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On the Spectrum of the Heisenberg Hamiltonian

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The quantum, antiferromagnetic, spin-1/2 Heisenberg Hamiltonian on the d-dimensional cubic lattice $\mathbb{Z}^d$ is considered for any dimension d. First the anisotropic case is considered for small transversal coupling and a convergent expansion is given for a family of eigenprojections which is complete in all finite-volume truncations. Then the general case is considered, for which an upper bound to the ground-state energy is given which is optimal for strong enough anisotropy. This bound is expressed through a functional involving the statistical expectation value at finite temperature of a certain correlation function of an Ising model defined on the lattice $\mathbb{Z}^d$ itself.

KEY WORDS: Antiferromagnetic Heisenberg model; perturbation theory; Monte Carlo method.

There are two reasons why I became interested in the spin-$\frac{1}{2}$, antiferromagnetic, quantum Heisenberg model in many dimensions and at zero temperature. First, this model describes a large class of antiferromagnetic insulators and it is attracting much interest because its understanding is of basic importance for the construction of a theory of high-temperature superconductivity. Second, this is one of the simplest nontrivial quantum many-body problems for which no exact solution is available. In this note I analyze this model perturbatively, starting from the Ising limit and treating the transversal coupling as the perturbation. The literature on this sort of perturbation theory is given in ref. 1. From the mathematical point of view, the problem of controlling the convergence of such expansions shows difficulties of a type scarcely considered so far. In fact, a straightforward application of Rayleigh–Schrödinger expansions is bound to fail

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because, as often happens in many-body problems, the perturbation is not relatively bounded with respect to the main part, i.e., the Ising Hamiltonian. To overcome this obstruction, I follow ref. 2 and make use of a dressing transformation which permits one at once to write a directly controllable expansion for the ground state, to define quasiparticles as local perturbations of the ground state, and to study their interactions. As in ref. 1, I end up with cluster expansions for all local observables. However, I do not use Matsubara–Feynman, but a new diagrammatic technique which has the property of yielding controllable expansions. Since the present series for any local observable are the same as those obtained with the methods of ref. 1, this provides an indirect proof of the convergence of their methods. Finally, I prove a formula which can be used to set up a variational Monte Carlo method to estimate the ground-state energy of the isotropic Heisenberg model in all dimensions. Such an estimate is actually an upper bound which is saturated for strong enough anisotropy. These numerical applications are discussed in ref. 5.

1. INTRODUCTION AND RESULTS

Let us consider the following family of Heisenberg Hamiltonians

$$H_\lambda = \sum_{\langle xy \rangle} (1 + \sigma_x^{(3)}\sigma_y^{(3)}) + \lambda(\sigma_x^{(1)}\sigma_y^{(1)} + \sigma_x^{(2)}\sigma_y^{(2)}) \tag{1.1}$$

Here $\sigma^{(1)}$, $\sigma^{(2)}$, and $\sigma^{(3)}$ are the Pauli matrices, λ is a parameter, and Λ is a torus obtained by gluing the opposite faces of a cube in $\mathbb{Z}^d$. The Hilbert space is $\mathscr{H} = \bigotimes_{i\in\Lambda} \mathbb{C}^2$. We are interested in the properties of (1.1) in the infinite-volume limit $\Lambda \uparrow \mathbb{Z}^d$.

To state the first result, let us introduce the function $a^d(\lambda)$, analytic for λ small, which is implicitly defined by the following equation:

$$a^d(\lambda) = \frac{1}{1+4d}\,[d(1+\lambda)\exp(4a^d(\lambda)) + (1-d)\lambda - d] \tag{1.2}$$

We have $a^d(0) = 0$. Let ρ_d be the radius of analyticity around $\lambda = 0$ of $a^d(\lambda)$. Moreover, let $\{E_n\}_{n=0,1,\ldots}$ denote the set of those integers which form the spectrum of the Ising Hamiltonian H_0 and let P_n be the spectral projection on the nth eigenspace. In Sections 2 and 3 I prove the following theorem.

Theorem 1. (i) For all $n \geqslant 0$, all $|\lambda|$ small enough, and all cubes Λ large enough, there exist eigenprojections P_n for the operator H_λ which depend analytically on n but not on Λ, and are such that $P_{n0} = P_n$. For $n = 0$, P_0 has a two-dimensional range and its radius of analyticity is not smaller than that of $a^d(\lambda)$, i.e., ρ_d. For $n \geqslant 1$, the radius of analyticity of P_n is not smaller than

$$[4e^2 k_d(E_n+2)+ek_d]^{-1} \tag{1.3}$$

where k_d is the smallest constant such that $\sum_{n=m}^{\infty} a_n^d |\lambda|^n \leqslant (k_d|\lambda|)^m$ for all $m \geqslant 0$, where $a^d(\lambda)=\sum_{n=1}^{\infty} a_n^d \lambda^n$.

(ii) For $|\lambda|$ small enough, the two eigenvalues $E'_{0\lambda}$ and $E''_{0\lambda}$ of H_λ restricted to $P_{0\lambda}\mathscr{H}$ are separated by a finite gap uniform in Λ as $\Lambda \uparrow \mathbb{Z}^d$, from the rest of the spectrum of H_λ. Moreover, we have

$$|E'_{0\lambda}-E''_{0\lambda}| = O(|\Lambda|\,(c_d\lambda)^{|\Lambda|/2})$$

as $\Lambda \uparrow \mathbb{Z}^d$, where c_d is a constant.

The two eigenstates of lowest energy, i.e., those which span the subspace $P_{0\lambda}\mathscr{H}$, have the form

$$\exp\left(-\frac{1}{2}\sum_{\gamma} J_\gamma(\lambda)\tau_\gamma\right)[|N\rangle \pm |N'\rangle] \tag{1.4}$$

Here the sum runs over all finite subsets γ of Λ; the $J_\gamma(\Lambda)$ are analytic functions of λ; $|N\rangle$ and $|N'\rangle$ are the two Néel states; and τ_γ is the operator

$$\tau_\gamma = \prod_{x\in\gamma} \tau_x \tag{1.5}$$

where τ_x is the operator which flips the spin on the site x,

$$\tau_x = \sigma_x^{(1)}: \quad \begin{cases} |\uparrow\rangle \to |\downarrow\rangle \\ |\downarrow\rangle \to |\uparrow\rangle \end{cases}$$

Since the energy difference among the two states (1.4) vanishes in the infinite-volume limit, it is natural to try a wave function of the form

$$|J\rangle = \exp\left(\frac{-1}{2}\sum_{\gamma} J_\gamma \tau_\gamma\right)|N\rangle \tag{1.6}$$

as a variational ansatz to bound from above the ground-state energy. Thanks to Theorem 1, in the infinite-volume limit and for strong enough anisotropy, this bound is optimal. The problem of evaluating the expectation value of the energy for states of the form (1.6) can easily be handled with a Monte Carlo procedure once one knows the identity reported below.

Theorem 2. For all λ, we have

$$\langle J|J\rangle^{-1}\langle J|H_\lambda|J\rangle=[\mathrm{Tr}(e^{-H_J})]^{-1}\,\mathrm{Tr}(P(J,\lambda)e^{-H_J}) \tag{1.7}$$

where H_J is the following Ising Hamiltonian:

$$H_J=\sum_\gamma J_\gamma\prod_{x\in\gamma}\sigma_x \tag{1.8}$$

with $\sigma_x=\sigma_x^{(3)}=\left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right)$ and

$$P(J,\lambda)=\sum_{\langle x_0y_0\rangle}\left\{1+(\lambda\sigma_{x_0}\sigma_{y_0}-1)\prod_{\gamma\not\supset\!\!\!\!\!\cap\,\langle x_0y_0\rangle}\left(\mathrm{ch}\,J_\gamma+\mathrm{sh}\,J_\gamma\prod_{x\in\gamma}\sigma_x\right)+\lambda\sigma_{x_0}\sigma_{y_0}\right\} \tag{1.9}$$

Here $\langle x_0y_0\rangle$ is any bond of $\mathbb{Z}^d$ and the notation $\gamma\not\supset\!\!\!\!\!\cap\,\langle x_0y_0\rangle$ means that the set γ touches but does not contain the bond $\langle x_0y_0\rangle$.

This result is proven in Section 4, while the discussion of its numerical applications is given in another paper.[5]

I conclude this section with a few words about the strategy of the proof of Theorem 1. To fix the notation, I anticipate that I found it convenient to rewrite the Hamiltonian (1.1) as follows:

$$H_\lambda=\sum_{\langle xy\rangle\subset\Lambda}(\sigma_x\sigma_y+1)+\lambda\tau_x\tau_y(1-\sigma_x\sigma_y) \tag{1.10}$$

where $\sigma=\sigma^{(3)}=\left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right)$ and τ was defined in (1.6). I shall also introduce the operators $S=\sum_{\langle xy\rangle}(\sigma_x\sigma_y+1)$ and $K=\sum_{\langle xy\rangle}\tau_x\tau_y(1-\sigma_x\sigma_y)$ so that

$$H_\lambda=S+\lambda K \tag{1.11}$$

The main difficulty of this problem of perturbation theory is that the perturbation λK is not relatively bounded with respect to S in the infinite-volume limit, so that Rayleigh–Schrödinger expansions cannot be applied directly. To get rid of this problem I follow ref. 2 and make a dressing transformation defined by a self-adjoint operator $R(\lambda)$ analytic for $|\lambda|$ small, such that

$$e^{-R(\lambda)}(S+\lambda K)e^{R(\lambda)}=S+V(\lambda)+E_0(\lambda)+F(\lambda)(|N\rangle\langle N'|+|N'\rangle\langle N|) \tag{1.12}$$

Here $E_0(\lambda)$ and $F(\lambda)$ are analytic functions with $F(\lambda)=O(|\Lambda|\,|c_d\lambda|^{|\Lambda|/2}$ as $\Lambda\uparrow\mathbb{Z}^d$, for some constant c_d. Here $V(\lambda)$ is an operator which annihilates the Néel states. The existence of $R(\lambda)$ proves that the subspace $e^{R(\lambda)}P_0\mathscr{H}$

is invariant under H_λ. Hence $P_{0\lambda}$ exists, is analytic, and is the orthogonal projection onto $e^{R(\lambda)}P_0\mathscr{H}$. Moreover, in Section 3 I shall verify that with the present choice of $R(\lambda)$, $V(\lambda)$ turns out to be relatively bounded with respect to S. Hence, after a dressing transformation and the subtraction of the infinite constant $E_0(\lambda)$ from (1.2), one is in a situation in which Rayleigh–Schrödinger expansions *can* be used to represent the other eigenprojections. This permits us to conclude the proof of Theorem 1.

2. THE DRESSING TRANSFORMATION

In this section I prove that, for every cube Λ, there are an operator $R(\lambda)$ and functions $E_0(\lambda)$ and $F(\lambda)$ analytic in a disc around $\lambda=0$ of size independent of Λ such that $F(\lambda)=O(|\Lambda|\ |c_d\lambda|^{|\Lambda|/2})$ for some constant c_d as the cubes Λ tend to $\mathbb{Z}^d$, and we have

$$e^{-R(\lambda)}H_\lambda e^{R(\lambda)}|N\rangle = E_0((\lambda)|N\rangle + F(\lambda)|N'\rangle \tag{2.1}$$

The operators solving the conjugacy problem (2.1) are not uniquely determined by this property. One way to take advantage of the freedom left is to look for a solution of the form $R(\lambda)=\sum_{n=1}^{\infty}\lambda^n R_n$, where

$$R_n=\sum_{\gamma} r_{n\gamma}\prod_{x\in\gamma}\tau_x \tag{2.2}$$

Note that with this choice of $R(\lambda)$, if (2.1) is satisfied, then also the equation obtained by interchanging $|N\rangle$ and $|N'\rangle$ holds, so that we find (1.12). The $r_{n\gamma}$ in (2.2) are constants determined by the following recursive relations, which are derived from (2.1):

$$\begin{aligned}[S, R_n]|N\rangle &= SR_n|N\rangle\\ &= -\sum_{\substack{i_1\leqslant\cdots\leqslant i_m\\ \# i\geqslant 2,\,|i|=n}}\frac{1}{(i)!}[\cdots[S, R_{i_1}],\dots, R_{i_m}]|N\rangle\\ &\quad -\sum_{\substack{j_1\leqslant\cdots\leqslant j_m\\ |j|=n-1}}\frac{1}{(j)!}[\cdots[K, R_{j_1}],\dots, R_{j_m}]|N\rangle\\ &\quad + E_{0n}|N\rangle + F_n|N'\rangle\end{aligned} \tag{2.3}$$

where E_{0n} and F_n are the nth coefficients of the power series expansions for $E_0(\lambda)$ and $F(\lambda)$, respectively. The operators S and K have been defined in

Section 1 and I use the following notations for the multi-indices $i=(i_1,..., i_m)$ of positive integers:

$$(i)! = \prod_{n=1}^{\infty} [\# \{i_j = n\}]! \tag{2.4}$$

$$|i| = i_1 + \cdots + i_m \tag{2.5}$$

For $n=1$, we have

$$R_1 = - \sum_{\langle xy \rangle} \frac{1}{4d-2} \tau_x \tau_y \tag{2.6}$$

i.e., the constants $r_{1\gamma}$ are nonzero only if γ is a bond and in this case they are equal to $-1/(4d-2)$.

For $n>1$, we have

$$[\cdots [\sigma_{x_0}\sigma_{y_0}, R_{i_1}] \cdots R_{i_m}] = (-2)^m \sum_{\gamma_1 \not\supseteq \langle x_0 y_0 \rangle} \cdots \sum_{\gamma_m \not\supseteq \langle x_0 y_0 \rangle} r_{i_1\gamma_1} \cdots r_{i_m\gamma_m} \tau_{\gamma_1} \cdots \tau_{\gamma_m} \sigma_{x_0}\sigma_{y_0} \tag{2.7}$$

Let $F_{i_1 \cdots i_m}$ be the coefficient of the operator $\tau_\Lambda \sigma_{x_0}\sigma_{y_0}$ in (2.7). Note that this coefficient vanishes if $|i| < \frac{1}{2}|\Lambda|$.

Let us introduce the notation $\varepsilon(\gamma)$ for the constant for which

$$S\tau_\gamma |N\rangle = \varepsilon(\gamma)\tau_\gamma |N\rangle \tag{2.8}$$

$\varepsilon(\gamma)$ is the number of frustrated bonds of the configuration $\tau_\gamma|N\rangle$. But $\varepsilon(\gamma)$ also has another interpretation. Observe that the constants $r_{m\gamma}$ are invariant under translations or rotations by an angle $\frac{1}{4}\pi$ of the set γ. Hence, the functions $r_{n\cdot}$ and $\varepsilon(\cdot)$ can be projected on the quotient set $\mathscr{C}$ between the set of all nonvoid subsets γ of Λ different by Λ, modulo the group generated by these symmetry operations. For each bond $\langle x_0 y_0 \rangle$ and class $\tilde{\gamma} \in \mathscr{C}$, we have

$$\# \{\gamma \in \tilde{\gamma} \text{ s.t. } \langle x_0 y_0 \rangle \not\supseteq \gamma\} = 2\varepsilon(\gamma) = 2\varepsilon(\tilde{\gamma}) \tag{2.9}$$

One can thus estimate as follows the norm of the operator (2.7) applied to $|N\rangle$ minus the component along $|N'\rangle$:

$$\begin{aligned} &\| [\cdots [\sigma_{x_0}\sigma_{y_0}, R_{i_1}] \cdots R_{i_m}] |N\rangle - F_{i_1 \cdots i_m} |N'\rangle \| \\ &\leqslant \sum_{\tilde{\gamma}_1 \cdots \gamma_m} 4^m |r_{i_1\tilde{\gamma}_1} \cdots r_{i_m\tilde{\gamma}_m}| \varepsilon(\tilde{\gamma}_1) \cdots \varepsilon(\tilde{\gamma}_m) \\ &= 4^m r^*_{i_1} \cdots r^*_{i_m} \end{aligned} \tag{2.10}$$

where

$$r_i^* = \sum_{\tilde{\gamma} \in \mathscr{C}} |r_{i\tilde{\gamma}}| \, \varepsilon(\tilde{\gamma}) \tag{2.11}$$

Hence, the norm of the first two terms on the right-hand side of (2.3) is bounded from above by

$$d|\Lambda| \, f(r_1,..., r_{n-1}) \tag{2.12}$$

where $d|\Lambda|$ is the number of bonds and

$$f(r_1,..., r_{n-1}) \equiv \sum_{\substack{i_1 \leqslant \cdots \leqslant i_m \\ \# i \geqslant 2, |i| = n}} \frac{4^m}{(i)!} r_{i_1}^* \cdots r_{i_m}^* + \sum_{\substack{j_1 \leqslant \cdots \leqslant j_m \\ |j| = n-1}} \frac{4^m}{(j)!} r_{j_1}^* \cdots r_{j_m}^* \tag{2.13}$$

On the other hand, thanks to (2.8), the norm of the left-hand side of (2.3) is equal to

$$\sum_{\gamma} |r_{n\gamma}| \, \varepsilon(\gamma) \geqslant |\Lambda| \sum_{\tilde{\gamma}} |r_{n\tilde{\gamma}}| \, \varepsilon(\tilde{\gamma}) = |\Lambda| \, r_n^* \tag{2.14}$$

In fact, $|\Lambda|$ gives a lower bound to the number of elements in a class of $\mathscr{C}$. Taking together (2.13) and (2.14), we find

$$r_n^* \leqslant df(r_1^*,..., r_{n-1}^*) \tag{2.15}$$

Let a_n^d be the sequence defined by the following recursive relations:

$$\begin{aligned} &a_1^d = r_1^* = 1 \\ &a_n^d = df(a_1^d,..., a_{n-1}^d) \qquad \text{for} \quad n \geqslant 2 \end{aligned} \tag{2.16}$$

We have $a_n^d \geqslant r_n^*$ for all $n \geqslant 1$. Thus, $R(\lambda)$ is analytic in a disc around the zero whose radius is not smaller than the radius of convergence of the series

$$a^d(\lambda) = \sum_{n=1}^{\infty} a_n^d \lambda^n \tag{2.17}$$

The function $a^d(\lambda)$ satisfies formally the following equation:

$$a^d(\lambda) = d(1 + \lambda) e^{4a^d(\lambda)} + (1 - d) \, \lambda - d - 4da^d(\lambda) \tag{2.18}$$

In fact, the right-hand side can be expanded as follows:

$$\begin{aligned} &\lambda + d \sum_{n=2}^{\infty} \frac{4^n}{n!} [a^d(\lambda)]^n + d\lambda \sum_{n=1}^{\infty} \frac{4^n}{n!} [a^d(\lambda)]^n \\ &\quad = \lambda + d \sum_{n=2}^{\infty} \lambda^n f(a_1^d,..., a_{n-1}^d) \end{aligned} \tag{2.19}$$

$a^d(\lambda)$ exists and it is analytic around $\lambda=0$ if and only if Eq. (2.18) admits such a solution. But this is a consequence of the implicit function theorem.

As a consequence of the estimates above, we also find the following bound:

$$|F(\lambda)| \leqslant \sum_{n=|\Lambda|/2}^{\infty} d|\Lambda| f(r_1,..., r_{n-1})\lambda^n$$
$$\leqslant |\Lambda| \sum_{n=|\Lambda|/2}^{\infty} a_n^d \lambda^n = O[|\Lambda| (c_d \lambda)^{|\Lambda|/2}]$$

as $\Lambda \uparrow \mathbb{Z}^d$, where c_d is a constant.

3. THE EXCITED STATES

In this section I study the operator $V(\lambda)$ such that

$$e^{-R(\lambda)}(S+\lambda K)e^{R(\lambda)} = E_0(\lambda) + S + V(\lambda) + F(\lambda)[|N\rangle\langle N'| + |N'\rangle\langle N|] \quad (3.1)$$

and prove that it is relatively bounded with respect to S (see Kato[4] for the definition of relative boundedness). The relative bound is not larger than $20a^d(\lambda)$, where $a^d(\lambda)$ is the function defined in (1.2). In particular, this bound is uniform in Λ as $\Lambda \uparrow \mathbb{Z}^d$ and it permits the control of the Rayleigh–Schrödinger expansion for the eigenprojection $P_{n\lambda}$ for any n, in the infinite-volume limit.

For the operator $V(\lambda)$ we have

$$V(\lambda) = \sum_{\langle x_0 y_0 \rangle} \left\{ \tau_{x_0}\tau_{y_0} + \sum_{n=1}^{\infty} \lambda^n \left[\sum_{\substack{i_1 \leqslant \cdots \leqslant i_m \\ |i|=n}} \frac{(-2)^m}{(i)!} \right.\right.$$
$$\times \sum_{\substack{\gamma_1 \not\supseteq \langle x_0 y_0 \rangle \\ \cdots \\ \gamma_m \not\supseteq \langle x_0 y_0 \rangle}} r_{i_1\gamma_1} \cdots r_{i_m\gamma_m} \tau_{\gamma_1} \cdots \tau_{\gamma_m} \sigma_{x_0}\sigma_{y_0}$$
$$\left.\left. - \sum_{\substack{j_1 \leqslant \cdots \leqslant j_m \\ |j|=n-1}} \frac{(-2)^m}{(i)!} \sum_{\substack{\gamma_1 \not\supseteq \langle x_0 y_0 \rangle \\ \cdots \\ \gamma_m \not\supseteq \langle x_0 y_0 \rangle}} r_{i_1\gamma_1} \cdots r_{i_m\gamma_m} \tau_{\gamma_1} \cdots \tau_{\gamma_m} \tau_{x_0}\tau_{y_0}\sigma_{x_0}\sigma_{y_0} \right]\right\} \quad (3.2)$$

The relative form boundedness of $V(\lambda)$ with respect to S is established by the following lemma.

Lemma 3.1. The following bound holds for the operator norm of $\tilde{V}(\lambda) = S^{-1/2}V(\lambda)S^{-1/2}$

$$\|S^{-1/2}V(\lambda)S^{-1/2}\|_1 \leqslant \frac{2e^2 k_d|\lambda|}{1-ek_d|\lambda|} \quad (3.3)$$

where k_d is the largest constant such that $\sum_{n=m}^{\infty} a_n^d |\lambda|^n \leqslant (k_d |\lambda|)^m$ for all $m > 0$.

Proof. We have

$$\|S^{-1/2} V(\lambda) S^{-1/2}\|_1$$
$$\leqslant \sup_{\gamma} \|S^{-1/2} V(\lambda) S^{-1/2} |\gamma\rangle\|_1$$
$$= \sup_{\gamma} \sum_{\langle xy\rangle \cap \gamma} \sum_{n=1}^{\infty} \sum_{\gamma' : d(\gamma,\gamma')=n} \varepsilon(\gamma)^{-1/2} \varepsilon(\gamma')^{-1/2} |\langle\gamma'| Q_{xy}(\lambda) |\gamma\rangle| \tag{3.4}$$

where

$$Q_{xy}(\lambda) = \sum_{m=1}^{\infty} \lambda^m Q_{x,y;m}$$
$$= e^{-R(\lambda)} H_{xy} e^{R(\lambda)} - 1 - \sigma_x^{(3)} \sigma_y^{(3)} - \frac{E_0(\lambda)}{2d|\Lambda|} \tag{3.5}$$

and

$$H_{xy} = 1 + \sigma_x^{(3)} \sigma_y^{(3)} + \lambda(\sigma_x^{(1)} \sigma_y^{(1)} + \sigma_x^{(2)} \sigma_y^{(2)}) \tag{3.6}$$

The distance $d(\gamma, \gamma')$ between two excitations γ and γ' is defined as the minimal length of a connected graph whose endpoints are $\gamma \Delta \gamma' = (\gamma \cup \gamma') \backslash (\gamma \cap \gamma')$. We have

$$(3.4) = \sup_{\gamma} \sum_{\langle xy\rangle \cap \gamma} \sum_{n=1}^{\infty} \sum_{\gamma' : d(\gamma,\gamma')=n} \sum_{m=n}^{\infty} |\lambda|^m$$
$$\times \varepsilon(\gamma)^{-1/2} \varepsilon(\gamma')^{-1/2} |\langle\gamma'| Q_{xy;m} |\gamma\rangle| \tag{3.7}$$

From the first part of the proof, we see that $\|Q_{xy;m}\|_1 \leqslant 2a_m^d$. Hence we have

$$(3.4) \leqslant \sup_{\gamma} \sum_{n=1}^{\infty} 2(k_d |\lambda|)^n \sup_{\gamma' : d(\gamma,\gamma')=n} \left[\frac{\varepsilon(\gamma)}{\varepsilon(\gamma')}\right]^{1/2}$$
$$\leqslant 2 \sum_{n=1}^{\infty} (k_d |\lambda|^n) \sup_{\gamma} \left[\frac{\varepsilon(\gamma)}{\max(1, \varepsilon(\gamma) - n)}\right]^{1/2}$$
$$\leqslant 2 \sum_{n=1}^{\infty} (k_d |\lambda|^n) e^{1+n} = \frac{2e^2 k_d |\lambda|}{1 - k_d e |\lambda|} \qquad \text{QED} \tag{3.8}$$

We can now complete the proof of Theorem 1.

(i) The projection $P_{n\lambda}$ for $n>0$ is given by the following contour integral:

$$P_{n\lambda}=\oint_{\mathscr{C}_n}\frac{d\zeta}{2\pi i}\frac{1}{\zeta-S_\lambda-V(\lambda)}$$

where $\mathscr{C}_n$ is a circle of radius $\frac{1}{2}$ in the complex plane with origin in E_n. Remark that $|\Lambda|$ is assumed to be so large that the distance between two eigenvalues of S_λ is at least 1, so that $\mathscr{C}_n$ encloses only one point of the spectrum of S, i.e., E_n. To control the resolvent in (3.14) one can expand it in a Rayleigh–Schrödinger series. We have

$$\frac{1}{\zeta-S_\lambda-V(\lambda)}=(S_\lambda+1)^{-1/2}\sum_{n=0}^{\infty}\frac{1}{\zeta(S_\lambda+1)^{-1}-S_\lambda(S_\lambda+1)^{-1}}$$
$$\times\left[\tilde{V}(\lambda)\frac{1}{\zeta(S_\lambda+1)^{-1}-S_\lambda(S_\lambda+1)}\right](S_\lambda+1)^{-1/2} \qquad (3.9)$$

Also,

$$\left\|\frac{1}{\zeta(S_\lambda+1)^{-1}-S_\lambda(S_\lambda+1)^{-1}}\right\|=\left\|\frac{S_\lambda+1}{\zeta-S_\lambda}\right\|\leqslant 1+\left\|\frac{1}{\zeta-S_\lambda}\right\|(1+|\zeta|)$$
$$\leqslant 1+2\left(E_n+\frac{3}{2}\right)=2E_n+4$$

Hence, due to (3.3) we have

$$\left\|\tilde{V}(\lambda)\frac{1}{\zeta(S_\lambda+1)^{-1}-S_\lambda(S_\lambda+1)^{-1}}\right\|\leqslant\frac{2e^2k_d|\lambda|}{1-ek_d|\lambda|}(2E_n+4)$$

The series (3.9) converges for those λ so small that (1.3) holds.

(ii) Let us consider the following contour integral:

$$\oint_{\mathscr{C}_0}\frac{d\zeta}{2\pi i}\frac{1}{\zeta-S_\lambda-V(\lambda)}$$

where $\mathscr{C}_0=\{|\zeta|=3/2\}$. One can prove as above that this integral is an analytic operator-valued function in a disc around $\lambda=0$. This integral gives the spectral projection on the eigenspace corresponding to the eigenvalues contained in the circle $\mathscr{C}_0$. Since the dimension of this space is an integer-valued analytic function of λ for λ small, it must be a constant so far as it is analytic. This proves that the two eigenvalues contained in $\mathscr{C}_0$ for $\lambda=0$ remain separated by a finite gap, uniform in Λ, from the rest of the spectrum of $S+V(\lambda)$. Moreover, these two eigenvalues can be explicitely computed in terms of the quantities introduced above and they are given by $\pm F(\lambda)$. Hence the lowest lying eigenvalues of H_λ are $E_0(\lambda)\pm F(\lambda)=E_0(\lambda)+O(|\Lambda|(c\lambda)^{d|\Lambda|})$. QED

4. AN UPPER BOUND ON THE GROUND-STATE ENERGY

In this section I prove the second theorem stated in Section 1. If Λ is a cube of $\mathbb{Z}^d$ to which we restrict our system by imposing periodic boundary conditions, we have to verify the following equality:

$$\langle J|J\rangle^{-1}\langle J|\,H_\lambda\,|J\rangle=\frac{\mathrm{Tr}(P(J,\lambda)e^{-H_J})}{\mathrm{Tr}(e^{-H_J})} \tag{4.1}$$

where $|J\rangle$ is the state

$$|J\rangle=\exp\left(-\frac{1}{2}\sum_\gamma J_\gamma\prod_{x\in\gamma}\tau_x\right)|N\rangle \tag{4.2}$$

and

$$P(J,\lambda)=1+(\lambda\sigma_{x_0}\sigma_{y_0}-1)\prod_{\gamma\not\supseteq\langle x_0y_0\rangle}\left(\mathrm{ch}\,J_\gamma+\mathrm{sh}\,J_\gamma\prod_{x\in\gamma}\sigma_{3x}\right)+\lambda\sigma_{x_0}\sigma_{y_0} \tag{4.3}$$

Let us begin by proving that

$$\langle J|J\rangle=2^{-|\Lambda|}\,\mathrm{Tr}(e^{-H_J}) \tag{4.4}$$

We have

$$\langle J|J\rangle=\langle N|\prod_\gamma\left(\mathrm{ch}\,J_\gamma-\mathrm{sh}\,J_\gamma\prod_{x\in\gamma}\tau_x\right)|N\rangle \tag{4.5}$$

$$=\left(\prod_\gamma\mathrm{ch}\,J_\gamma\right)\left[1+\sum(-1)^n\,\mathrm{th}\,J_{\gamma_1}\cdots\mathrm{th}\,J_{\gamma_n}\right] \tag{4.6}$$

where the sum runs over all collections of subsets $(\gamma_i)_{i=1,\dots,n}$ such that

$$\prod_{x_1\in\gamma_1}\cdots\prod_{x_n\in\gamma_n}\tau_{x_1}\cdots\tau_{x_n}=\mathbb{1} \tag{4.7}$$

where $\mathbb{1}$ denotes the identity operator. Equation (4.6) derives from (4.5) because the expectation value in the state $|N\rangle$ of a product of τ operators on distinct sites is zero. On the other hand, we have

$$\mathrm{Tr}(e^{-H_J})=\sum_{\{\sigma\}}\prod_\gamma\left(\mathrm{ch}\,J_\gamma-\mathrm{sh}\,J_\gamma\prod_{x\in\gamma}\sigma_x\right) \tag{4.8}$$

where the sum runs over all the eigenstates that the operators σ_x have in common. If we expand the product and sum over all the Ising configurations, the terms containing the product of an odd number of spins σ_x on one site cancel each other. We thus find (4.4).

Next, let us compute $\langle J|\,\sigma_{x_0}\sigma_{y_0}\,|J\rangle$. We have

$$\sigma_{x_0}\sigma_{y_0}|J\rangle = \prod_\gamma \left(\operatorname{ch}\frac{J_\gamma}{2} \pm \operatorname{sh}\frac{J_\gamma}{2}\prod_{x\in\gamma}\tau_x\right)\sigma_{x_0}\sigma_{y_0}|N\rangle \tag{4.9}$$

where the plus sign appears if $\gamma \underset{\not\supset}{\cap} \langle x_0 y_0\rangle$; otherwise the minus sign is there. Hence we have

$$\langle J|\,\sigma_{x_0}\sigma_{y_0}\,|J\rangle = -\left(\prod_\gamma \operatorname{ch} J_\gamma\right)\left[1+\sum{}'\,(-1)^n \operatorname{th} J_{\gamma_1}\cdots \operatorname{th} J_{\gamma_n}\right] \tag{4.10}$$

where the sum runs over all collections $(\gamma_i)_{i=1,\dots,n}$ fulfilling (4.7) and such that $\gamma_i \underset{\not\supset}{\cap} \langle x_0 y_0\rangle$. We have

$$\operatorname{Tr}\left(\left[\prod_{\gamma \underset{\not\supset}{\cap} \langle x_0 y_0\rangle}\left(\operatorname{ch} J_\gamma + \operatorname{sh} J_\gamma \prod_{x\in\gamma}\sigma_x\right)\right]e^{-H_J}\right) = -2^{|\Lambda|}\langle J|\,\sigma_{x_0}\sigma_{y_0}\,|J\rangle \tag{4.11}$$

Analogously, one can find the equalities

$$\langle J|\,\tau_{x_0}\tau_{y_0}\,|J\rangle = 2^{-|\Lambda|}\operatorname{Tr}(\sigma_{x_0}\sigma_{y_0}e^{-H_J}) \tag{4.12}$$

and

$$\langle J|\,\tau_{x_0}\tau_{y_0}\sigma_{x_0}\sigma_{y_0}\,|J\rangle$$
$$= -2^{-|\Lambda|}\operatorname{Tr}\left\{\sigma_{x_0}\sigma_{y_0}\left[\prod_{\gamma \underset{\not\supset}{\cap} \langle x_0 y_0\rangle}\left(\operatorname{ch} J_\gamma + \operatorname{sh} J_\gamma \prod_{x\in\gamma}\sigma_x\right)\right]e^{-H_J}\right\} \tag{4.13}$$

which, together with (4.11) and (4.4), imply (4.1). QED.

Note added. After the completion of this paper I learned that T. Kennedy has proved some of the results I discuss here, with different methods; his work has not yet appeared. See, however, ref. 3.

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