. (4.10). It is clear that N_a^C is equal to the number of elements in the set $S_a = \{\mathbf{i} \in L \mid a(\mathbf{i}) \cap L^C \neq \phi\}$, and that it is independent of the labeling of the standard clusters. The same is true for example for a lattice on a cylinder. If we allow the diameter of the cylinder to become infinite we see that Eq. (4.24) also applies to a system which is infinite along one direction and finite along another direction. However, because the set S_a itself is not independent of the labeling of the standard clusters we must always be careful and investigate both boundaries in this case; N_a^C is not just twice the number of clusters which extend into L^C across one of the boundaries. Because of the same reason Eq. (4.24) is not well defined for half spaces.

Perturbation theory now leads to

$$\sigma = \sum_{n=1}^{U} \sigma^{(n)} , \tag{4.25}$$

where U is an upper bound, which depends on the size of the system. The successive terms in this sum are given by

$$\sigma^{(n)} = -\lim_{\alpha\to 0} i\frac{\partial}{\partial t}\sum_a f_a \bar{X}_n^t(a)\big|_{t=0} , \tag{4.26}$$

where $f_a = N_a^C / N_{\partial L}$.

V. THE ISING MODEL

The one-dimensional Ising model in a transverse magnetic field provides an excellent test case for the theory described in the preceding section. The Hamiltonian of this model is one of the simplest Hamiltonians which fit in with the general scheme of Sec. III. The exact formulas with which the results can be compared are derived by Pfeuty.[17]

The Hamiltonian of the model is

$$H(\lambda) = \sum_i [1-\sigma_3(i)] - \lambda\sum_i \sigma_1(i)\sigma_1(i+1) . \tag{5.1}$$

where σ_1 and σ_3 are two of the three Pauli spin matrices. The ground state of the unperturbed Hamiltonian $H_0 = \sum[1-\sigma_3(i)]$ is given by Eq. (3.3) with $|0\rangle = \binom{1}{0}$; the corresponding ground state energy is $E_0^0 = 0$. Products of the Pauli matrices are given by $\sigma_\mu\sigma_\mu = \mathbf{1}$ and $\sigma_\mu\sigma_\nu = i\epsilon_{\mu\nu\lambda}\sigma_\lambda (\mu \neq \nu)$, where the Einstein summation convention has been used and where $\epsilon_{\mu\nu\lambda}$ is an element of the Levi-Civita tensor. Use of these product rules leads to

$$\Phi^t(\lambda) = -\lambda e^{\alpha t}\sum_i \sigma_1^t(i)\sigma_1^t(i+1) , \tag{5.2}$$

with

$$\sigma_1^t = \sigma_1\cos 2t + \sigma_2 \sin 2t . \tag{5.3}$$

A. The ground state energy

The basic quantities that we need are the $\langle 0|V_n^t(a)|0\rangle$ for all a and n. Now, $V_n^t(a)$ is a sum of integrals over products of n interactions $-\lambda e^{\alpha t_l}\sigma_1^{t_l}(i)\sigma_1^{t_l}(i+1)$ with i, $i+1 \in a$ and $l = 1, 2, \ldots, n$, and with each product being irreducible on a. So the integrand of each term is a product of factors, one for each $i \in a$. As a result the expectation value $\langle 0|V_m^t(a)|0\rangle$ is a sum of integrals whose integrands also factorize into a factor for each $i \in a$. The one-particle factors are expectation values in D of products of several $\sigma_1^{t_l}$ at different times t_l. These expectation values can easily be shown to be given by

$$\begin{aligned} &\langle 0|\sigma_1^{t_n}\sigma_1^{t_{n-1}}\ldots\sigma_1^{t_2}\sigma_1^{t_1}|0\rangle = 0, && n = \text{odd} , \\ &= \exp\{2i(t_1 - t_2 + \cdots + t_{n-1} - t_n)\}, && n = \text{even} . \end{aligned} \tag{5.4}$$

It is clear from this that $\langle 0|V_n^t(a)|0\rangle$ can only be nonzero if n = even.

As an example we now give the complete calculation of $\langle 0|V_4^t(a_2)|0\rangle$, where a_2 is the cluster consisting of three vertices and two edges: $X-X-X$. (In general we use the convention that a_n denotes the connected cluster with n edges.) From its definition it follows that:

$$\begin{aligned} \langle 0|V_4^t(a_2)|0\rangle = {} & X\tfrac{1}{2}X\tfrac{3}{4}X + X\tfrac{1}{3}X\tfrac{2}{4}X \\ & + X\tfrac{1}{4}X\tfrac{2}{3}X + X\tfrac{2}{3}X\tfrac{1}{4}X \\ & + X\tfrac{2}{4}X\tfrac{1}{3}X + X\tfrac{3}{4}X\tfrac{1}{2}X , \end{aligned} \tag{5.5}$$

where we have made use of

$$\begin{aligned} X\tfrac{1}{2}X\tfrac{3}{4}X = {} & (i\lambda)^4 \int_{-\infty}^{t} dt_4\, e^{\alpha t_4} \int_{-\infty}^{t_4} dt_3 e^{\alpha t_3} \int_{-\infty}^{t_3} dt_2\, e^{\alpha t_2} \int_{-\infty}^{t_2} dt_1\, e^{\alpha t_1} \\ & \times \langle 0|\sigma_1^{t_4}(2)\sigma_1^{t_4}(3)\sigma_1^{t_3}(2)\sigma_1^{t_3}(3)\sigma_1^{t_2}(1)\sigma_1^{t_2}(2)\sigma_1^{t_1}(1)\sigma_1^{t_1}(2)|0\rangle , \end{aligned} \tag{5.6}$$

and of analogous definitions for the other terms. On introducing Eq. (5.6) into Eq. (5.5), taking the expectation value and using Eq. (5.4) we find the result given in Table I. In order to simplify the notation we have defined

$$(l_1, l_2, \ldots, l_n) = e^{n\alpha t}\prod_{k=1}^{n}\frac{1}{il_k + k\alpha} . \tag{5.7}$$

In Table I all $\langle 0|V_n^t(a_l)|0\rangle$ are given with n up to 6 in-

TABLE I. $\langle 0 | V_n^t(a_l) | 0 \rangle$ for all n up to 6.

l	n	$(-\lambda)^{-n} \langle 0 \| V_n^t(a_l) \| 0 \rangle$[a]
1	2	$-(4,0)$
	4	$(4,0,4,0)$
	6	$-(4,0,4,0,4,0)$
2	4	$2(4,0,4,0)+4(4,4,4,0)$
	6	$-6(4,0,4,0,4,0)-8(4,0,4,4,4,0)$
		$-8(4,4,4,4,4,0)-8(4,4,4,0,4,0)$
3	6	$-24(4,4,4,4,4,0)-16(4,8,4,4,4,0)$
		$-16(4,4,4,8,4,0)-8(4,0,4,4,4,0)$
		$-8(4,4,4,0,4,0)-6(4,0,4,0,4,0)$
		$-4(4,8,4,0,4,0)-4(4,0,4,8,4,0)$
		$-4(4,8,4,8,4,0)$

[a]The entries in this column are defined in Eq. (5.7).

clusive. Actually we have also performed the calculations for $n=8$, but the presentation of the results would be too lengthy. The results have been used however to calculate $\Delta\epsilon^{(8)}$.

The next step is to calculate $X_n^t(a_l)$ for all n and l. This can be done by use of Eq. (4.9). For example it follows from this equation that:

$$\langle 0 | V^t(a_2) | 0 \rangle = X^t(a_1)^2 + X^t(a_2)\{1+X^t(a_1)\}^2 . \tag{5.8}$$

Putting $X^t(a_1) = \langle 0 | V^t(a_1) | 0 \rangle$ and equating equal powers of λ left and right one easily derives the results given in Table II. The other entries in this table can be calculated analogously.

The final step is to calculate the cumulants $\tilde{X}_m^t(a)$ from Eq. (4.15) and then $\Delta\epsilon^{(n)}$ from Eq. (4.14). It is important that the limit $\alpha \to 0$ be taken after all other operations have been performed, because most of the separate terms in Eq. (4.14) are singular even after the differentiation to t. The results of these calculations are presented in Table III.

B. The magnetization

The total magnetization of the lattice is defined as the ground state expectation value of $\sum \sigma_3(i)$. According to Eq. (2.12) this can be calculated once the eigenvalues of

TABLE II. $X_n^t(a_l)$ in terms of $\langle 0 | V_n^t(a_l) | 0 \rangle$.

l	n	$X_n^t(a_l)$
1	2	$\langle 0 \| V_2^t(a_1) \| 0 \rangle$
	4	$\langle 0 \| V_4^t(a_1) \| 0 \rangle$
	6	$\langle 0 \| V_6^t(a_1) \| 0 \rangle$
2	4	$\langle 0 \| V_4^t(a_2) \| 0 \rangle - \langle 0 \| V_2^t(a_1) \| 0 \rangle^2$
	6	$\langle 0 \| V_6^t(a_2) \| 0 \rangle - 2\langle 0 \| V_4^t(a_2) \| 0 \rangle \langle 0 \| V_2^t(a_1) \| 0 \rangle$
		$-2\langle 0 \| V_4^t(a_1) \| 0 \rangle \langle 0 \| V_2^t(a_1) \| 0 \rangle + 2\langle 0 \| V_2^t(a_1) \| 0 \rangle^3$
3	6	$\langle 0 \| V_6^t(a_3) \| 0 \rangle - 2\langle 0 \| V_4^t(a_2) \| 0 \rangle \langle 0 \| V_2^t(a_1) \| 0 \rangle$
		$+\langle 0 \| V_2^t(a_1) \| 0 \rangle^3$

TABLE III. Perturbation results for the Ising model.

n	$(-\lambda)^{-n} \Delta\epsilon^{(n)}$	$(-\lambda)^{-n} m^{(n)}$	$(-\lambda)^{-n} \omega^{(n)}$
1	0	0	2
2	$-1/2^2$	$-1/2^2$	0
3	0	0	0
4	$-1/2^6$	$-3/2^6$	
5	0	0	
6	$-1/2^8$	$-5/2^8$	
7	0	0	
8	$-25/2^{14}$	$-175/2^{14}$	

$$H(\lambda, y) = H(\lambda) + y \sum_{i=1}^{N} \sigma_3(i)$$
$$= yN + (1-y) H[\lambda/(1-y)] \tag{5.9}$$

are known. From the second identity in Eq. (5.9) and the previously derived results for the ground state energy of $H(\lambda)$ the reader can easily check that the magnetization per particle is given by

$$m = 1 + \sum_{n=1}^{\infty} m^{(n)} = 1 + \sum_{n=1}^{\infty} (n-1)\Delta\epsilon^{(n)} . \tag{5.10}$$

C. The first excited state

Before we can use the formulas of Sec. IV C to calculate the energy of the first excited state, we must check the condition stated just before Eq. (4.17). Therefore suppose $i \neq 0$. Then, if $0 \notin A_l$ for all $l = 1, 2, \ldots, m$, $\langle 0 | \psi(0) V^t(A_1 \cdots A_m) \psi^\dagger(i) | 0 \rangle = 0$ because of the orthogonality of $|0\rangle$ and $|1\rangle$. So suppose $0 \in A_l$ for some $l = 1, 2, \ldots, m$. Then, using formulas analogous to Eq. (5.4), we conclude that the only nonzero contributions to $\langle 0 | \psi(0) V^t(A_1 \cdots A_m) \psi^\dagger(i) | 0 \rangle$ come from terms which have an odd number of factors $\sigma_1^{\dagger j}(0)$ in the integrand. This will lead to an odd number of factors $\sigma_1^{\dagger j}(k)$ at some vertex $k \in A_l$. Then, if $i \neq k$, all terms will vanish. As a result $\langle 0 | \psi(0) V^t(A_1 \cdots A_m) \psi^\dagger(i) | 0 \rangle$ can only be nonzero if 0 and i belong to the same cluster A_l for some $l = 1, 2, \ldots, m$.

All calculations are now completely analogous to those of Sec. V A. For reference we give some results in Tables III, IV, and V. Here $b_{l,k}$ represents

TABLE IV. $\langle 0 | W_n^t(b_{l,k}) | 0 \rangle$ for all n up to 3.

l	k	n	$(-\lambda)^{-n} \langle 0 \| W_n^t(b_{l,k}) \| 0 \rangle$[a]
1	1,2	1	$-i(0)$
		2	$-(0,0)$
		3	$i(0,0,0)$
2	1,3	2	$-(0,0)-(4,0)$
		3	$i(0,0,0)+2i(0,4,0)$
	2	2	
		3	$4i(4,0,0)+2i(0,0,0)$
3	1,4	3	$i(0,0,0)+i(4,0,0)+i(0,4,0)+3i(4,4,0)$
	2,3	3	

[a]The entries in this column are defined in Eq. (5.7).

TABLE V. $Y_n^t(b_{l,k})$ in terms of $\langle 0|\, W_n^t(b_{l,k})\,|0\rangle$ and $\langle 0|\, V_n^t(a_l)\,|0\rangle$.

l	k	n	$Y_n^t(b_{l,k})$
1	1,2	1	$\langle 0\|\, W_1^t(b_{1,1})\,\|0\rangle$
		2	$\langle 0\|\, W_2^t(b_{1,1})\,\|0\rangle$
		3	$\langle 0\|\, W_3^t(b_{1,1})\,\|0\rangle$
2	1,3	2	$\langle 0\|\, W_2^t(b_{2,1})\,\|0\rangle$
		3	$\langle 0\|\, W_3^t(b_{2,1})\,\|0\rangle$
			$-\langle 0\|\, W_2^t(b_{2,1})\,\|0\rangle\langle 0\|\, W_1^t(b_{1,1})\,\|0\rangle$
			$-\langle 0\|\, V_2^t(a_1)\,\|0\rangle\langle 0\|\, W_1^t(b_{1,1})\,\|0\rangle$
	2	2	$\langle 0\|\, W_2^t(b_{2,2})\,\|0\rangle - \langle 0\|\, W_1^t(b_{1,1})\,\|0\rangle^2$
		3	$\langle 0\|\, W_3^t(b_{2,2})\,\|0\rangle$
			$-2\langle 0\|\, W_2^t(b_{2,2})\,\|0\rangle\langle 0\|\, W_1^t(b_{1,1})\,\|0\rangle$
			$-2\langle 0\|\, W_2^t(b_{1,1})\,\|0\rangle\langle 0\|\, W_1^t(b_{1,1})\,\|0\rangle$
			$+2\langle 0\|\, W_1^t(b_{1,1})\,\|0\rangle^3$
3	1,4	3	$\langle 0\|\, W_3^t(b_{3,1})\,\|0\rangle$
	2,3	3	$\langle 0\|\, W_3^t(b_{3,2})\,\|0\rangle$
			$-\langle 0\|\, W_2^t(b_{2,1})\,\|0\rangle\langle 0\|\, W_1^t(b_{1,1})\,\|0\rangle$

a cluster with l edges and with the kth vertex coinciding with the origin of the lattice, i.e., with site number 0. Because the calculations soon become cumbersome we stop at the terms of order three in perturbation.

VI. DISCUSSION

In the preceding sections we have developed a perturbation theory for lattice Hamiltonians based on the adiabatic theorem, and applied it to the one-dimensional Ising model in a transverse magnetic field. This model is of interest because it corresponds[2,18] to a two-dimensional classical spin model in which a phase transition can take place. In the original model the phase transition manifests itself as the crossing of the ground state energy level with some excited state level as the magnetic field strength λ is varied. From the exact results[17] we know that this occurs when $\lambda = \lambda_c = 1$, and we are mainly interested in the values of λ of this order of magnitude. In Table III we have collected the final results of our calculations. Comparing them with the coefficients in the power series expansion of the analytical results[17] we find that all entries in this table are exact. In the case of the excitation energy, low order perturbation theory even leads to the full analytical expression $\omega = 2(1-\lambda)$, from which we find the exact result $\lambda_c = 1$. From the first two columns in Table III we can calculate the ground state energy and the ground state magnetization to the eighth order in λ. For the values of $\lambda \leqq 1$ this will give us nearly the exact results. As an example we mention $\Delta\epsilon(\lambda = 1) = -0.271$ from Table III, whereas the exact result is -0.273. For the values of $\lambda \geqq 1$ good results can be obtained[8] from the perturbation series by the method of Padé approximants. An alternative is to do the calculations on $H(\lambda)/\lambda$ and let λ^{-1} be the perturbation parameter. For a discussion of the properties of the model we refer to the literature.[17]

From the results of Sec. V we may conclude that the assumptions made in the application of the adiabatic theorem are fully justified, at least for the Hamiltonian under investigation in this paper. As to the amount of work involved in the application of our method it is interesting to mention that all entries in Table III, except for those with $n = 8$, were easily obtained by hand. Although the formulas in Sec. IV look somewhat formidable they provide a simple algorithm to calculate the perturbation series. This will be so even if the interaction in the Hamiltonian is more complicated than the one in Sec. V; the main reason for this is that all combinatorial calculations are restricted to finite clusters. Because of the same reason our method can be readily applied to finite systems or to systems with impurities.

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