

# Expansions for One Quasiparticle States in Spin 1/2 Systems

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Convergent expansions of the wavefunctions for the ground state and low-lying excited states of quantum transverse Ising systems are obtained. These expansions are employed to prove that the dispersion relation for a single quasi-particle has a convergent expansion.

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**KEY WORDS:** Quantum spins; quasiparticles; expansions; transverse Ising model.

## 1. INTRODUCTION

The ground state and low-lying excited states of a quantum spin system, governed by a Hamiltonian  $H$ , are usually studied by considering a low temperature expansion of its partition function, e.g., refs. 1–4. This involves an analysis of the trace of the operator,  $\exp(-\beta H)$ , in the limit of large  $\beta$  (with  $\beta = 1/k_B T$ ,  $k_B$  being the Boltzmann constant). The analysis is usually done by applying the method of cluster expansions to the Trotter product representation of the operator. In contrast, Kirkwood and Thomas<sup>(5)</sup> studied the ground state of such systems by working directly with the Schrödinger equation,  $H|\Psi\rangle = E|\Psi\rangle$ . They considered a class of Hamiltonians of quantum spin-1/2 systems, which were small perturbations of classical Hamiltonians. By making a clever ansatz for the form of the ground state, they were able to develop a convergent expansion for the ground state which they used to show that the infinite volume limit of the ground state exists and has exponential decay of the truncated correlation functions.

The method of Kirkwood and Thomas has been employed, in the  $C^*$ -algebraic framework, to establish the uniqueness of translationally

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invariant ground states in quantum spin-1/2 systems<sup>(6)</sup> and has also been extended to study the ground states of models of arbitrary (though finite) spin, e.g., the quantum Potts model.<sup>(7)</sup>

The approach of Kirkwood and Thomas can, however, be applied only to a restricted class of Hamiltonians, namely to ones that satisfy a Perron–Frobenius condition. In this paper, we greatly extend the class of Hamiltonians to which the Kirkwood–Thomas approach can be applied by removing the requirement of this condition. We also simplify their method—the simplification being in the estimates which show that the expansions converge. The methods of this paper are applicable to any lattice Hamiltonian of the form

$$H = -\sum_i \sigma_i^x + \epsilon \sum_X V_X \quad (1)$$

where  $V_X$  is a local operator that acts only on the spins at sites in  $X$ . There is a finite constant  $R$  such that  $X$  is only summed over subsets with  $g(X) < R$ , where  $g(X)$  is the number of bonds in the smallest connected set of sites containing  $X$ . Kirkwood and Thomas required that the matrix representing the local operator,  $V_X$ , satisfies a Perron–Frobenius condition; we do not need such a condition.

Throughout this paper we will work with a specific example of such a Hamiltonian, the Ising model in a transverse field.

$$H = -\sum_i \sigma_i^x + \epsilon \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z \quad (2)$$

(The sum over  $\langle ij \rangle$  is over all nearest neighbor sites in the lattice.) Usually perturbation theory in  $\epsilon$  is done with the unitarily equivalent Hamiltonian

$$\tilde{H} = -\sum_i \sigma_i^z + \epsilon \sum_{\langle ij \rangle} \sigma_i^x \sigma_j^x \quad (3)$$

However, following Kirkwood and Thomas, we use (2) in our approach. (When  $\epsilon = 0$  the groundstate of (2), in the usual basis in which the  $\sigma^z$  are diagonal, is the constant wave function. The Kirkwood–Thomas approach is an expansion around this constant wavefunction.) An example of a Hamiltonian to which our methods apply, but the original approach of Kirkwood and Thomas does not, is the following.

$$H = -\sum_i \sigma_i^x + \epsilon \sum_{\langle ij \rangle} [\sigma_i^z \sigma_j^z + J \sigma_i^y \sigma_j^y] \quad (4)$$

with  $J \neq 1$ .

A Hamiltonian of the form

$$H = -\sum_i \sigma_i^z + \epsilon \sum_X V'_X \quad (5)$$

is unitarily equivalent to a Hamiltonian of the form (1). A more general class of Hamiltonians one might consider is

$$H = \sum_X D_X + \epsilon \sum_Y V'_Y \quad (6)$$

where  $D_X$  is a local *diagonal* operator. If the classical Hamiltonian  $\sum_X D_X$  has a unique ground state, then  $\text{Tr}(e^{-\beta H})$ , and hence the ground state, may be studied by standard expansion methods. It would be interesting to extend the methods of Kirkwood and Thomas and this paper to this class of models.

It is of interest to study, not only the properties of the ground state, but also the low-lying excited states of quantum spin systems. There have been a series of papers<sup>(8-13)</sup> devoted to the investigation of the low-lying spectra of infinite-dimensional quantum lattice systems. In ref. 8 this has been done by reducing the problem to the spectral analysis of an operator which is unitarily equivalent to the Hamiltonian governing the lattice system, and is also the generator of an infinite-dimensional Markov diffusion process. The method of cluster expansions has been employed to analyse the low-lying spectral properties. In particular, the spectrum of the Hamiltonian has been analysed in the one-particle invariant subspaces, which describe the elementary excitations of the ground state. In refs. 9 and 10 it has been shown that the one-particle excitations form a segment of absolutely continuous spectrum, which is separated by energy gaps from the ground state eigenvalue, and from the rest of the spectrum.

In the second part of this paper, we study one quasi-particle excitations in a quantum spin-1/2 system by employing a method different from the ones mentioned above. Our method uses techniques, based on the Kirkwood-Thomas approach, that we develop for the ground state analysis. The key idea is that the lowest excited states have a definite momentum. We make an ansatz for the form of these states based on their momentum, and use it to develop a convergent expansion for them. As an application of this expansion we study the dispersion relation for a single quasi-particle and show that it has a convergent expansion.

Kirkwood and Thomas also considered models with two ground states related by the global spin flip, e.g., the highly anisotropic XY- and Heisenberg models.<sup>(5)</sup> The simplifications and generalizations of their method that we introduce in this paper also apply to these types of models

as will be explained elsewhere.<sup>(14)</sup> We will also show that interfaces (kink states) in these models may be studied in much the same way that we study the excited states with one quasiparticle in the models of this paper.

We consider the Hamiltonian to be restricted to finite volumes,  $\Lambda$ , which are hypercubes, and impose periodic boundary conditions. This restriction is essential for our treatment of the one quasi-particle excited states which relies on the translation symmetry of the model. However, for our treatment of the ground state we could consider more general  $\Lambda$  and other boundary conditions.

It has been shown<sup>(12)</sup> that the spectrum of the Hamiltonian (2) above the lowest energy level contains a *continuous* part and is separated from the lowest level by an energy gap. In this paper we make no further analysis of the *nature* of the spectrum above the ground state eigenvalue.

Section 2 of this paper is devoted to our version of the Kirkwood–Thomas approach to the ground state of quantum spin-1/2 systems, in particular to the Hamiltonian in (2). We prove that the wavefunction of the Hamiltonian can be expressed in the form

$$\psi(\sigma) = \exp\left(\sum_X h_X(\sigma)\right) \quad (7)$$

where  $\sum_X h_X$  is a function of the configuration on the lattice which can be thought of as a *classical* Hamiltonian. It is infinite range ( $h_X \neq 0$  for arbitrarily large  $X$ ), but the size of  $h_X$  decays exponentially as  $X$  grows. This is the form of the Kirkwood–Thomas ansatz for the wavefunction, but we emphasize that our approach shows that it holds even for models without a Perron–Frobenius condition. (Depending on the model, the function  $\sum_X h_X$  may be complex-valued.) The one-particle excitations of the system are analysed in Section 3. We obtain an expression for the wavefunction of the lowest excited state in a subspace of fixed momentum, and use it to prove that the infinite volume dispersion relation for the spectral gap above the ground state eigenvalue has a convergent expansion. This shows that this gap persists in the infinite-volume limit and allows us to prove properties of the gap, e.g., that it is minimized at a particular value of  $k$ , depending on the sign of  $\epsilon$ . Unfortunately, the analysis of two-particle excitations lies outside the scope of our method.

## 2. THE GROUND STATE

A classical spin configuration on the lattice is an assignment of a  $+1$  or a  $-1$  to each site in the lattice. So for each  $i \in \Lambda$ ,  $\sigma_i = \pm 1$ . We will abbreviate the classical spin configuration  $\{\sigma_i\}_{i \in \Lambda}$  by  $\sigma$ . For each such  $\sigma$

we let  $|\sigma\rangle$  be the state in the Hilbert space which is the tensor product of a spin up state at each site with  $\sigma_i = +1$  and a spin down state at each site with  $\sigma_i = -1$ . Thus  $|\sigma\rangle$  is an eigenstate of all the  $\sigma_i^z$  with  $\sigma_i^z |\sigma\rangle = \sigma_i |\sigma\rangle$ . Any state  $|\Psi\rangle$  can be written in terms of this basis:

$$|\Psi\rangle = \sum_{\sigma} \psi(\sigma) |\sigma\rangle \quad (8)$$

where  $\psi(\sigma)$  is a complex-valued function on the spin configurations  $\sigma$ .

The form of the Hamiltonian in Eq. (3) seems natural for perturbation theory in  $\epsilon$  since the Hamiltonian is diagonal when  $\epsilon = 0$ . However, following Kirkwood and Thomas, we study a unitarily equivalent Hamiltonian

$$H = -\sum_i \sigma_i^x + \epsilon \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z \quad (9)$$

For a single site the ground state of  $-\sigma^x$  is the vector  $|+1\rangle + |-1\rangle$ . Thus the unnormalized ground state of the Hamiltonian (9) with  $\epsilon = 0$  is given by (8) with  $\psi(\sigma) = 1$  for all  $\sigma$ .

For a subset  $X$  of the lattice  $\mathcal{A}$ , let

$$\sigma(X) = \prod_{i \in X} \sigma_i$$

and we use the convention that  $\sigma(\emptyset) = 1$ . Let  $f(\sigma)$  be a complex-valued function of the  $\sigma$ 's. Then  $f(\sigma)$  can be written in a unique way as

$$f(\sigma) = \sum_X g(X) \sigma(X)$$

where the  $g(X)$  are complex numbers and  $X$  is summed over all subsets of  $\mathcal{A}$  (including  $\mathcal{A}$  itself and the empty set). The Fourier coefficients  $g(X)$  are given by

$$g(X) = 2^{-|\mathcal{A}|} \sum_{\sigma} \sigma(X) f(\sigma)$$

where  $|\mathcal{A}|$  is the number of sites in  $\mathcal{A}$  and the sum is over all  $2^{|\mathcal{A}|}$  spin configurations on  $\mathcal{A}$ . [In general, let  $|X|$  denote the number of sites in any subset  $X$  of the lattice.]

The heart of the Kirkwood Thomas method is the following. We expand the ground state with respect to the basis as in Eq. (8) and assume that  $\psi(\sigma)$  can be written in the form

$$\psi(\sigma) = \exp \left[ -\frac{1}{2} \sum_X g(X) \sigma(X) \right] \quad (10)$$

(The factor of  $-\frac{1}{2}$  is introduced for later convenience.) Kirkwood and Thomas use a Perron–Frobenius argument to show that  $\psi(\sigma) > 0$  for all  $\sigma$ , and so the ground state can be written in this form with real  $g(X)$ . The Perron–Frobenius argument requires that the off-diagonal terms in the Hamiltonian are all non-positive, and so it appears that the Kirkwood Thomas approach only applies to a very restricted class of models. This is not the case. We will show how to eliminate the Perron–Frobenius argument entirely. We proceed in two steps. First, we will make the ansatz (10) and prove that there is an eigenstate of this form. Later we will give a short argument to show that this eigenstate must in fact be the ground state.

Consider the eigenvalue equation

$$H |\Psi\rangle = E_0 |\Psi\rangle \quad (11)$$

The operator  $\sigma_i^z \sigma_j^z$  is diagonal, so

$$\sigma_i^z \sigma_j^z \sum_{\sigma} \psi(\sigma) |\sigma\rangle = \sum_{\sigma} \sigma_i \sigma_j \psi(\sigma) |\sigma\rangle \quad (12)$$

The operator  $\sigma_i^x$  just flips the spin at site  $i$ , i.e.,  $\sigma_i^x |\sigma\rangle = |\sigma^{(i)}\rangle$ , where  $\sigma^{(i)}$  is the spin configuration  $\sigma$  but with  $\sigma_i$  replaced by  $-\sigma_i$ . Hence

$$\sigma_i^x \sum_{\sigma} \psi(\sigma) |\sigma\rangle = \sum_{\sigma} \psi(\sigma) |\sigma^{(i)}\rangle = \sum_{\sigma} \psi(\sigma^{(i)}) |\sigma\rangle \quad (13)$$

The last equality follows by a change of variables in the sum.

Thus if we use (8) in the Schrödinger Eq. (11) and pick out the coefficient of  $|\sigma\rangle$ , then for each spin configuration  $\sigma$  we have

$$-\sum_i \psi(\sigma^{(i)}) + \epsilon \sum_{\langle ij \rangle} \sigma_i \sigma_j \psi(\sigma) = E_0 \psi(\sigma) \quad (14)$$

Dividing both sides by  $\psi(\sigma)$ , we have

$$-\sum_i \frac{\psi(\sigma^{(i)})}{\psi(\sigma)} + \epsilon \sum_{\langle ij \rangle} \sigma_i \sigma_j = E_0 \quad (15)$$

Now  $\sigma^{(i)}(X)$  is just  $\sigma(X)$  if  $i \notin X$  and  $-\sigma(X)$  if  $i \in X$ . Thus

$$\psi(\sigma^{(i)}) = \exp \left[ -\frac{1}{2} \sum_{X: i \notin X} g(X) \sigma(X) + \frac{1}{2} \sum_{X: i \in X} g(X) \sigma(X) \right]$$

and so we have

$$\frac{\psi(\sigma^{(i)})}{\psi(\sigma)} = \exp \left[ \sum_{X:i \in X} g(X) \sigma(X) \right]$$

Thus the Schrödinger equation is now

$$-\sum_i \exp \left[ \sum_{X:i \in X} g(X) \sigma(X) \right] + \epsilon \sum_{\langle ij \rangle} \sigma_i \sigma_j = E_0 \quad (16)$$

This equation must hold for every configuration  $\sigma$ . This is the magic step in the Kirkwood Thomas method because of the cancellation between terms in  $\psi(\sigma)$  and  $\psi(\sigma^{(i)})$ . As  $|A| \rightarrow \infty$ , the sum  $\sum_X g(X) \sigma(X)$  will diverge, but the sum  $\sum_{X:i \in X} g(X) \sigma(X)$  that appears in the above equation will remain bounded. We will refer to Eq. (16) as the Kirkwood Thomas equation.

We define

$$\exp^{(2)}(x) = e^x - 1 - x \quad (17)$$

and rewrite (16) as

$$\begin{aligned} -\sum_i \exp^{(2)} \left( \sum_{X:i \in X} g(X) \sigma(X) \right) + \epsilon \sum_{\langle ij \rangle} \sigma_i \sigma_j &= E_0 + |A| + \sum_i \sum_{X:i \in X} g(X) \sigma(X) \\ &= E_0 + |A| + \sum_X |X| g(X) \sigma(X) \end{aligned} \quad (18)$$

So the Kirkwood Thomas equation becomes

$$\sum_X |X| g(X) \sigma(X) + E_0 + |A| = -\sum_i \exp^{(2)} \left( \sum_{X:i \in X} g(X) \sigma(X) \right) + \epsilon \sum_{\langle ij \rangle} \sigma_i \sigma_j \quad (19)$$

Expanding  $\exp^{(2)}$  in a power series we have

$$\begin{aligned} \sum_X |X| g(X) \sigma(X) + E_0 + |A| &= -\sum_i \sum_{n=2}^{\infty} \frac{1}{n!} \left( \sum_{X:i \in X} g(X) \sigma(X) \right)^n + \epsilon \sum_{\langle ij \rangle} \sigma_i \sigma_j \\ &= -\sum_i \sum_{n=2}^{\infty} \frac{1}{n!} \sum_{X_1, X_2, \dots, X_n: i \in X_j} \prod_{j=1}^n g(X_j) \sigma(X_j) + \epsilon \sum_{\langle ij \rangle} \sigma_i \sigma_j \end{aligned} \quad (20)$$

The notation  $i \in X_j$  means that  $i$  belongs to  $X_j$  for all  $j = 1, 2, \dots, n$ . Since  $\sigma_i^2 = 1$ ,  $\sigma(X)\sigma(Y) = \sigma(X \Delta Y)$  where the symmetric difference  $X \Delta Y$  of  $X$  and  $Y$  is defined by  $X \Delta Y = (X \cup Y) \setminus (X \cap Y)$ . Thus  $\prod_{j=1}^n \sigma(X_j) = \sigma(X_1 \Delta \dots \Delta X_n)$ . Eq. (20) implies that the coefficients of  $\sigma(X)$  on both sides of the equation must be equal. So for  $X \neq \emptyset$  we have

$$g(X) = -\frac{1}{|X|} \sum_i \sum_{n=2}^{\infty} \frac{1}{n!} \sum_{\substack{X_1, X_2, \dots, X_n: i \in X_j, \\ X_1 \Delta \dots \Delta X_n = X}} g(X_1) g(X_2) \cdots g(X_n) + \frac{1}{|X|} \epsilon 1_{\text{nn}}(X) \quad (21)$$

where  $1_{\text{nn}}(X)$  is 1 if  $X$  consists of two nearest neighbor sites and is 0 otherwise.

Similarly, for  $X = \emptyset$ , we obtain the equation

$$E_0 + |A| = -\sum_i \sum_{n=2}^{\infty} \frac{1}{n!} \sum_{\substack{X_1, X_2, \dots, X_n: i \in X_j, \\ X_1 \Delta \dots \Delta X_n = \emptyset}} g(X_1) g(X_2) \cdots g(X_n) \quad (22)$$

since  $\sigma(\emptyset) = 1$ .

We let  $g$  denote the collection of coefficients  $\{g(X) : X \subset A, X \neq \emptyset\}$ , and think of Eq. (21) as a fixed point equation,  $g = F(g)$ . We define a norm by

$$\|g\| = \sum_{X \ni i} |g(X)| |X| (|\epsilon| M)^{-w(X)} \quad (23)$$

where  $w(X)$  is the number of bonds in the smallest connected set of bonds that contains  $X$ . (We make the convention that a bond contains its end-points.) If  $X$  just contains the single site  $i$ , then  $w(X) = 0$ . With periodic boundary conditions we need only consider  $g(X)$  which are translation invariant, and so the above quantity does not depend on  $i$ . With other boundary conditions we would need to define the norm to be the supremum over  $i$  of the above. The constant  $M$  will be chosen later. It will only depend on the lattice. We will prove that the fixed point equation has a solution in the Banach space defined by this norm if  $|\epsilon|$  is sufficiently small by applying the contraction mapping theorem.

**Theorem 1.** There exists a constant  $M > 0$  which depends only on the number of dimensions such that if  $|\epsilon| M \leq 1$ , then the fixed point equation (21) has a solution  $g$ , and  $\|g\| \leq c$  for some constant  $c$  which depends only on the lattice.

*Proof.* We will prove that  $F$  is a contraction on a small ball about the origin, and that it maps this ball back into itself. The contraction mapping theorem will then imply that  $F$  has a fixed point in this ball. We denote the radius of the ball by  $\delta$  and let

$$\delta = \frac{4d}{M} \quad (24)$$

(The factor of  $4d$  is for the lattice  $Z^d$ . In general this factor is twice the coordination number of the lattice.) For the sake of concreteness, we will prove  $F$  is a contraction with constant  $1/2$ , but there is nothing special about the choice of  $1/2$ . So we need to show

$$\|F(g) - F(g')\| \leq \frac{1}{2} \|g - g'\| \quad \text{for } \|g\|, \|g'\| \leq \delta \quad (25)$$

and

$$\|F(g)\| \leq \delta \quad \text{for } \|g\| \leq \delta \quad (26)$$

The proof of (25) proceeds as follows.

$$\begin{aligned} & \|F(g) - F(g')\| \\ & \leq \sum_i \sum_{n=2}^{\infty} \frac{1}{n!} \sum_{\substack{X_1, \dots, X_n: i \in X_j, \\ 0 \in X_1 \Delta \dots \Delta X_n}} |g(X_1) \cdots g(X_n) - g'(X_1) \cdots g'(X_n)| (|\epsilon| M)^{-w(X_1 \Delta \dots \Delta X_n)} \end{aligned} \quad (27)$$

If  $0 \in X_1 \Delta \dots \Delta X_n$ , then  $0$  is in at least one  $X_j$ . Using the symmetry under permutations of the  $X_j$ , we can take  $0 \in X_1$  at the cost of a factor of  $n$ . We claim that if  $i \in X_j$  for  $j = 1, 2, \dots, n$ , then

$$w(X_1 \Delta \dots \Delta X_n) \leq \sum_{j=1}^n w(X_j) \quad (28)$$

To prove the claim, let  $C_j$  be connected sets of bonds such that  $X_j \subset C_j$  and  $|C_j| = w(X_j)$ . Define  $C = \bigcup_{j=1}^n C_j$ . Since all the  $X_j$  contain  $i$ , all the  $C_j$  contain  $i$ . So  $C$  is connected. Clearly,  $X_1 \Delta \dots \Delta X_n \subset C$ . So

$$w(X_1 \Delta \dots \Delta X_n) \leq |C| \leq \sum_{j=1}^n |C_j| = \sum_{j=1}^n w(X_j) \quad (29)$$

which proves the claim (28). So

$$\begin{aligned}
 \|F(g) - F(g')\| &\leq \sum_i \sum_{n=2}^{\infty} \frac{1}{(n-1)!} \sum_{X_1, \dots, X_n: i \in X_j, 0 \in X_1} \left| \prod_{j=1}^n g(X_j) - \prod_{j=1}^n g'(X_j) \right| \\
 &\quad \times (|\epsilon| M)^{-w(X_1) - w(X_2) - \dots - w(X_n)} \\
 &\leq \sum_{n=2}^{\infty} \frac{1}{(n-1)!} \sum_{X_1 \ni 0} \sum_{i \in X_1} \sum_{X_2 \dots X_n \ni i} \sum_{k=1}^n \left( \prod_{j=1}^{k-1} |g(X_j)| \right) \\
 &\quad \cdot |g(X_k) - g'(X_k)| \left( \prod_{j=k+1}^n |g'(X_j)| \right) \\
 &\quad \times (|\epsilon| M)^{-w(X_1) - w(X_2) - \dots - w(X_n)} \\
 &\leq \sum_{n=2}^{\infty} \frac{1}{(n-1)!} \sum_{X_1 \ni 0} \sum_{i \in X_1} |g(X_1) - g'(X_1)| (|\epsilon| M)^{-w(X_1)} \\
 &\quad \times \sum_{X_2 \dots X_n \ni i} \left( \prod_{j=2}^n |g'(X_j)| (|\epsilon| M)^{-w(X_j)} \right) \\
 &\quad + \sum_{n=2}^{\infty} \frac{1}{(n-1)!} \sum_{X_1 \ni 0} \sum_{i \in X_1} |g(X_1)| (|\epsilon| M)^{-w(X_1)} \\
 &\quad \times \sum_{X_2 \dots X_n \ni i} \sum_{k=2}^n \left( \prod_{j=2}^{k-1} |g(X_j)| (|\epsilon| M)^{-w(X_j)} \right) \\
 &\quad \times |g(X_k) - g'(X_k)| (|\epsilon| M)^{-w(X_k)} \left( \prod_{j=k+1}^n |g'(X_j)| (|\epsilon| M)^{-w(X_j)} \right) \\
 &\leq \|g - g'\| \sum_{n=2}^{\infty} \frac{1}{(n-1)!} \left[ \|g'\|^{n-1} + \sum_{k=2}^n \|g\|^{k-1} \|g'\|^{n-k} \right] \tag{30}
 \end{aligned}$$

where we have bounded various sums by  $\|g - g'\|$ ,  $\|g\|$  and  $\|g'\|$  in obvious ways. Since  $\|g\|$  and  $\|g'\|$  are both bounded by  $\delta$ , it follows from (30) that

$$\|F(g) - F(g')\| \leq K \|g - g'\| \tag{31}$$

where

$$K = \sum_{n=2}^{\infty} \frac{n}{(n-1)!} \delta^{n-1} = e^\delta - 1 + \delta e^\delta \tag{32}$$

Recalling that  $\delta = 4d/M$ , if  $M$  is large enough then  $K \leq 1/2$ .

To prove (26), we use (25) with  $g' = 0$ . Using (21) to compute  $F(0)$ , it follows that

$$\begin{aligned} \|F(g)\| &\leq \|F(g) - F(0)\| + \|F(0)\| \leq \frac{1}{2} \|g\| + \sum_{X \ni 0} |\epsilon| 1_{\text{nn}}(X) (|\epsilon| M)^{-w(X)} \\ &\leq \frac{1}{2} \|g\| + 2d |\epsilon| (|\epsilon| M)^{-1} \leq \frac{\delta}{2} + 2dM^{-1} = \delta \quad \blacksquare \end{aligned} \quad (33)$$

At this point all we have shown is that we can find an eigenfunction of the form (10). Kirkwood and Thomas show that this eigenfunction is the ground state by a Perron–Frobenius argument. This limits their method to models in which the off-diagonal matrix elements of the Hamiltonian are non-positive. We give a different argument which does not impose any restrictions on the signs of the matrix elements of the Hamiltonian.

When  $\epsilon = 0$ , we have  $g = 0$ , and we know that our eigenfunction is the ground state. Since we are working on a finite lattice, we are considering a finite dimensional eigenvalue problem. So the only way our eigenvalue can cease being the ground state energy is if it crosses another eigenvalue. So if we can show that our eigenfunction is nondegenerate for all  $\epsilon$  with  $|\epsilon| < 1/M$ , then it follows that our eigenfunction is the ground state for all such  $\epsilon$ . Suppose that there is some  $\epsilon$  such that the degeneracy of the eigenvalue of our eigenfunction is greater than one. Recall that our eigenfunction is denoted by  $\psi(\sigma)$ . Let  $\phi(\sigma)$  denote a different eigenfunction with the same eigenvalue. Define

$$\psi_\alpha(\sigma) = \psi(\sigma) + \alpha\phi(\sigma) \quad (34)$$

So  $\psi_\alpha$  is also an eigenfunction with the same eigenvalue. Since  $\psi(\sigma) > 0$  for all  $\sigma$ , and there are finitely many  $\sigma$ , if  $\alpha$  is sufficiently small, then  $\psi_\alpha(\sigma) > 0$  for all  $\sigma$ . Thus it can be written in the form

$$\psi_\alpha(\sigma) = \exp \left[ -\frac{1}{2} \sum_X g_\alpha(X) \sigma(X) \right] \quad (35)$$

Moreover, as  $\alpha \rightarrow 0$ ,  $\|g - g_\alpha\| \rightarrow 0$ . Since  $\psi_\alpha$  is an eigenfunction,  $g_\alpha$  satisfies the fixed point equation. For sufficiently small  $\alpha$ ,  $g_\alpha$  is in the ball of radius  $\delta$  about the origin. But this contradicts the uniqueness of the solution of the fixed point equation in this ball. Thus the eigenvalue is nondegenerate, and so the eigenfunction we have constructed is indeed the ground state. In the preceding argument, how small  $\alpha$  must be depends on  $\mathcal{A}$ . This is not a problem. For each  $\mathcal{A}$  we need only find one value of  $\alpha$  which leads to a

contradiction and so implies that the eigenfunction is not degenerate. This argument works for all  $\epsilon$  with  $|\epsilon| < 1/M$ , and  $M$  does not depend on  $\Lambda$ .

Finally, we consider the question of convergence to the infinite volume limit. One approach would be to show that the coefficients  $g(X)$  have convergent expansions in  $\epsilon$  and that these expansions agree up to order  $\epsilon^L$  where  $L$  is the length of the smallest side in  $\Lambda$ . We will sketch a different approach based on the fixed point equation. It takes advantage of the fact that if we have a  $g$  which is near the origin and very close to being a fixed point, then it must be very close to the true fixed point.

We start by asking where the volume dependence is in the fixed point equation (21). The  $X_i$  in this equation must be subsets of the volume  $\Lambda$ , and the notion of nearest neighbor in the term  $1_{\text{nn}}(X)$  in (21) depends on the volume because of the periodic boundary conditions. To make the volume dependence of  $F(g)$  explicit, we write it as  $F_\Lambda(g)$ . We can define a fixed point equation which should give the infinite volume limit directly. To do this, in (21) we let the  $X_i$  be subsets of  $Z^d$  and interpret  $1_{\text{nn}}(X)$  to mean nearest neighbors in  $Z^d$  in the usual sense. We denote the resulting function by  $F_\infty(g)$ . Our proof of Theorem 1 also shows that there is a small neighborhood of the origin in which the fixed point equation  $F_\infty(g) = g$  has a unique solution.

Let  $g_\Lambda$  and  $g_\infty$  denote the fixed points of  $F_\Lambda$  and  $F_\infty$ . We want to show that as the volume  $\Lambda$  converges to  $Z^d$ ,  $g_\Lambda$  converges to  $g_\infty$ . Note that  $g_\Lambda$  and  $g_\infty$  are defined for different collections of subsets, so it is not immediately clear in what sense  $g_\Lambda$  should converge to  $g_\infty$ . In fact, if a set  $X$  is near the boundary,  $g_\Lambda(X)$  and  $g_\infty(X)$  need not be close. Consider one dimension and let  $\Lambda = \{1, 2, \dots, L\}$ , and let  $X = \{1, L\}$ . Because of the periodic boundary conditions, the two sites in  $X$  are actually nearest neighbors. So  $g_\Lambda(X)$  is of order  $\epsilon$ . But  $g_\infty(X)$  will be of order  $\epsilon^L$ .

To compare  $g_\Lambda$  and  $g_\infty$  correctly, we proceed as follows. We take our volume to be centered about the origin and let  $L$  be the length of the shortest side. So the closest sides are a distance  $L/2$  from the origin. Recall that  $w(X)$  is the number of bonds in the smallest set of bonds which contains  $X$ . We claim that

$$\sum_{X \ni 0: w(X) \leq L/4} |g_\Lambda(X) - g_\infty(X)| \quad (36)$$

converges to zero exponentially fast as  $\Lambda$  converges to  $Z^d$ . Note that the terms we are neglecting,

$$\sum_{X \subset \Lambda: 0 \in X, w(X) > L/4} |g_\Lambda(X)| \quad (37)$$

and

$$\sum_{X \subset Z^d : 0 \in X, w(X) > L/4} |g_\infty(X)| \tag{38}$$

are both of order  $(|\epsilon| M)^{L/4}$  by our bounds on the solution of the fixed point equations.

Our strategy is to show that  $g_A$  is almost a fixed point of  $F_\infty$ . This then implies that  $g_A$  is close to the exact fixed point  $g_\infty$  of  $F_\infty$ . To show that  $g_A$  is almost a fixed point of  $F_\infty$  we need to estimate

$$F_\infty(g_A) - g_A = F_\infty(g_A) - F_A(g_A) \tag{39}$$

However,  $g_A$  is only defined on subsets of  $A$ , so we cannot plug  $g_A$  directly into  $F_\infty$ . We define a function  $g'_A$  which is defined for all  $X \subset Z^d$  as follows. For sets  $X$  with  $0 \in X$  and  $w(X) \leq L/4$ , we let  $g'_A(X) = g_A(X)$ . We then extend the definition to sets which are translates of such  $X$  by taking  $g'_A(X+t) = g'_A(X)$ . (These translations are done in  $Z^d$ .) Finally we define  $g'_A(X)$  to be zero for the sets for which it is not yet defined. Note that there is a consistency issue here. If we have two sets  $X$  and  $Y$  which both contain 0, have  $w(X), w(Y) \leq L/4$  and are translates of each other in  $Z^d$ , then we need to be sure  $g_A(X) = g_A(Y)$ . These conditions on  $X$  and  $Y$  ensure that they are also translates in  $A$ , so this follows from the translation invariance of  $g_A$ .

We will now show that  $g'_A$  is close to  $g_\infty$  by showing that  $g'_A$  is almost a fixed point of  $F_\infty$ . We will estimate

$$\sum_{X \ni 0} |F_\infty(g'_A)(X) - g'_A(X)| \tag{40}$$

where  $F_\infty(g'_A)(X)$  is the coefficient of  $\sigma(X)$  in  $F_\infty(g'_A)$ . Note that we are now using a norm without the weighting factor of  $(|\epsilon| M)^{-w(X)}$ . We divide the terms in this sum into two classes, those with  $w(X) \leq L/4$  and those with  $w(X) > L/4$ . For the latter,  $g'_A(X) = 0$  and

$$\begin{aligned} \sum_{X \ni 0 : w(X) > L/4} |F_\infty(g'_A)(X)| &\leq (|\epsilon| M)^{L/4} \sum_{X \ni 0 : w(X) > L/4} |F_\infty(g'_A)(X)| (|\epsilon| M)^{-w(X)} \\ &= (|\epsilon| M)^{L/4} \|F_\infty(g'_A)\| \end{aligned} \tag{41}$$

where  $\|F_\infty(g'_A)\|$  is the original norm with the exponential weight. Now consider an  $X$  containing 0 for which  $w(X) \leq L/4$ . Then  $g'_A(X) = g_A(X) = F_A(g_A)(X)$ . So we need to compare  $F_\infty(g'_A)(X)$  and  $F_A(g_A)(X)$ .

Consider a term  $X_1, \dots, X_n$  in  $F_\infty$  with  $\sum_i w(X_i) \leq L/4$  and  $X_1 \triangle \dots \triangle X_n = X$ , with  $X$  containing the origin. If  $w(X_i) \leq L/4$ , then  $X_i$  has a translate  $X_i + t$  with  $0 \in X_i + t$  and  $w(X_i + t) \leq L/4$ . So we have  $g'_A(X_i) = g_A(X_i)$ , and the contribution of this term to  $F_\infty(g'_A)(X)$  will be the same as the contribution of this term to  $F_A(g_A)(X)$ . So the difference between  $F_\infty(g'_A)(X)$  and  $F_A(g_A)(X)$  comes from terms with  $\sum_i w(X_i) > L/4$ . Their total contribution to (40) is of order  $(|\epsilon| M)^{L/4}$ . Combining this with (41), we have shown (40) is of order  $(|\epsilon| M)^{L/4}$ . If we apply the contraction mapping theorem with the norm without the weighting factor  $(|\epsilon| M)^{w(X)}$ , this implies

$$\sum_{X \ni 0} |g'_A(X) - g_\infty(X)| \quad (42)$$

is of order  $(|\epsilon| M)^{L/4}$ . And so (36) converges to zero like  $(|\epsilon| M)^{L/4}$  in the infinite volume limit.

### 3. EXCITED STATES

In this section we study the low-lying excited states with one quasi-particle for the model defined by (9) when  $\epsilon$  is small. When  $\epsilon$  is 0, these states for the Hamiltonian (3) have all spins pointing in the  $z$ -direction except for one spin pointing in the opposite direction. Thus the energy of the first excited state is  $|A|$ -fold degenerate ( $|A|$  is the number of sites). When  $\epsilon$  is small but not zero, this degenerate eigenvalue should open up into a band of continuous spectrum in the infinite volume limit. The goal is to get a convergent expansion for the eigenfunctions corresponding to this continuous spectrum. This looks impossible since there is no gap around these eigenvalues. However, these excited states are uniquely determined by their momentum. If  $T_l$  denotes translation by  $l$ , then an eigenstate with momentum  $k$  satisfies

$$T_l |\Psi\rangle = e^{-ikl} |\Psi\rangle \quad (43)$$

(For  $d > 1$ ,  $k$  and  $l$  are vectors, and  $kl$  will denote their dot product.) If you look in the subspace with momentum  $k$ , then the first excited state has an isolated eigenvalue. We will show that by building into the wave function the constraint that it has momentum  $k$ , one can get a convergent expansion for the eigenfunction. One of the consequences of our expansion is the following theorem about the energy dispersion relation.

We will always work on a hyper-rectangle:

$$A = \{(i_1, \dots, i_d) : 1 \leq i_j \leq L_j, j = 1, 2, \dots, d\} \quad (44)$$

where  $L_i$  is the length in the  $i$ th direction. The possible momenta are given by  $k = (k_1, \dots, k_d)$  where  $k_i = \frac{2\pi n_i}{L_i}$  and  $n_i = 0, 1, \dots, L_i - 1$ . We denote the ground state energy for a volume  $A$  by  $E_0$ . We let  $E_1(k)$  denote the lowest eigenvalue in the subspace of momentum  $k$  if  $k \neq 0$  and the next to lowest eigenvalue if  $k = 0$ . (We think of this as the energy of the state with one quasiparticle with momentum  $k$ .) These eigenvalues depend on the volume  $A$ . When we wish to emphasize this dependence, we will write them as  $E_0^A$  and  $E_1^A(k)$ . The dispersion relation is

$$\Delta^A(k) = E_1^A(k) - E_0^A \quad (45)$$

When  $\epsilon = 0$ ,  $\Delta^A(k) = 2$  for all  $k$ . For small nonzero  $\epsilon$  we expect  $\Delta^A(k)$  to equal 2 plus a function that is of order  $\epsilon$ . The following theorem essentially says that this function has an infinite volume limit, and this limit has a convergent expansion. We state the theorem in terms of the Fourier coefficients of  $\Delta^A(k)$  rather than the function itself since  $\Delta^A(k)$  is defined for different values of  $k$  for different  $A$ .

**Theorem 2.** There exists an  $\epsilon_0 > 0$  such that for all  $|\epsilon| < \epsilon_0$  the following is true. Write  $\Delta^A(k)$  as a Fourier series:

$$\Delta^A(k) = 2 + \sum_{s \in A} e_s^A e^{iks} \quad (46)$$

There are coefficients  $e_s$ , defined for all  $s \in \mathbb{Z}^d$ , such that for any sequence of finite volumes which are hyper-rectangles and converge to  $\mathbb{Z}^d$ , the coefficients  $e_s^A$  converge uniformly to  $e_s$ . The coefficients  $e_0^A$  and  $e_0$  are at least first order in  $\epsilon$ , and  $e_s^A$  and  $e_s$  are at least of order  $\epsilon^{|s|}$  in the sense that there is a constant  $c$  such that

$$|e_s| \leq (c |\epsilon|)^{|s|} \quad (47)$$

Thus the infinite volume dispersion relation may be defined by

$$\Delta(k) = 2 + \sum_{s \in \mathbb{Z}^d} e_s e^{iks} \quad (48)$$

**Remark.** The bounds on the  $e_s$  are only upper bounds. Some of the  $e_s$  may be higher order in  $\epsilon$  than the theorem indicates.

We start the proof by considering what states with momentum  $k$  look like. A function  $\psi(\sigma)$  has momentum  $k$  if

$$T_j \psi(\sigma) = e^{-ikj} \psi(\sigma) \quad (49)$$

If  $X$  is any subset of the lattice, then we can form such a function by letting

$$\phi_{X,k}(\sigma) = \sum_l e^{ikl} \sigma(X+l) \quad (50)$$

where  $X+l$  is the set of sites  $\{i+l : i \in X\}$ . The above sum is over sites in  $\mathcal{A}$ . All subsequent sums in this section will be over sites in  $\mathcal{A}$  unless otherwise indicated. We claim that these functions span the subspace of momentum  $k$ . It suffices to show that if we consider all  $k$ , then these functions span the entire state space. Since

$$\sum_k \phi_{X,k}(\sigma) = |\mathcal{A}| \sigma(X) \quad (51)$$

the span of the functions  $\phi_{X,k}(\sigma)$  includes the functions  $\sigma(X)$  for all  $X$ . The latter form a basis for the state space, so the  $\phi_{X,k}$  span the state space.

While these functions span the subspace of momentum  $k$ , they are not linearly independent. For some choices of  $X$  and  $k$ ,  $\phi_{X,k}(\sigma)$  will be zero. For example, if  $X = \emptyset$  or  $\mathcal{A}$ , then the function is zero unless  $k = 0$ . Furthermore,

$$\phi_{X+t,k}(\sigma) = e^{-ikt} \phi_{X,k}(\sigma) \quad (52)$$

So if two  $X$ 's are translates of each other, then the corresponding functions will be the same up to a multiplicative constant. Define  $X$  and  $Y$  to be translationally equivalent if  $X = Y + n$  for some  $n \in \mathcal{A}$ . Then the subsets of  $\mathcal{A}$  can be partitioned into equivalence classes. Pick one set from each equivalence class and let  $\mathcal{X}$  be the resulting collection of sets. Every subset of  $\mathcal{A}$  can be written in the form  $X + n$  for some  $X \in \mathcal{X}$ . While  $X$  is uniquely determined,  $n$  is not. (For example, consider  $X = \emptyset$  or  $\mathcal{A}$ .) If we consider the collection  $\phi_{X,k}$  for  $X \in \mathcal{X}$ , then this collection spans the subspace of momentum  $k$ .

Now suppose that for each  $k$  we have an eigenstate  $\psi_k(\sigma)$  with momentum  $k$ . Let  $\psi(\sigma)$  denote the groundstate wavefunction, (10), obtained in Section 2. Then  $\psi_k(\sigma)/\psi(\sigma)$  also has momentum  $k$ . So it can be written in the form

$$\frac{\psi_k(\sigma)}{\psi(\sigma)} = \sum_{X \in \mathcal{X}} c(X, k) \phi_{X,k}(\sigma) \quad (53)$$

for some coefficients  $c(X, k)$ , which depend on  $k$ . For each  $X$ ,  $c(X, k)$  has a Fourier series

$$c(X, k) = \sum_n e^{-ikn} e(X, n) \quad (54)$$

(The sum over  $n$  is over the sites in  $\Lambda$ .) Then

$$\psi_k(\sigma) = \psi(\sigma) \sum_{X \in \mathcal{X}} \sum_n e^{-ikn} e(X, n) \phi_{X, k}(\sigma) \quad (55)$$

Using (52) this becomes

$$\psi_k(\sigma) = \psi(\sigma) \sum_{X \in \mathcal{X}} \sum_n e(X, n) \phi_{X+n, k}(\sigma) = \psi(\sigma) \sum_X e(X) \phi_{X, k}(\sigma) \quad (56)$$

where the coefficients  $e(X)$  are given by

$$e(X) = \sum_{Y \in \mathcal{X}, n: Y+n=X} e(Y, n) \quad (57)$$

We now have

$$\psi_k(\sigma) = \psi(\sigma) \sum_l e^{ikl} \sum_X e(X) \sigma(X+l) \quad (58)$$

If we define

$$\phi(\sigma) = \sum_X e(X) \sigma(X) \quad (59)$$

then

$$\psi_k(\sigma) = \psi(\sigma) \sum_l e^{ikl} T_l \phi(\sigma) \quad (60)$$

Note that the only momentum dependence in the above is in the explicit factor of  $e^{ikl}$ .

When  $\epsilon = 0$ , the lowest excited states with momentum  $k$  of the Hamiltonian  $H$  defined in (9) are

$$\psi_k(\sigma) = \sum_l e^{ikl} \sigma_l \quad (61)$$

In the above formulation this corresponds to  $c(\{0\}, k) = 1$  for all  $k$  and  $c(X, k) = 0$  for all  $k$  and all  $X \in \mathcal{X}$  other than  $\{0\}$ . This is equivalent to  $e(\{0\}) = 1$  and  $e(X) = 0$  for all  $X$  other than  $\{0\}$ . For nonzero  $\epsilon$  we can normalize the eigenstates so that  $c(\{0\}, k) = 1$  for all  $k$ . This is equivalent to taking  $e(\{0\}) = 1$  and  $e(\{l\}) = 0$  for  $l \neq 0$ . We will show that the other

$e(X)$  are small and localized near 0 when  $\epsilon$  is small. As we showed in the last section, the ground state wave function  $\psi(\sigma)$  can be written as

$$\psi(\sigma) = \exp \left[ -\frac{1}{2} \sum_X g(X) \sigma(X) \right]$$

The ground state is translationally invariant, so  $g(X+l) = g(X)$ .

The action of the Hamiltonian on the wavefunction (58) is

$$\begin{aligned} (H\psi_k)(\sigma) &= \psi(\sigma) \sum_l e^{ikl} \left[ -\sum_j \exp \left( \sum_{Y \ni j} g(Y) \sigma(Y) \right) \right. \\ &\quad \times \left[ \sum_{X \ni j-l} e(X) \sigma(X+l) - \sum_{X \ni j+l} e(X) \sigma(X+l) \right] \\ &\quad \left. + \epsilon \sum_{\langle ij \rangle} \sigma_i \sigma_j \sum_X e(X) \sigma(X+l) \right] \end{aligned}$$

The above needs to equal

$$E_1(k) \psi_k(\sigma) = E_1(k) \psi(\sigma) \sum_l e^{ikl} \sum_X e(X) \sigma(X+l)$$

Cancelling the common factor of  $\psi(\sigma)$ , the Schrödinger equation for the excited state becomes

$$\begin{aligned} \sum_l e^{ikl} \left[ -\sum_j \exp \left( \sum_{Y \ni j} g(Y) \sigma(Y) \right) \left[ \sum_{X \ni j-l} e(X) \sigma(X+l) - \sum_{X \ni j+l} e(X) \sigma(X+l) \right] \right. \\ \left. + \epsilon \sum_{\langle ij \rangle} \sigma_i \sigma_j \sum_X e(X) \sigma(X+l) - E_1(k) \sum_X e(X) \sigma(X+l) \right] = 0 \end{aligned} \quad (62)$$

Recall that the ground state wave function satisfies

$$-\sum_j \exp \left( \sum_{Y \ni j} g(Y) \sigma(Y) \right) + \epsilon \sum_{\langle ij \rangle} \sigma_i \sigma_j = E_0 \quad (63)$$

Multiplying this equation by  $\sum_l e^{ikl} \sum_X e(X) \sigma(X+l)$  and subtracting the result from Eq. (62), we have

$$\begin{aligned} 2 \sum_l e^{ikl} \sum_j \exp \left( \sum_{Y \ni j} g(Y) \sigma(Y) \right) \sum_{X \ni j-l} e(X) \sigma(X+l) \\ = \sum_l e^{ikl} [E_1(k) - E_0] \sum_X e(X) \sigma(X+l) \end{aligned} \quad (64)$$

Define  $h(Y)$  by

$$\exp\left(\sum_{Y \ni 0} g(Y) \sigma(Y)\right) = 1 + \sum_Y h(Y) \sigma(Y) \quad (65)$$

Explicitly,

$$h(Y) = \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{\substack{Y_1, \dots, Y_n: 0 \in Y_j, \\ Y_1 \Delta \dots \Delta Y_n = Y}} g(Y_1) \cdots g(Y_n) \quad (66)$$

Note that  $h(Y)$  is localized near the origin. Using the translation invariance of the  $g(Y)$ , we have

$$\exp\left(\sum_{Y \ni j} g(Y) \sigma(Y)\right) = 1 + \sum_Y h(Y) \sigma(Y+j) \quad (67)$$

Inserting this in (64)

$$\begin{aligned} & 2 \sum_l e^{ikl} \sum_j \left[ 1 + \sum_Y h(Y) \sigma(Y+j) \right] \sum_{X \ni j-l} e(X) \sigma(X+l) \\ & = \sum_l e^{ikl} [E_1(k) - E_0] \sum_X e(X) \sigma(X+l) \end{aligned} \quad (68)$$

The change of variables  $j \rightarrow j+l$  changes this to

$$\begin{aligned} & 2 \sum_l e^{ikl} \sum_j \left[ 1 + \sum_Y h(Y) \sigma(Y+j+l) \right] \sum_{X \ni j} e(X) \sigma(X+l) \\ & = \sum_l e^{ikl} [E_1(k) - E_0] \sum_X e(X) \sigma(X+l) \end{aligned} \quad (69)$$

Using

$$\sum_j \sum_{X \ni j} e(X) \sigma(X+l) = \sum_X |X| e(X) \sigma(X+l) \quad (70)$$

this becomes

$$\begin{aligned} & 2 \sum_l e^{ikl} \sum_X |X| e(X) \sigma(X+l) \\ & \quad + 2 \sum_l e^{ikl} \sum_Y \sum_X \sum_{j \in X} h(Y) e(X) \sigma([(Y+j) \Delta X] + l) \\ & = \sum_l e^{ikl} [E_1(k) - E_0] \sum_X e(X) \sigma(X+l) \end{aligned} \quad (71)$$

We can write  $E_1(k) - E_0$  as a Fourier series in  $k$ . Since this quantity equals 2 when  $\epsilon = 0$ , it is natural to write it in the form

$$E_1(k) - E_0 = 2 + \sum_m e^{-ikm} e_m \quad (72)$$

Inserting this in (71) and making the change of variables  $l \rightarrow l + m$  and then  $X \rightarrow X - m$  in the second term, the right side of (71) becomes

$$2 \sum_l e^{ikl} \sum_X e(X) \sigma(X+l) + \sum_{l,m} e^{ikl} e_m \sum_X e(X-m) \sigma(X+l) \quad (73)$$

Thus Eq. (71) is of the form

$$\sum_l e^{ikl} \sum_X f(X) \sigma(X+l) = 0 \quad (74)$$

where

$$f(X) = 2 |X| e(X) + 2 \sum_{Y,Z,j \in \mathbb{Z}: (Y+j)\Delta Z = X} h(Y) e(Z) - 2e(X) - \sum_m e_m e(X-m) \quad (75)$$

Obviously, if  $f(X) = 0$  for all  $X$ , then Eq. (74) holds. We will argue that the converse is true.

We rewrite (74) as

$$\sum_l e^{ikl} \sum_X f(X-l) \sigma(X) = 0 \quad (76)$$

This must hold for all  $\sigma$ , so for all  $X$  and  $k$  we must have

$$\sum_l e^{ikl} f(X-l) = 0 \quad (77)$$

Fix an  $X$  and regard  $f(X-l)$  as a function of  $l$ . Since the above equation holds for all  $k$ , we must have  $f(X-l) = 0$  for all  $l$ . This proves the converse, and so eq. (74) is equivalent to  $f(X) = 0$  for all  $X$ .

We now assume that  $e(\{0\}) = 1$  and  $e(\{l\}) = 0$  for all  $l \neq 0$ . A priori there is no reason that a solution with these properties must exist, but we will show that it does. As we saw before this is essentially a normalization condition on the eigenstates. If  $X = \{s\}$ , then the  $2|X|e(X)$  and  $2e(X)$

terms in  $f(X)$  cancel. For such an  $X$ ,  $e(X-m)$  is zero except when  $m=s$ , in which case it is 1. So for such  $X$ ,  $f(X) = 0$  becomes

$$e_s = 2 \sum_{Y, Z, j \in Z: (Y+j) \Delta Z = \{s\}} h(Y) e(Z) \quad (78)$$

For  $X$  with  $|X| \neq 1$  (including the case of  $X = \emptyset$ ), the equation  $f(X) = 0$  can be written as

$$e(X) = \frac{1}{2(|X|-1)} \left[ -2 \sum_{Y, Z, j \in Z: (Y+j) \Delta Z = X} h(Y) e(Z) + \sum_m e_m e(X-m) \right] \quad (79)$$

We will show these equations have a solution by writing them as a fixed point equation. Consider the set of variables

$$e := \{e(X) : |X| \neq 1\} \cup \{e_s : s \in \Lambda\} \quad (80)$$

Equations (78) and (79) form a fixed point equation for  $e$

$$F(e) = e \quad (81)$$

Let us introduce the norm

$$\|e\| := \sum_s |e_s| (|\epsilon| M)^{-|s|} + 2 \sum_{X: |X| \neq 1} |e(X)| \left| |X| - 1 \right| (|\epsilon| M)^{-w_0(X)} \quad (82)$$

The factor of 2 is included merely for convenience. Here  $w_0(X)$  denotes the number of bonds in the smallest connected set of bonds containing  $X$  and the origin, and  $|s|$  is the  $l^1$  norm of the site  $s$ . Note that  $|s| = w_0(\{s\})$ . If  $X = X_1 \Delta \cdots \Delta X_n$ , then

$$w_0(X) \leq w_0(X_1) + \cdots + w_0(X_n) \quad (83)$$

We prove that the fixed point equation for  $e$  has a solution by using the contraction mapping theorem as we did in the previous section. We must show that there is a  $\delta > 0$  such that

$$\|F(e) - F(e')\| \leq \frac{1}{2} \|e - e'\| \quad \text{for } \|e\|, \|e'\| \leq \delta \quad (84)$$

$$\|F(e)\| \leq \delta \quad \text{for } \|e\| \leq \delta \quad (85)$$

To verify (84), we use (78) and (79) to see that

$$\begin{aligned} \|F(e) - F(e')\| &\leq \sum_{X: |X| \neq 1} (|\epsilon| M)^{-w_0(X)} \\ &\quad \times \left[ 2 \sum_{Y, Z, j \in Z: (Y+j) \Delta Z = X} |h(Y)[e(Z) - e'(Z)]| \right. \\ &\quad \left. + \sum_s |e_s e(X-s) - e'_s e'(X-s)| \right] \\ &\quad + 2 \sum_l (|\epsilon| M)^{-|l|} \sum_{Y, Z, j \in Z: (Y+j) \Delta Z = \{l\}} |h(Y)[e(Z) - e'(Z)]| \end{aligned} \tag{86}$$

For a site  $l$ , we have  $w_0(\{l\}) = |l|$ , so the above

$$\begin{aligned} &= 2 \sum_{Y, Z, j \in Z} (|\epsilon| M)^{-w_0((Y+j) \Delta Z)} |h(Y)[e(Z) - e'(Z)]| \\ &\quad + \sum_s \sum_{X: |X| \neq 1} (|\epsilon| M)^{-w_0(X)} |e_s e(X-s) - e'_s e'(X-s)| \end{aligned} \tag{87}$$

We claim that for  $j \in Z$  we have  $w_0((Y+j) \Delta Z) \leq w_0(Y) + w_0(Z)$ . To see this, let  $A$  and  $B$  be connected sets of bonds containing the origin such that  $Y \subset A$ ,  $Z \subset B$  and  $|A| = w_0(Y)$  and  $|B| = w_0(Z)$ . Since the origin is in  $A$ , the site  $j$  is in  $A+j$ . The site  $j$  is also in  $Z$  and so is in  $B$ . Since each of  $A+j$  and  $B$  is connected and they both contain  $j$ , their union is connected. So if we define  $C = (A+j) \cup B$ , then  $C$  is a connected set of bonds which contains the origin and  $(Y+j) \Delta Z$ . So

$$w_0((Y+j) \Delta Z) \leq |C| \leq |A+j| + |B| = |A| + |B| = w_0(Y) + w_0(Z) \tag{88}$$

We also have  $w_0(X) \leq w_0(X-s) + |s|$ . The sum over  $j$  in (87) then produces a factor of  $|Z|$ . So (87) is

$$\begin{aligned} &\leq 2 \sum_{Y, Z} (|\epsilon| M)^{-w_0(Y) - w_0(Z)} |Z| |h(Y)[e(Z) - e'(Z)]| \\ &\quad + \sum_s \sum_{X: |X| \neq 1} (|\epsilon| M)^{-w_0(X-s) - |s|} |e_s e(X-s) - e'_s e'(X-s)| \end{aligned} \tag{89}$$

Since  $e(Z) = e'(Z)$  if  $|Z| = 1$ , and  $|Z| \leq 2 ||Z| - 1|$  if  $|Z| \neq 1$ , we have

$$\begin{aligned} &\sum_Z (|\epsilon| M)^{-w_0(Z)} |Z| |e(Z) - e'(Z)| \\ &\leq \sum_{Z: |Z| \neq 1} (|\epsilon| M)^{-w_0(Z)} 2 ||Z| - 1| |e(Z) - e'(Z)| \leq \|e - e'\| \end{aligned} \tag{90}$$

So the first of the two terms in (89) is bounded by

$$2 \sum_Y (|\epsilon| M)^{-w_0(Y)} |h(Y)| \|e - e'\| \tag{91}$$

After the change of variables  $X \rightarrow X + s$ , the second term in (89) equals

$$\begin{aligned} & \sum_s \sum_{X: |X| \neq 1} (|\epsilon| M)^{-w_0(X) - |s|} |e_s e(X) - e'_s e'(X)| \\ & \leq \sum_s \sum_{X: |X| \neq 1} (|\epsilon| M)^{-w_0(X) - |s|} [|e_s e(X) - e_s e'(X)| + |e_s e'(X) - e'_s e'(X)|] \\ & \leq \frac{1}{2} \|e\| \|e - e'\| + \frac{1}{2} \|e - e'\| \|e'\| \leq \delta \|e - e'\| \end{aligned} \tag{92}$$

where we have used the triangle inequality and the fact that  $\|e\|$  and  $\|e'\|$  are no greater than  $\delta$ . Combining (91) and (92), we have

$$\|F(e) - F(e')\| \leq K \|e - e'\| \tag{93}$$

where

$$K = 2 \sum_Y (|\epsilon| M)^{-w_0(Y)} |h(Y)| + \delta \tag{94}$$

From (66) and (83)

$$\begin{aligned} & \sum_Y (|\epsilon| M)^{-w_0(Y)} |h(Y)| \\ & \leq \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{Y_1 \ni 0, \dots, Y_n \ni 0} (|\epsilon| M)^{-w_0(Y_1) - \dots - w_0(Y_n)} |g(Y_1) \cdots g(Y_n)| = e^{\|g\|} - 1 \end{aligned} \tag{95}$$

So

$$K \leq 2(e^{\|g\|} - 1) + \delta \tag{96}$$

If  $\delta$  and  $\epsilon$  are small enough, then  $K \leq 1/2$ .

To prove (85), we use (78) and (79) to compute  $F(0)$ . Note that  $e = 0$  means that  $e(X) = 0$  for all  $X$  except  $X = \{0\}$ . We always have  $e(\{0\}) = 1$ . Letting  $e'$  denote  $F(0)$ , we have

$$e'_i = 2 \sum_{Y: Y \Delta \{0\} = \{i\}} h(Y) \tag{97}$$

and for  $X$  with  $|X| \neq 1$  (including the case of  $X = \emptyset$ ),

$$e'(X) = -\frac{1}{(|X|-1)} \sum_{Y: Y \Delta \{0\} = X} h(Y) \quad (98)$$

Thus

$$\|F(0)\| \leq 2 \sum_Y (|\epsilon| M)^{-w_0(Y)} |h(Y)| \leq 2(e^{\|g\|} - 1) \quad (99)$$

Hence, for  $\|e\| \leq \delta$  and  $\epsilon$  small enough that  $2(e^{\|g\|} - 1) < \delta/2$ ,

$$\|F(e)\| \leq \|F(e) - F(0)\| + \|F(0)\| \leq \frac{1}{2} \|e\| + \|F(0)\| \leq \delta \quad (100)$$

This completes the proof that the fixed point equation has a solution.

We still must prove that for each  $k$ , the eigenstate we have constructed has the lowest eigenvalue in the subspace of momentum  $k$  if  $k \neq 0$  and has the next to lowest eigenvalue if  $k = 0$ . When  $\epsilon = 0$  we know that this is true. So if we can prove that within the subspace of momentum  $k$ , our eigenstate is never degenerate for  $|\epsilon| \leq \epsilon_0$ , then we are done. We will use the local uniqueness of solutions to the fixed point equation to prove this.

Let  $\psi_k(\sigma)$  continue to denote the eigenfunctions constructed above with eigenvalues  $E_1(k)$ . Suppose that for some  $k_0$  there is another eigenfunction  $\psi'(\sigma)$  with momentum  $k_0$  and eigenvalue  $E_1(k_0)$ . We can write it in the form

$$\psi'(\sigma) = \psi(\sigma) \sum_{X \in \mathcal{X}} c'(X) \phi_{X, k_0}(\sigma) \quad (101)$$

For small  $\alpha$  we define

$$\psi_k^\alpha(\sigma) = \psi_k(\sigma) \quad (102)$$

for  $k \neq k_0$  and

$$\psi_{k_0}^\alpha(\sigma) = \frac{\psi_{k_0}(\sigma) + \alpha \psi'(\sigma)}{1 + \alpha c'(\{0\})} \quad (103)$$

(We need only consider small  $\alpha$ , so we are not dividing by zero in the above.) Then for all small  $\alpha$ ,  $\psi_k^\alpha(\sigma)$  is an eigenstate of  $H$  with eigenvalue  $E_1(k)$  and momentum  $k$  for all  $k$ . These states can be written in the form

$$\psi_k^\alpha(\sigma) = \psi(\sigma) \sum_{X \in \mathcal{X}} c_\alpha(X, k) \phi_{X, k}(\sigma) \quad (104)$$

where  $c_\alpha(X, k)$  is just  $c(X, k)$  for  $k \neq k_0$  and

$$c_\alpha(X, k_0) = \frac{c(X, k_0) + \alpha c'(X, k_0)}{1 + \alpha c'(\{0\})} \quad (105)$$

As before we can write this in the form

$$\psi_k^\alpha(\sigma) = \psi(\sigma) \sum_X e_\alpha(X) \phi_{X,k}(\sigma) \quad (106)$$

where

$$c_\alpha(X, k) = \sum_n e^{-ikn} e_\alpha(X, n) \quad (107)$$

and

$$e_\alpha(X) = \sum_{Y \in \mathcal{X}, n: Y+n=X} e_\alpha(Y, n) \quad (108)$$

We have normalized things so that  $e_\alpha(\{0\}) = 1$  and  $e_\alpha(\{l\}) = 0$  for  $l \neq 0$ . It follows from what we have done before that for small  $\alpha$ ,  $e_\alpha(X)$  is a solution of the fixed point equation (75). As  $\alpha \rightarrow 0$ ,  $e_\alpha(X) \rightarrow e(X)$ . However, our solution of the fixed point equation is locally unique by the contraction mapping theorem. Thus  $e_\alpha(X) = e(X)$  for small  $\alpha$ . This implies that the second eigenfunction  $\psi'$  is in fact just a multiple of  $\psi_{k_0}$ . This completes the proof that the eigenfunctions we have constructed are indeed the lowest excited states.

The existence of the infinite volume limit and the convergence of  $e_s^A$  to  $e_s$  follow from the estimates of this section and the arguments of the previous section. In the fixed point equation, (78) and (79),  $h(Y)$  depends on the volume. However, the difference between it and its infinite volume limit is exponentially small in  $L$ . The extension of  $e(X)$  to a function  $e'(X)$  that is defined for all  $X$  is simpler than the definition of  $g'(X)$  in the previous section. We can simply define  $e'(X)$  to be  $e(X)$  if  $X$  is in  $A$  and 0 otherwise. The bounds on the  $e_s$  follow from our choice of norm (82) which implies that

$$|e_s| \leq (\epsilon |M|)^{|s|} \|e\| \quad (109)$$

and so  $e_s$  is of order  $|\epsilon|^{|s|}$ . This completes the proof of Theorem 2. ■

As an application of the theorem, we show that the minimum of the dispersion relation occurs at  $k = (\pi, \dots, \pi)$  if  $\epsilon > 0$  and at  $k = (0, \dots, 0)$  if  $\epsilon < 0$ . We can use our expansion for the dispersion relation to compute the order  $\epsilon$  contribution to the dispersion relation. Consider Eq. (78) for the

coefficients  $e_s$ . Recall that  $e(\{0\}) = 1$ . Otherwise,  $e(Z)$  is always at least order  $\epsilon$ . For all  $Y$ ,  $h(Y)$  is at least order  $\epsilon$ . So  $e_s$  can get an order  $\epsilon$  contribution from the sum in (78) only for  $Z = \{0\}$ . In this case  $j$  must be zero. The constraint on the sum is  $Y \Delta \{0\} = \{s\}$ , which is equivalent to  $Y = \{0\} \Delta \{s\}$ . From (21) we see that the only  $Y$ 's for which  $g(Y)$  has a nonzero contribution at first order in  $\epsilon$  are the sets containing two sites which are nearest neighbors. For such sets  $g(Y) = \epsilon/2 + O(\epsilon^2)$ . Thus from (66) we see that  $h(Y)$  has a nonzero contribution at first order in  $\epsilon$  only if  $Y$  is a set consisting of two nearest neighbors, one of which is the origin. For such sets  $h(Y) = \epsilon/2 + O(\epsilon^2)$ . Since  $Y = \{0\} \Delta \{s\}$ ,  $e_s$  has a first order contribution only if  $s$  is a nearest neighbor of 0, i.e.,  $|s| = 1$ . In this case Eq. (78) gives  $e_s = \epsilon + O(\epsilon^2)$ . Thus

$$\Delta(k) = 2 + \epsilon \sum_{s: |s|=1} e^{iks} + \sum_{s \in \mathbb{Z}^d} e'_s e^{iks} = 2 + 2\epsilon \sum_{i=1}^d \cos(k_i) + \sum_{s \in \mathbb{Z}^d} e'_s e^{iks} \quad (110)$$

where the  $e'_s$  are all of order  $\epsilon^2$ , and  $k_i$  are the components of the vector  $k$ .

We consider the case of  $\epsilon > 0$ . The argument in the other case is analogous. Obviously,  $2 + 2\epsilon \sum_{i=1}^d \cos(k_i)$  has its minimum at  $k = (\pi, \dots, \pi)$ . To show this is true for  $\Delta(k)$  we consider two cases. It is easy to see that  $k = (\pi, \dots, \pi)$  is a critical point of  $\Delta(k)$  and by computing the Hessian that this critical point must be a local minimum. So there is a  $\delta > 0$  so that  $\Delta(k)$  is greater than its value at  $(\pi, \dots, \pi)$  provided  $|k_i - \pi| < \delta$  for all  $i$ . If any  $k_i$  has  $|k_i - \pi| \geq \delta$ , then  $2 + 2\epsilon \sum_{i=1}^d \cos(k_i)$  is greater than its minimum value by at least  $O(\delta^2)$ . The difference between  $2 + 2\epsilon \sum_{i=1}^d \cos(k_i)$  and  $\Delta(k)$  is  $O(\epsilon^2)$ , so  $|k_i - \pi| \geq \delta$  implies  $\Delta(k)$  is greater than its value at  $k = (\pi, \dots, \pi)$  provided  $\epsilon$  is small compared to  $\delta$ .

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