

## Spin Waves in Quantum Ferromagnets

J. L. van Hemmen,<sup>1,3</sup> A. A. S. Brito,<sup>2,4</sup> and W. F. Wreszinski<sup>2,5</sup>

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Low-temperature properties of Heisenberg quantum ferromagnets ("spin waves") are derived within a *configuration* space formalism. Most of the work is done without explicitly assuming translational invariance. We provide a general criterion, classical domination, to decide about the nature and uniqueness of ground states for a large class of quantum ferromagnets. We also analyze and clarify the Dyson formalism and indicate why an energy gap between the physical ground state and the improper (unphysical) states does not exist. This is of particular relevance to the kinematical interaction. Using reflection positivity we provide upper and lower bounds to the contribution of the dynamical interaction to the free energy. In a certain approximation, these bounds imply that the dynamical interaction may be dropped if the inverse temperature  $\beta$  and the spin quantum number  $S$  are large enough.

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### 1. INTRODUCTION AND SYNOPSIS

For quite a long time spin-wave theory has called for a simple and transparent, yet mathematically rigorous, formulation. The present situation is well illustrated by quoting a definition of the notion of spin wave as it still holds, but was given by Dyson in his monumental work<sup>(1,2)</sup> on the subject: "a single reversed spin distributed *coherently* over a large number of

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<sup>1</sup> Sonderforschungsbereich 123, Universitaet Heidelberg 6900 Heidelberg 1, Federal Republic of Germany.

<sup>2</sup> Instituto de Física, Universidade de São Paulo, Caixa Postal 20516-01000 São Paulo, Brazil.

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otherwise aligned atomic spins in a crystal lattice” (the italization is ours). This definition clearly isolates two important ingredients of the usual spin-wave theory: (a) the system is translation invariant, and (b) the temperature is low, far below the critical point (if any), so that the situation may be described as a small deviation from the ground state. But whereas the second condition is necessary to obtain a justification of linear spin-wave theory,<sup>6</sup> the former condition seems less relevant and is certainly not appropriate in the study of *random* systems.<sup>(6)</sup>

There are two, at first sight different, approaches to spin-wave theory. The first and earliest stems from Bloch himself<sup>(7)</sup> and corresponds to the definition referred to above. The second originated from the work of Holstein and Primakoff<sup>(8)</sup> and was further developed by van Kranendonk and van Vleck.<sup>(9)</sup> It consists in introducing first a certain Boson representation at each site, in terms of which the Hamiltonian is expressed. Then the Hamiltonian is reduced to a bilinear form and diagonalized exactly. It turns out that the latter approach, which *explicitly* reduces the original dynamical system to an ideal Bose gas of magnons, is more fruitful and that, in the translation invariant case, it is fully equivalent to the original Bloch approach.

Our present considerations apply to ferromagnets only. Ferromagnets have a well-defined and, under suitable conditions, unique ground state, which is known explicitly—a fact which will be crucial to our analysis later on. Nevertheless, it still remains quite remarkable that as Anderson<sup>(10)</sup> has shown, the ground-state energy of a Heisenberg spin-1/2 *anti*-ferromagnet in the linear spin-wave approximation is only 3% off the exact value. We have verified that the error for the one-dimensional spin-1/2 *XY* model with various degrees of anisotropy amounts to approximately 5%. In both models the ground state of the infinite system was taken to be the classical one, which is expected to become exact for large values of the spin quantum number  $S$ .

In Section 2 we present a classical domination principle. It enables us to decide quickly—for any  $S$  and any dimension  $\nu$ —whether a Hamiltonian has a ferromagnetic ground state and, if so, whether this ground state is unique. In Section 3 we introduce the physical Hamiltonian, which is positive and of direct relevance to later work, analyze the Holstein–Primakoff formalism, and shed new light on Dyson’s work.<sup>(1,2)</sup> Everything is done in *configuration* space, and nowhere do we invoke translational invariance. In contrast to Dyson,<sup>(2)</sup> we find a multitude of states in the so-called improper Hilbert space, with the same energy as the physical ground state (see Appendix A).

<sup>6</sup> More recently, it was proven that spin waves play a slightly different role near the critical point, in the form of “infrared bounds”.<sup>(3–5)</sup>

Hence there is *no* volume-independent energy gap between the improper Hilbert space and the ground state.

The Holstein–Primakoff approach directly aims at constructing a *quadratic* boson Hamiltonian in configuration space. To obtain this Hamiltonian one has to drop both the kinematical interaction, which refers to the restriction that the number of boson excitations at any site  $x$  should not exceed  $2S$ , and the dynamical interaction, which incorporates some quartic terms. The nonexistence of the energy gap referred to above directly bears on the study of the kinematical interaction. In view of the existing difficulties (Appendix A) we did not spend too much effort on this problem, however.

What can be said if we first drop the dynamical interaction so as to obtain the “kinematical” Hamiltonian? Employing reflection positivity (whose present usage requires translational invariance—see Section 4) and admitting a plausible approximation (for large  $S$ ) discussed in Section 4, we are able to obtain satisfying results (Theorem 4.6) on the asymptotic equality of the full and the kinematical free energy provided  $\beta$  and  $S$  are large enough. This is an important step into the direction of a low-temperature expansion of the free energy,<sup>7</sup> and we hope our paper may provide additional stimulation for further research on the subject.

## 2. CLASSICAL DOMINATION

Ground states of quantum Heisenberg models have received considerable interest ever since the conception of the model. The most famous Ansatz was given by Bethe<sup>(12)</sup> for an antiferromagnetic chain of spins  $1/2$ . But, to determine the ground state, one would like to have a general principle that is valid, at least in the ferromagnetic case, in any dimension, and not only for spins  $1/2$ .

Throughout this paper we adopt the following Hamiltonian:

$$H_A = \frac{1}{2} \sum_{x,y \in A} \{J(x,y)[S_1(x)S_1(y) + S_2(x)S_2(y)] + J_3(x,y)[S_2(x)S_3(y) - S^2]\} + h \sum_{x \in A} [S_3(x) + S] \quad (2.1)$$

with

$$J_3(x,y) \geq |J(x,y)| \quad (2.2)$$

<sup>7</sup> A complete low-temperature asymptotic expansion for the free energy of the classical  $XY$  model has been achieved recently.<sup>(11)</sup> The methods used in Ref. 11 are, however, inherently classical.

and  $\hbar \geq 0$ . For the moment we put  $\hbar = 0$ . As usual,  $\Lambda$  is a finite domain in the (hyper) cubic lattice  $\mathbb{Z}^p$ . At each site  $x$  we have a spin angular momentum  $\mathbf{S}(x)$ . The spin quantum number  $S$  may assume any of its allowed values:  $0, 1/2, 1, \dots$ . But all spins are to be equal. So, once chosen,  $S$  is fixed for the whole lattice. Finally we suppose  $J$  and  $J_3$  to be short range, with  $J(x, x) = J_3(x, x) = 0$ .

Is it true that (2.1) has a ferromagnetic ground state for any  $S$ , and is the ground state unique if some, or all, of the inequalities are strict? These questions arise in a very natural way. So it is desirable, as we noted above, to provide the answers by means of a general, but simple, principle: *classical domination*.

We mean by classical domination that the  $z$  terms in (2.1) dominate the  $xy$  terms. More specifically,

$$S^2 - S_3(x) S_3(y) \geq \pm [S_1(x) S_1(y) + S_2(x) S_2(y)] \quad (2.3)$$

For the special case  $S = 1/2$  this operator inequality was proved by Hepp.<sup>(13)</sup> He proposed to verify (2.3) explicitly by using the  $4 \times 4$  matrix representation of the spin operators. For higher  $S$  values this proposal is not very practical, however.

To prove (2.3) let us start with the case where the plus sign holds, viz.,  $S^2 \geq \mathbf{S}(x) \cdot \mathbf{S}(y)$ . Adding the two spin operators  $\mathbf{S}(x)$  and  $\mathbf{S}(y)$  we obtain the total spin  $\mathbf{S} = \mathbf{S}(x) + \mathbf{S}(y)$ , with the spin quantum number  $L$  ranging from 0 up to  $2S$ . Proving the inequality

$$\mathbf{S}(x) \cdot \mathbf{S}(y) \leq S^2 \quad (2.4)$$

is equivalent to verifying

$$[\mathbf{S}(x) + \mathbf{S}(y)]^2 \leq 2S(2S + 1) \quad (2.5)$$

which is evident since  $0 \leq L \leq 2S$ . So we have shown

$$S^2 - S_3(x) S_3(y) \geq + [S_1(x) S_1(y) + S_2(x) S_2(y)] \quad (2.6)$$

Let us now perform a canonical transformation,

$$S_1(y) \rightarrow -S_1(y), \quad S_2(y) \rightarrow -S_2(y), \quad S_3(y) \rightarrow S_2(y) \quad (2.7)$$

which is nothing but a rotation of  $\mathbf{S}(y)$  through  $\pi$  about the  $z$  axis. The new spin angular momentum is as good as the old one, so it obeys (2.6), and thus we find

$$S^2 - S_3(x) S_3(y) \geq - [S_1(x) S_1(y) + S_2(x) S_2(y)] \quad (2.8)$$

The classical domination inequality may be used to advantage if we want to determine the ground state of the Hamiltonian (2.1), given the condition (2.2). First we notice that the state with all spins down, parallel to the negative  $z$  axis, is an eigenstate of  $H_\Lambda$  with eigenvalue *zero*. Then we apply (2.3) so as to obtain

$$H_\Lambda \geq \frac{1}{2} \sum_{x,y \in \Lambda} [J_3(x,y) - |J(x,y)|] [S^2 - S_3(x) S_3(y)] \quad (2.9)$$

where, by (2.2), the coefficients are positive. The right-hand side of (2.9) is *classical* and, clearly, positive. Thus  $H_\Lambda \geq 0$ , and an eigenstate with eigenvalue zero is a ground state. In a similar vein we could have shown that all spins up represent another ground state. If  $h > 0$ , the spin-flip symmetry is broken, and the configuration with all spins down remains as the only ground state. Plainly, if  $J_3(x,y) = J(x,y) > 0$  and  $h > 0$ , even the full rotation symmetry is broken.

The uniqueness problem associated with the ferromagnetic ground state has already been touched upon. We now prove that between the ground-state energy  $E_0$  and the energy of the first excited state there exists a gap, whose width does not depend on  $\Lambda$ , provided for each  $x$  in  $\Lambda$  we can find a  $y$  in  $\Lambda$  such that

$$J_3(x,y) - |J(x,y)| \geq \varepsilon > 0 \quad (2.10)$$

for some fixed  $\varepsilon$ . Moreover, the state with all spins down represents the *unique* ground state of (2.1), up to spin flip symmetry.

If  $h > 0$ , the assertion is trivial and (2.10) is superfluous. So let us suppose  $h = 0$ . Given  $\Lambda$ , let  $\mathbf{S}$  denote the total spin in  $\Lambda$ ;  $S_3$  is its  $z$  component.  $S_3$  and  $H_\Lambda$  commute, so they may be diagonalized simultaneously in the Hilbert space  $\mathfrak{H}_\Lambda$  that is used to describe the composite system of  $|\Lambda|$  spins. ( $|\Lambda|$  is the number of sites in  $\Lambda$ ). In the orthogonal complement of the two states with all spins up and all spins down *at least one* spin has been flipped. Then (2.9) and (2.10) imply that in this orthogonal complement  $H_\Lambda$  satisfies the relation  $H_\Lambda \geq \varepsilon S > 0$ , so that the gap between  $E_0$  and the energy of the first excited state is at least  $\varepsilon S$ , independent of  $\Lambda$ . An example where (2.10) is realized is provided by a ferromagnetic Heisenberg model with finite anisotropy and periodic boundary conditions; cf. Section 4.

### 3. PHYSICAL HAMILTONIAN, HOLSTEIN-PRIMAKOFF APPROACH, AND DYSON'S FORMALISM

The spin wave formalism amounts to a boson representation of the *low*-temperature elementary excitations of a spin system. It, therefore, is natural

to study the ground-state ( $T=0$ ) representation first (Section 3.1). This representation gives rise to the so-called physical Hamiltonian, which is basic to all that follows. In Section 3.2 we provide the prerequisites for the Holstein–Primakoff approach, and in Section 3.3 we shed new light on the Dyson formalism.

### 3.1. The Physical Hamiltonian

The more usual Hamiltonian describing a Heisenberg ferromagnet is given by

$$H^F = -\frac{1}{2} \sum_{x,y} \{J(x,y)[S_1(x)S_1(y) + S_2(x)S_2(y)] + J_3(x,y)[S_3(x)S_3(y)]\} + h \sum_x S_3(x) \quad (3.1)$$

Here  $x$  and  $y$  range through  $\mathbb{Z}^v$ , and  $F$  stands for formal. The coefficients  $J(x,y)$  and  $J_3(x,y)$  obey (2.2). With  $h > 0$  the model gives rise to a unique ground state, which, for any  $S$  and  $v$ , is represented by all spins down. We wish to derive some properties of the physical Hamiltonian, an object which is intimately related to both the ground state and  $H^F$ .

The lattice being infinite, we consider the incomplete tensor product

$$\mathfrak{H} = \bigotimes_{x \in \mathbb{Z}^v} \mathbb{C}^{2S+1} \quad (3.2)$$

with respect to the ground state  $\bigotimes_x \varphi \downarrow(x) = |0\rangle$ , where  $\varphi \downarrow(x)$  is the state with spin down at  $x$ . The Hilbert space  $\mathfrak{H}$  is generated by

$$\prod_x S_+(x)^{m(x)} |0\rangle \quad (3.3)$$

with

$$m(x) = 0, 1, \dots, 2S \quad \text{and} \quad \sum_x m(x) < \infty \quad (3.4)$$

that is, by finite products of spin creation operators working on  $|0\rangle$ . The linear space of these generating vectors we call  $\mathcal{D}_S$ . The vectors (3.3) constitute an orthogonal, though not yet normalized, basis for  $\mathfrak{H}$ . If we restrict  $x$  to a finite domain  $\mathcal{A}$ , we find the local Hilbert space  $\mathfrak{H}_{\mathcal{A}}$  that fully suffices to describe the finite system inside  $\mathcal{A}$  (whatever the temperature).

Finite products of local spin operators  $\{S_+(x), S_-(x), \text{ and } S_3(x)\}$  generate the local algebra  $\mathfrak{A}_{\mathcal{L}}$ . Its completion, the quasilocal algebra, is

denoted by  $\mathfrak{A}$ . In  $\mathfrak{A}$  we have a dynamical evolution  $\alpha_t$  generated by  $H^F$ .<sup>(14,15)</sup> Now the *physical Hamiltonian* is defined as the (unique) self-adjoint operator  $H$  in  $\mathfrak{H}$  such that

$$\begin{aligned} \mathfrak{A}_L \ni A \mapsto \alpha_t(A) &= \lim_{\Lambda \rightarrow \infty} e^{iH_\Lambda^F t} A e^{-iH_\Lambda^F t} \\ &= e^{iHt} A e^{-iHt} \end{aligned} \quad (3.5)$$

gives the time-evolution automorphism of  $\mathfrak{A}$ , and

$$e^{iHt} |0\rangle = |0\rangle \Leftrightarrow H|0\rangle = 0 \quad (3.6)$$

i.e.,  $H$  annihilates the ground state.  $\mathfrak{H}$  itself is nothing but the GNS Hilbert space<sup>(16)</sup> of the ground-state expectation functional. The operator  $H$  is well defined on a dense domain in  $\mathfrak{H}$ , viz.,  $\mathcal{D}_S$  as given by (3.3), though<sup>(14)</sup>

$$H \left( \prod_x S_+(x)^{m(x)} \right) |0\rangle = \left[ H^F, \prod_x S_+(x)^{m(x)} \right] |0\rangle \quad (3.7)$$

A slightly modified  $\mathcal{D}_S$  where we replace  $S_+(x)$  by  $S_i(x)$ ,  $i = +, -, 3$ , would do as well. That is, for  $A$  in  $\mathfrak{A}_L$  we could define  $HA|0\rangle = [H^F, A]|0\rangle$ . Finally, it turns out<sup>(16)</sup> that  $H$  is *positive*.

Conversely, to obtain an explicit expression for the physical Hamiltonian, we have to find a positive operator  $H$  such that  $H$  has the same commutation relations as  $H^F$ , and  $H|0\rangle = 0$ . In a more mathematical language  $H$  and  $H^F$  give rise to the same derivation. It is not hard to see that  $H$ , when restricted to a finite region  $A$ , must be given by (2.1). The positivity follows from (2.9), and  $H|0\rangle = 0$  is evident, as is (3.7). Since, for any *local*  $A$ ,  $\alpha_t A$  is analytic in  $t$  in a neighborhood of the origin,<sup>(16)</sup> we may infer directly that  $H$  has  $\mathcal{D}_S$  as a dense domain of analytic vectors and, thus, is essentially self-adjoint on  $\mathcal{D}_S$ .

In conclusion,  $H_\Lambda$  as given by (2.1) is the *restriction to  $\Lambda$*  of the physical Hamiltonian  $H$ . Since  $H$  is obtained from  $H^F$  by adding an “infinite positive constant,” their restrictions to finite domains generate essentially the same thermodynamics—at any temperature. It, therefore, suffices to study the system  $\{H_\Lambda; \Lambda \subseteq \mathbb{Z}^v\}$ . In fact, to make sense out of spin waves we need the limit  $S \rightarrow \infty$  together with a certain scaling and the inverse temperature  $\beta$  as adjustable parameter and it is then even imperative to use the physical Hamiltonian.

### 3.2. The Holstein–Primakoff Approach

In the limit  $S \rightarrow \infty$  two methods of scaling are rather natural. One method consists in scaling each spin operator  $\mathbf{S}(x)$  by  $S^{-1}$  so as to get

$S^{-1}\mathbf{S}(x)$ . Then<sup>(17)</sup> the quantum mechanical model becomes *classical* as  $S \rightarrow \infty$  in the sense that the quantum free energy (ground-state energy) and expectation values of intensive observables converge to their classical values, with vectors  $\mathbf{S}(x)$  ranging over the unit sphere. Moreover, the order of taking the limits  $A \rightarrow \infty$  and  $S \rightarrow \infty$  is immaterial.

Since Bloch<sup>(7)</sup> another method has been practiced in solid-state physics. It was rationalized up to a certain extent by Holstein and Primakoff<sup>(8)</sup> and, roughly, amounts to scaling each  $\mathbf{S}(x)$  by  $S^{-1/2}$  so as to obtain *boson* modes. As we will discuss Dyson's work<sup>(1,2)</sup> later on, we quickly turn to the method itself. Our exposition is akin to, but in certain details different from some known constructions,<sup>(18)</sup> which do not seem to be standard, however, and it is germane to applications in subsequent work.

At the site  $x$  the "vacuum" is taken to be  $\varphi^\dagger(x)$ , and denote by  $|0\rangle$  (par abus de langage).  $S_+(x)$  operates repeatedly on  $|0\rangle$  to generate an orthonormal system of  $2S + 1$  eigenvectors of  $S_3(x)$

$$|n(x)\rangle = F(n)^{-1/2} \frac{1}{\sqrt{n!}} \left[ \frac{S_+(x)}{(2S)^{1/2}} \right]^n |0\rangle \quad (3.8)$$

Following Dyson<sup>(1)</sup> we define the *metric tensor*  $F$  by

$$F(n) = 1 \left(1 - \frac{1}{2S}\right) \cdots \left(1 - \frac{n-1}{2S}\right), \quad n = 0, 1, \dots, 2S \quad (3.9)$$

$$F(n) = 0, \quad n \geq 2S + 1$$

and introduce the function  $f_s$  via

$$f_s(n) = 1 - \frac{n}{2S}, \quad n = 0, 1, \dots, 2S \quad (3.10)$$

$$f_s(n) = 0, \quad n \geq 2S + 1$$

Then one may verify

$$\frac{1}{(2S)^{1/2}} S_+ |n\rangle = f_s^{1/2}(n) (n+1)^{1/2} |n+1\rangle \quad (3.11)$$

$$\frac{1}{(2S)^{1/2}} S_- |n\rangle = f_s^{1/2}(n) \sqrt{n} |n-1\rangle$$

which is to be compared with  $a|n\rangle = \sqrt{n}|n-1\rangle$  and  $a^+|n\rangle = (n+1)^{1/2}|n+1\rangle$  for a boson pair  $a$  and  $a^+$  satisfying  $[a, a^+] = 1$ . An *orthonormal* basis for  $\mathfrak{H}$  is defined through

$$|\{n(x)\}\rangle = \bigotimes_{x \in \mathbb{Z}^p} |n(x)\rangle \quad (3.12)$$



where, as before in (3.4),

$$0 \leq n(x) \leq 2S \quad \text{and} \quad \sum_x n(x) < \infty \quad (3.13)$$

Besides  $\mathfrak{H}$  we introduce the boson Fock space  $\mathcal{F}$  with vacuum  $|0\rangle$ , where (magnon) creation and annihilation operators  $a^+(x)$  and  $a(x)$ , with  $x$  in  $R^v$ , act irreducibly,

$$\begin{aligned} [a(x), a^+(y)] &= \delta_{x,y}, & [a(x), a(y)] &= 0 \\ a(x)|0\rangle &= 0 & \forall x \in \mathbb{Z}^v \end{aligned} \quad (3.14)$$

These requirements determine  $\mathcal{F}$  uniquely. If we restrict  $x$  to  $\Lambda \subseteq \mathbb{Z}^v$ , we obtain the local Fock space  $\mathcal{F}_\Lambda$ . An orthonormal basis of  $\mathcal{F}$  is given by

$$|\{m(x)\}\rangle = \prod_{x \in \mathbb{Z}^v} [m(x)!]^{-1/2} a(x)^{m(x)} |0\rangle \quad (3.15)$$

with

$$m(x) = 0, 1, 2, \dots \quad \text{and} \quad \sum_x m(x) < \infty \quad (3.16)$$

The finite linear space of the vectors  $|\{m(x)\}\rangle$  is denoted by  $\mathcal{D}$ .

We now embed  $\mathfrak{H}$  one-to-one into the boson Fock space  $\mathcal{F}$  by

$$\mathcal{Q} |\{m(x)\}\rangle = |\{m(x)\}\rangle \quad (3.17)$$

Note, however, that  $m(x)$  in (3.15) and (3.16) may range from 0 to  $+\infty$ , whereas  $m(x)$  in (3.17) is restricted to the range  $0 \leq m(x) \leq 2S$ . Thus  $\mathfrak{H}$  is a proper subspace of  $\mathcal{F}$ , which is called the *physical Hilbert space*.  $\mathcal{Q}$  being an isometry,  $\mathfrak{H}$  and  $\mathcal{Q}\mathfrak{H}$  are unitarily equivalent.<sup>8</sup> So we may safely limit our discussion to the boson Fock space  $\mathcal{F}$ —more specifically, to the physical Hilbert space which we now again call  $\mathfrak{H}$ .

Let  $P(x)$  be the projection onto the first  $2S + 1$  boson states at the site  $x$ , i.e.,  $|n(x)\rangle$  with  $0 \leq n(x) \leq 2S$ . Then

$$P_\Lambda = \prod_{x \in \Lambda} P(x) \quad (3.18)$$

projects  $\mathcal{F}_\Lambda$  onto  $\mathfrak{H}_\Lambda$ . When there is no fear of confusion we will drop the index  $\Lambda$ . Moreover, let

$$a_s^\#(x) = P(x) a^\#(x) P(x) \quad (3.19)$$

<sup>8</sup> Doing the mapping the other way around we would have obtained Hepp's<sup>(18)</sup> contraction  $T$ .

One easily verifies (we now also drop the argument  $x$ )

$$\begin{aligned} aP &= a_s, & Pa^+ &= a_s^+ \\ a_s^+ a_s &= Pa^+ aP = Pa^+ a = a^+ aP \end{aligned} \quad (3.20)$$

and, with some more effort,

$$\begin{aligned} \frac{1}{(2S)^{1/2}} S_+(x) &\simeq a_s^+(x) f_s^{1/2}(x), & \frac{1}{(2S)^{1/2}} S(x) &\simeq f_s^{1/2}(x) a_s(x) \\ S_3(x) + S &\simeq Pa^+(x) a(x)P \end{aligned} \quad (3.21)$$

with

$$f_s(x) = f_s(n(x)), \quad n(x) = a^+(x) a(x) \quad (3.22)$$

and  $\simeq$  as a unitary equivalence.  $f_s$  is zero outside the physical Hilbert space because of (3.10).  $P$  and  $f_s$  commute.

Returning to  $H_\Lambda$  as given by (2.1), we rescale  $h$  by  $h \rightarrow hS$ , and rewrite the physical Hamiltonian  $H$  in the form

$$\begin{aligned} H &= -\frac{1}{2} \sum_{x,y} \{ \frac{1}{2} J(x,y) [S_+(x) S_-(y) + S_-(x) S_+(y)] \\ &\quad + J_3(x,y) [S_3(x) S_3(y) - S^2] \} + hS \sum_x [S_3(x) + S] \end{aligned} \quad (3.23)$$

Taking advantage of (3.21) we obtain

$$\begin{aligned} S^{-1}H &\simeq P \left\{ -\sum_{x,y} J(x,y) [f_s^{1/2}(x) a(x) a^+(y) f_s^{1/2}(y)] \right. \\ &\quad \left. + \sum_{x,y} \frac{1}{2} J_3(x,y) \left[ n(x) + n(y) - \frac{n(x)n(y)}{S} \right] + h \sum_x n(x) \right\} P \end{aligned} \quad (3.24)$$

or, succinctly,

$$S^{-1}H \simeq P \mathcal{H}_S P, \quad \mathcal{H}_S = \mathcal{H}_S^{xy} + \mathcal{H}_S^z + hN \quad (3.25)$$

where  $N$  is the number operator. Let us consider the main term in  $\mathcal{H}_S^z$ , keeping in mind that at the end we have to multiply by  $P$ ,

$$\begin{aligned} n(x) + n(y) - \frac{n(x)n(y)}{S} &= n(x) f_s(y) + n(y) f_s(x) \\ &= n(x) f_s(x) + n(y) f_s(y) + \frac{1}{2S} [n(x) - n(y)]^2 \end{aligned} \quad (3.26)$$

define

$$\lambda(x) = \sum_y J_3(x, y)$$

and note that

$$\mathcal{H}_S^z = \sum_x \lambda(x) f_S(x) n(x) + \frac{1}{4S} \sum_{x,y} J_3(x, y) [n(x) - n(y)]^2 \quad (3.27)$$

We may absorb the terms with  $\lambda$  into  $\mathcal{H}_S^{xy}$  so as to get a new operator which describes our *kinematical* interaction,

$$\mathcal{H}_S^{\text{kin}} = \sum_{x,y} f_S^{1/2}(x) a(x) [\lambda(x) \delta_{x,y} - J(x, y)] a^\dagger(y) f_S^{1/2}(y) \quad (3.28)$$

The quadratic terms in (3.27) represent our dynamical interaction,

$$\mathcal{H}_S^{\text{dyn}} = \frac{1}{4S} \sum_{x,y} J_3(x, y) [n(x) - n(y)]^2 \quad (3.29)$$

while the remaining *diagonal* terms are represented by

$$\mathcal{H}_S^{\text{diag}} = h \sum_x n(x) - \sum_x \lambda(x) f_S(x) \quad (3.30)$$

The boson Hamiltonian  $\mathcal{H}_S$  is now given by

$$\mathcal{H}_S = \mathcal{H}_S^{\text{kin}} + \mathcal{H}_S^{\text{dyn}} + \mathcal{H}_S^{\text{diag}} \quad (3.31)$$

Suppose for the moment  $h > 0$ . At “low” temperatures “most”  $n(x)$  are expected to be “zero.” To exploit this idea the Ansatz of Holstein and Primakoff<sup>(8)</sup> consisted in taking  $S$  large, putting  $f_S(x) \rightarrow 1$  in (3.29) and (3.30), and dropping  $\mathcal{H}_S^{\text{dyn}}$  altogether. Then one is left with a quadratic boson Hamiltonian  $\mathcal{H}$  whose interaction matrix is determined by

$$D(x, y) = \lambda(x) \delta_{x,y} - J(x, y) \quad (3.32)$$

Invoking, for instance, the Gersgorin circle theorem,<sup>(19)</sup> one easily verifies that  $D$  is positive definite. If  $D$  is strictly positive [if (2.10) holds, or if  $h > 0$ ], the quadratic Hamiltonian may be diagonalized exactly,<sup>(20)</sup> and the thermodynamics, including the free energy and the magnetization [cf. Eq. (3.21)], trivially follows.

In the above derivation we already see the relevance of the physical Hamiltonian (2.1) being positive. Let us trace back the line of argument to see why. Consider  $H^F$  as defined by (3.1) with  $h = 0$ .  $H^F$  is bilinear in the

spin operators. We could find a ground state for  $H^F$  which may be written as a tensor product of one-spin states. These states are eigenstates<sup>9</sup> of  $S_3(x)$  with *maximal* or *minimal*  $z$  component. Subtracting the ground-state energy, which is known, we get a positive operator  $H$ , the physical Hamiltonian. At each site  $x$  we now may apply the substitution (3.21), which is local and refers to the ground state we have found. Since  $H_A$  is also bilinear, as is brought out by Eq. (2.1), the resulting operator  $\mathcal{H}_S$  in (3.24) is bound to be positive, and so is its limit, as  $S \rightarrow \infty$ . The trace of  $\exp(-\beta\mathcal{H}_A)$  would be completely ill-defined and the whole formalism would be meaningless if  $\mathcal{H}_S$  and, hence,  $\mathcal{H}$  had zero or negative eigenvalues. The gist of the argument is, however, that the transformation (3.21) is local because the ground state to which it refers is a tensor product of suitable one-spin states. Counterexamples where the ground state is a tensor product of *two*-spin states are known<sup>(22)</sup>; here the spin wave formalism breaks down. In antiferromagnets with nearest-neighbor interactions<sup>(10)</sup> the *classical* ground state still can be found as a tensor product of one-spin states (up and down), and this, in fact, suffices to make the quadratic boson Hamiltonian  $\mathcal{H}$  positive definite.

Returning to (3.25) or (3.31) and restricting our attention to a bounded region  $A$ , we note that the finite linear space  $\mathcal{D}_A$  of (3.15) with  $x$  in  $A$  is a core of  $\mathcal{H}_A$ , and  $\mathcal{H}_{S,A}$  converges on  $\mathcal{D}_A$  to  $\mathcal{H}_A$  as  $S \rightarrow \infty$ . In view of this observation and the inequality  $\mathcal{H} \geq \hbar N$  it is not hard to show that

$$Z_A(S) = \text{Tr} \exp(-\beta H_A) = \text{Tr} \exp(-\beta P \mathcal{H}_{S,A} P) \quad (3.33)$$

converges to  $\text{Tr} \exp(-\beta \mathcal{H}_A)$ . However, as it stands this result is not very useful. We need an estimate of the difference between the free energy  $f_A(\beta, S)$  of  $H_A$  and  $f_A(\beta)$  of the quadratic boson Hamiltonian  $\mathcal{H}_A$ , which is *uniform* in  $A$ . We anticipate from Section 4 that this difference is small if  $S$  and  $\beta$  are chosen suitably.

### 3.3. The Dyson Formalism

Though intuitively appealing, the Holstein–Primakoff procedure has long called for a justification. Dyson<sup>(1,2)</sup> introduced a new, non-Hermitian, Hamilton operator  $\mathcal{H}_D$ . Since his original derivation was quite involved and delicate, we will present here some simple arguments to elucidate the Dyson formalism. We need not assume any translational invariance.

The equilibrium thermodynamics of a finite region  $A$  is determined by the partition function  $Z_A(S)$ . We want to prove

$$Z_A(S) = \text{Tr} \exp -\beta P \mathcal{H}_{S,A} P = \text{Tr} \exp -\beta P \mathcal{H}_{D,A} P \quad (3.34)$$

<sup>9</sup> Possibly after a local rotation at  $x$ .

where  $\mathcal{H}_{D,\Lambda}$  is the restriction to  $\Lambda$  of the Dyson Hamiltonian  $\mathcal{H}_D$  to be defined below.

We start by mapping the orthonormal basis (3.25) onto an orthogonal one through the “diagonal” transformation

$$\mathbb{F}^{1/2} |\{n(x)\}\rangle \mapsto \prod_x f(x)^{1/2} |\{n(x)\}\rangle \quad (3.35)$$

operating in the physical Hilbert space, with  $n(x) \leq S$  for all  $x$ .  $\mathbb{F}^{1/2}$  is extended to the whole boson Fock space through the identity. The transformation  $\mathbb{F}$  is defined analogously.  $P$  and  $\mathbb{F}$  commute. With respect to this new basis (3.35)  $P\mathcal{H}_S P$  is given by

$$P\mathbb{F}^{1/2}\mathcal{H}_S\mathbb{F}^{-1/2}P = P\mathcal{H}_D P \quad (3.36)$$

i.e., as far as the physical Hilbert space is concerned,  $\mathcal{H}_D$  is obtained by a *similarity transformation*. Let us quickly check the consequences of (3.36) and then return to its definition proper. Denote by  $A$  the diagonal matrix which multiplies by  $a(x)$  at the site  $x$ . Then  $\mathcal{H}_S^{xy}$  may be rewritten [see Eq. (3.24)]

$$\mathcal{H}_S^{xy} = -\mathbb{F}^{1/2} A J A^+ \mathbb{F}^{1/2} \quad (3.37)$$

and thus, by (3.36),

$$\mathcal{H}_D = -\mathbb{F} A J A^+ + \mathcal{H}_S^z + hN \quad (3.38)$$

since  $\mathbb{F}$  is diagonal. In full,

$$\mathcal{H}_D = -\sum_{x,y} J(x,y) f_S(x) a(x) a^+(y) + \mathcal{H}_S^z + hN \quad (3.39)$$

In these equations it is understood that we sandwich by  $P$ . Though  $\mathcal{H}_D$  is non-Hermitian, the spectrum of  $P\mathcal{H}_{D,\Lambda}P$  is real and positive because a similarity transformation preserves the spectrum; cf. (3.36). Moreover, a similarity transformation also leaves invariant the trace. Hence (3.34) holds.

There is a little subtlety, however, in the above argument. As it stands,  $\mathbb{F}$  is not invertible since  $f_S(2S) = 0$ ; cf. Eq. (3.10). We, therefore, modify the function  $f_S$  and define  $f_S(2S) = \varepsilon > 0$ . The modified operators  $\mathcal{H}_{S,\Lambda}^\varepsilon$  and  $\mathcal{H}_{D,\Lambda}^\varepsilon$  are defined accordingly, and

$$\text{Tr} \exp(-\beta P \mathcal{H}_{S,\Lambda}^\varepsilon P) = \text{Tr} \exp(-\beta P \mathcal{H}_{D,\Lambda}^\varepsilon P) \quad (3.40)$$

Now let  $\varepsilon$  go to zero. Equation (3.34) follows. From now on  $f_S(2S) = 0$  holds again.

We finish the argument by noting that

$$P\mathcal{H}_S P = P\mathcal{H}_S \quad \text{and} \quad P\mathcal{H}_D P = P\mathcal{H}_D \quad (3.41)$$

The only case which needs some checking is

$$f_S(x) a(x) |2S + 1\rangle = 0 \quad (3.42)$$

But this is evident once  $f_S(2S) = 0$ . Thus we may write

$$Z_\Lambda(S) = \text{Tr } P \exp(-\beta \mathcal{H}_{D,\Lambda}) P \quad (3.43)$$

Note that  $\mathcal{H}_D$  does not commute with  $P$ , although  $\mathcal{H}_S$  does. This last observation directly follows from (3.41) and from  $\mathcal{H}_S$  being self-adjoint. Accordingly, the physical Hilbert space and its orthogonal complement (the “improper” states) reduce  $\mathcal{H}_S$  but *not*  $\mathcal{H}_D$ . Nevertheless (3.43) holds, which is the starting point of Dyson’s analysis.

#### 4. DROPPING THE DYNAMICAL INTERACTION

A first step towards justifying the Holstein–Primakoff approach consists in dropping the dynamical interaction  $P\mathcal{H}_S^{\text{dyn}}P$  given by (3.29). To this end we require translational invariance and, hence, assume periodic boundary conditions throughout. Furthermore, we restrict our attention to a nearest-neighbor (n.n.) anisotropic Heisenberg model with exchange interactions

$$\begin{cases} J_3(x, y) = \tilde{J}(x, y) \\ J(x, y) = \alpha \tilde{J}(x, y) \end{cases} \quad (4.1)$$

where

$$\tilde{J}(x, y) = \tilde{J}(x - y) = \begin{cases} J & \text{if } |x - y| = 1 \\ 0 & \text{otherwise} \end{cases} \quad (4.2)$$

and  $0 < \alpha < 1$ . The problem will be analyzed in terms of *spin* operators.

We write (3.28)–(3.31) in terms of spin operators:

$$H_\Lambda = H_\Lambda^{\text{kin}} + H_\Lambda^{\text{dyn}} \quad (4.3)$$

where

$$H_\Lambda^{\text{dyn}} = \frac{J}{4S} \sum_{\substack{x, y \in \Lambda \\ (x, y) \text{ n.n.}}} [S_3(x) - S_3(y)]^2 \quad (4.4)$$

and

$$H_\Lambda^{\text{kin}} = \frac{1}{2S} \sum_{x, y \in \Lambda} S_+(x) D_\alpha(x, y) S_-(y) - \frac{Jz}{2S} \sum_{x \in \Lambda} [S_3(x) + S] \quad (4.5)$$

with

$$D_\alpha(x, y) = Jz \delta_{x,y} - \alpha \tilde{J}(x - y) \quad (4.6)$$

As usual,  $z = 2\nu$  is the number of nearest neighbors of a point in  $\mathbb{Z}^\nu$ . Above, we inverted the order of  $a(x)$  and  $a^+(y)$  in the diagonal term in (3.28), leading to a new  $\mathcal{H}_\Lambda^{\text{diag}}$ , which is given in spin language by the second term in (4.5). The latter is “small” near the ferromagnetic ground state  $S_3(x) \approx -S$  if  $S$  is sufficiently large, and was therefore included in  $H_\Lambda^{\text{kin}}$  for convenience. We also set  $h = 0$  in (3.30) and replaced the matrix in (3.28) by  $D_\alpha(x, y)$ , given by (4.6) [which is equivalent to (4.1)]. The anisotropy plays to some extent the role of the external field we left out, and is easier to handle. Note that the spin-wave normalization has already been incorporated in (4.3)–(4.5).

To simplify the notation we denote the free energy of  $H_\Lambda$  by  $f(H_\Lambda)$  and the one related to  $H_\Lambda^{\text{kin}}$  by  $f(H_\Lambda^{\text{kin}})$ , the dependence upon  $\beta$  and  $S$  being understood. For any Hamiltonian  $H$  the expectation value of an observable  $O$  is defined by

$$\langle O \rangle_H = \text{Tr}(e^{-\beta H} O) / \text{Tr} e^{-\beta H}$$

In this section we show that the difference between  $f(H_\Lambda)$  and  $f(H_\Lambda^{\text{kin}})$  is small if  $\beta$  and  $S$  are chosen conveniently. The physics is clear. If the temperature is low, i.e.,  $\beta$  is large, nearly all the spins are down (or up) so that  $[S_3(x) - S_3(y)]^2 / 4S$  is small. Taking suitable linear combinations of these few magnon states we get spin waves. On the other hand, those states which have large values of  $[S_3(x) - S_3(y)]^2$  are energetically unfavorable, in particular at low temperatures, and, hence, will not contribute appreciably to  $f(H_\Lambda)$ . However, making these ideas precise is not that simple. We will tackle the problem via a series of lemmas.

**Lemma 4.1.**

$$0 \leq f(H_\Lambda) - f(H_\Lambda^{\text{kin}}) \leq \frac{1}{|\Lambda|} \langle H_\Lambda^{\text{dyn}} \rangle_{H_\Lambda^{\text{kin}}} \quad (4.7)$$

*Proof.* By the Bogoliubov–Peierls inequality<sup>(23)</sup>

$$\frac{1}{|\Lambda|} \langle H_\Lambda^{\text{dyn}} \rangle_{H_\Lambda} \leq f(H_\Lambda) - f(H_\Lambda^{\text{kin}}) \leq \frac{1}{|\Lambda|} \langle H_\Lambda^{\text{dyn}} \rangle_{H_\Lambda^{\text{kin}}}$$

By (4.4)  $H_\Lambda^{\text{dyn}}$  is positive, and (4.8) follows. ■

The remaining part of this section is devoted to deriving upper bound for the right-hand side of (4.7). Let  $|\sigma(x)\rangle$  denote an eigenfunction of  $S_3(x)$

with eigenvalue  $-S \leq \sigma(x) \leq +S$ , and define projection operators  $P^{\pm\delta}(x)$  by requiring that  $P^{+\delta}(x)$  and  $P^{-\delta}(x)$  project on all the spin states  $|\sigma(x)\rangle$  with  $\sigma(x) \geq \delta$  and  $\sigma(x) \leq -\delta$ , respectively;  $0 \leq \delta \leq S$ . Then

$$P^{<\delta}(x) = 1 - P^{\delta}(x) - P^{-\delta}(x) \quad (4.8)$$

projects onto  $|\sigma(x)\rangle$  with  $|\sigma(x)| < \delta$ . Finally

$$P^{\pm}(x) = P^{\pm(\delta=0)}(x) \quad (4.9)$$

projects onto all states  $|\sigma(x)\rangle$  with  $\sigma(x) \geq 0$  or  $\sigma(x) \leq 0$ .

Our main general estimate is Proposition 4.2. In principle, it does not need any assumption of translational invariance.

**Proposition 4.2.** Let  $x$  be an arbitrary point in  $\mathcal{A}$ . If  $0 < \delta < S$ , then

$$\begin{aligned} \frac{1}{|\mathcal{A}|} \langle H_{\Lambda}^{\text{dyn}} \rangle_{H_{\Lambda}^{\text{kin}}} &\leq \frac{J}{4S} \sum_{y \text{ n.n. of } x} [(S - \delta)^2 \\ &\quad + 2(S + \delta)(3S - \delta) \langle P^{+}(x) P^{-}(y) \rangle_{H_{\Lambda}^{\text{kin}}} \\ &\quad + 8S\delta \langle P^{<\delta}(x) \rangle_{H_{\Lambda}^{\text{kin}}}] \end{aligned} \quad (4.10)$$

*Proof.* We omit lower index  $H_{\Lambda}^{\text{kin}}$  in  $\langle \cdot \rangle_{H_{\Lambda}^{\text{kin}}}$ . By translational invariance we have

$$\frac{1}{|\mathcal{A}|} \langle H_{\Lambda}^{\text{dyn}} \rangle = \frac{J}{4S} \sum_{y \text{ n.n. of } x} \langle [S_3(x) - S_3(y)]^2 \rangle \quad (4.11)$$

where  $x$  may be any point in  $\mathcal{A}$ . Now we get, for any pair  $\langle x, y \rangle$  of nearest neighbours in  $\mathcal{A}$ ,

$$\begin{aligned} \langle (S_3(x) - S_3(y))^2 \rangle &= \langle [P^{\delta}(x) + P^{-\delta}(x) + P^{<\delta}(x)] \\ &\quad \times [P^{\delta}(x) + P^{-\delta}(x) + P^{<\delta}(x)] \cdot [S_3(x) - S_3(y)]^2 \rangle \\ &\leq 4\delta^2 \langle P^{<\delta}(x) P^{<\delta}(y) \rangle + (S - \delta)^2 \{ \langle P^{\delta}(x) P^{\delta}(y) \rangle \\ &\quad + \langle P^{-\delta}(x) P^{-\delta}(y) \rangle \} + 8S^2 \langle P^{-\delta}(x) P^{\delta}(y) \rangle \\ &\quad + 2(S + \delta)^2 \langle (1 - P^{<\delta}(x)) P^{<\delta}(y) \rangle \end{aligned} \quad (4.12)$$

and

$$\begin{aligned} &\langle P^{+\delta}(x) P^{+\delta}(y) + P^{-\delta}(x) P^{-\delta}(y) \rangle \\ &= 1 - \langle P^{<\delta}(x) \rangle - 2 \langle P^{\delta}(x) P^{-\delta}(y) \rangle \\ &\quad - \langle (1 - P^{<\delta}(x)) P^{<\delta}(y) \rangle \end{aligned} \quad (4.13)$$



Substitution of (4.13) into (4.12) yields

$$\begin{aligned} & \langle \{S_3(x) - S_3(y)\}^2 \rangle \\ & \leq (S - \delta)^2 + 2(S + \delta)(3S - \delta) \cdot \langle P^{+\delta}(x) P^{-\delta}(y) \rangle \\ & \quad + 8S\delta \langle P^{<\delta}(x) \rangle + (3\delta^2 - 6S\delta - S^2) \langle P^{<\delta}(x) P^{<\delta}(y) \rangle \end{aligned} \quad (4.14)$$

To improve the inequality we may drop the last term from (4.14) since  $3\delta^2 - 6S\delta - S^2 < 0$  for  $0 \leq \delta \leq S$ . Equation (4.10) then follows if we sum over the nearest neighbors  $y$  of  $x$ , take (4.11) into account, and use the obvious inequality

$$\langle P^{+\delta}(x) P^{-\delta}(y) \rangle \leq \langle P^+(x) P^-(y) \rangle \quad \blacksquare$$

In order to transform the local estimates above into *global* ones (i.e., involving all points of  $\Lambda$ ), the notion of reflection positivity (RP)<sup>(4,5,21)</sup> is useful. Let  $\pi$  be a plane between lattice sites dividing  $\Lambda$  into two disjoint congruent parts  $\Lambda_+$  and  $\Lambda_-$ . Let  $\mathfrak{A}(x)$  denote the algebra of all bounded functions of the spins  $\{S_i(x), i = 1, 2, 3\}$  and

$$\mathfrak{A}_\pm = \bigotimes_{x \in \Lambda_\pm} \mathfrak{A}(x), \quad \mathfrak{A} = \mathfrak{A}_+ \otimes \mathfrak{A}_-$$

Given  $B \in \mathfrak{A}$ , define  $\theta B$  by

$$\begin{aligned} (\theta B) & [ \{S_i(x); i = 1, 2, 3; x \in \Lambda\} ] \\ & = B [ \{(\theta S_i)(x); i = 1, 2, 3; x \in \Lambda\} ] \end{aligned}$$

where

$$(\theta S_i)(x) = S_i(\theta x), \quad i = 1, 2, 3$$

and  $\theta x$  is a reflection of  $x$  through  $\pi$ . We now state the definition of RP which we need in the proofs (see also Ref. 21, Theorem 2.1):

**Definition 4.1.** A Hamiltonian  $H_\Lambda$  is said to satisfy reflection positivity (RP) if

$$\langle F(\overline{\theta F}) \rangle_{H_\Lambda} \geq 0 \quad (4.15)$$

for  $F$  any bounded function of  $\{S_3(x); x \in \Lambda\}$  belonging to  $\mathfrak{A}_+$ . The bar denotes complex conjugation.

**Proposition 4.3.**  $H_\Lambda^{\text{kin}}$  satisfies RP.

*Proof.* By (4.5) and (4.6)

$$\begin{aligned}
 H_\Lambda^{\text{kin}} &= \frac{Jz}{2S} \sum_{x \in \Lambda} [S^2 - S_3(x)^2] \\
 &\quad - \frac{\omega J}{2S} \sum_{\substack{\langle x, y \rangle \text{ n.n.} \\ x, y \in \Lambda}} [S_1(x) S_1(y) + S_2(x) S_2(y)] \quad (4.16)
 \end{aligned}$$

Performing a counterclockwise rotation of  $\pi/2$  around the  $x$  axis at each site,  $S_1(x) \rightarrow S_1(x)$ ,  $S_2(x) \rightarrow S_3(x)$ , and  $S_3(x) \rightarrow -S_2(x)$ . Hence the second term in (4.18) goes over to the “ $X$ - $Z$ ” model with the proper sign, which is RP,<sup>(21)</sup> while the first term is *real* and of the form  $(A + \theta A)$ , with

$$A = \frac{Jz}{2S} \sum_{x \in \Lambda_+} [S^2 - S_2(x)^2]$$

This  $\pi/2$  rotation is a unitary transformation which *commutes* with the  $\theta$  operation (in contrast to a rotation of  $\pi$  around the  $x$  axis at each point of a sublattice). This proves (4.15). ■

Note that the above proof implies (4.15) for any bounded function  $F$  of all the  $\{S_i(x), i = 1, 2, 3\}$ , and hence that  $H_\Lambda^{\text{kin}}$  is RP according to the stronger criterion of Ref. 21.

Let now for definiteness  $\nu = 3$ ,  $M = \frac{1}{4}N$ , with  $N^3 = |\Lambda|$ . We define (cf. Fig. 1 of Ref. 21):

$$\begin{aligned}
 P_\Lambda &= \prod_{m=0}^{M-1} \left[ \prod_{k=0}^{N-1} \prod_{n=0}^{N-1} P^+(4m, n, k) P^-(4m + 1, n, k) \right. \\
 &\quad \left. \times P^-(4m + 2, n, k) P^+(4m + 3, n, k) \right] \quad (4.17)
 \end{aligned}$$

and

$$P_\Lambda^{<\delta} = \bigotimes_{x \in \Lambda} P^{<\delta}(x) \quad (4.18)$$

Proposition 4.3 and Ref. 21 imply the following corollary.

**Lemma 4.4.**

$$\begin{aligned}
 \langle P^+(x) P^-(y) \rangle_{H_\Lambda^{\text{kin}}} &\leq \langle P_\Lambda \rangle_{H_\Lambda^{\text{kin}}}^{1/|\Lambda|}(x, y \text{ n.n. in } \Lambda) \\
 \langle P^{<\delta}(x) \rangle_{H_\Lambda^{\text{kin}}} &\leq \langle P_\Lambda^{<\delta} \rangle_{H_\Lambda^{\text{kin}}}^{1/|\Lambda|} \quad \forall x \in \Lambda
 \end{aligned} \quad (4.19)$$

We wish to prove that  $\langle H_\Lambda^{\text{dyn}} \rangle_{H_\Lambda^{\text{kin}}}$  is sufficiently small if  $\beta$  and  $S$  are large enough. By Proposition 4.2 and Lemma 4.4 it suffices to show that the right-hand sides of (4.19) and (4.20) are small under such conditions. The

main tool is the powerful exponential localization theorem of Ref. 21. In order to understand what is involved, write

$$H_{\Lambda}^{\text{kin}} = \frac{1}{2S} \sum_{x,y \in \Lambda} S_+(x) D_{\alpha}(x,y) S_-(y) + C_{\Lambda} \quad (4.21)$$

where

$$C_{\Lambda} = -\frac{Jz}{2S} \sum_{x \in \Lambda} [S + S_3(x)] \quad (4.22)$$

We shall first assume that the contribution of  $C_{\Lambda}$  in the right-hand side of (4.19) and (4.20) may be neglected. This is the approximation mentioned in the Abstract and the Introduction, to be discussed at the end of this section. Under this assumption,  $H_{\Lambda}^{\text{kin}}$  is just the first term in (4.21), which may also be written

$$H_{\Lambda}^{\text{kin}} = A_{\Lambda} + B_{\Lambda} \quad (4.23)$$

where

$$\begin{aligned} A_{\Lambda} &= \frac{Jz}{2S} \sum_{x \in \Lambda} S_+(x) S_-(x) \\ &= \frac{Jz}{2S} \sum_{x \in \Lambda} \{S(S+1) - S_3(x)[S_3(x) - 1]\} \end{aligned} \quad (4.24)$$

is positive and diagonal, and

$$B_{\Lambda} = -\frac{\alpha J}{2S} \sum_{\substack{\langle x,y \rangle \text{ n.n.} \\ x,y \in \Lambda}} S_+(x) S_-(y) \quad (4.25)$$

As in Section 2, we denote by  $|0\rangle = \bigotimes_{x \in \Lambda} |\sigma(x) = -S\rangle$  the state with all spins down.

**Lemma 4.5.**  $|0\rangle$  is the (unique) ground state of both  $A_{\Lambda}$  and  $H_{\Lambda}^{\text{kin}}$ , corresponding to zero energy. Furthermore,  $B_{\Lambda}$  is denominated by  $A_{\Lambda}$ ,

$$\pm B_{\Lambda} \leq \alpha A_{\Lambda} \quad (4.26)$$

*Proof.* Plainly,  $H_{\Lambda}^{\text{kin}}|0\rangle = A_{\Lambda}|0\rangle = 0$ . We shall prove that  $H_{\Lambda}^{\text{kin}}$  is a positive operator with  $|0\rangle$  as its (unique) ground state. This follows from  $D_{\alpha}(x,y)$  being a positive-definite matrix,  $0 \leq \alpha \leq 1$ . In fact, take  $\alpha = 1$ . Then both the matrix  $[Jz\delta_{x,y} - J(x-y)]$  and  $[Jz\delta_{x,y} + J(x-y)]$  are positive-definite by the Gersgorin disk theorem.<sup>(19)</sup> Equation (4.26) is an immediate

consequence of this observation. Hence  $|0\rangle$  is a ground state of  $H_A^{\text{kin}}$ . It follows from (4.26) that  $H_A^{\text{kin}} \geq (1 - \alpha)A_\Lambda$  and  $A_\Lambda$  has  $|0\rangle$  as its unique ground state, therefore  $|0\rangle$  is also the unique ground state of  $H_A^{\text{kin}}$ . ■

The main idea of the forthcoming proof is the following.  $P_A^{\delta}$  (for suitable  $\delta$ ) and  $P_A$  project onto configurations which have a higher  $A_\Lambda$  energy than the ground state of  $A_\Lambda$ , and  $B_\Lambda$  is dominated by  $A_\Lambda$  through (4.26). Hence the right-hand sides of (4.19) and (4.20) are expected to become small for suitable  $\delta$ , and  $\beta$  and  $S$  sufficiently large. Notice that the choice of  $H_A^{\text{kin}}$ , with just  $|0\rangle$  and *not*  $\otimes_{x \in \Lambda} |\sigma(x) = +S\rangle$  as its unique ground state, plays a crucial role. [A positive external field has the same effect.] Our main result of this section is the following theorem.

**Theorem 4.6.** Let  $S > 2$  and  $2 < \varepsilon < 4$ . Then

$$\begin{aligned}
 & |f(H_\Lambda) - f(H_\Lambda^{\text{kin}})| \\
 & \leq \frac{J\varepsilon^2 z}{16S} + zJ(2S - \varepsilon)[(2S + 1) \exp(-\beta^{1/4}) + \sigma^{d_2}] \\
 & \quad + 2Jz \left( S - \frac{\varepsilon^2}{16S} \right) [(2S + 1) \exp(-\beta^{1/4}) + \sigma^{d_1}] \quad (4.27)
 \end{aligned}$$

where  $\sigma = (1 + \alpha)/2 < 1$  and in three dimensions ( $\nu = 3$ )

$$d_1 = \left\{ \frac{S}{32} \left[ \frac{Jz(1 - \alpha)}{2(1 + \alpha)} \right]^{1/3} \beta^{1/4} \right\}_+ \quad (4.28a)$$

$$d_2 = \left\{ \frac{\varepsilon}{64} \left[ \frac{(1 - \alpha)}{2(1 + \alpha)} \Gamma \right]^{1/3} \beta^{1/4} \right\}_+ \quad (4.28b)$$

here  $\{x\}_+$  is the greatest integer  $\leq x$ , and

$$\Gamma = \frac{Jz\varepsilon}{4} \left( 1 + \frac{1}{2S} - \frac{\varepsilon}{8S} \right) \quad (4.28c)$$

Some remarks are in order. First, the expressions for  $d_1$  and  $d_2$  depend on the dimension  $\nu$  and may be obtained for values of  $\nu$  other than three by the procedure outlined in Appendix B. Second, the correlation between  $\beta$  and  $S$ , apparent from (4.27), arises from the spin wave normalization  $S^{-1/2}$  of the spin operators—in contrast to the scaling by  $S^{-1}$  for the classical limit.<sup>(21,17)</sup> Third, if  $\beta$  and  $S$  are chosen suitably, the error we make in replacing  $H_\Lambda$  by  $H_\Lambda^{\text{kin}}$  is exponentially small in  $\beta^{1/4}$ .

In view of Lemma 4.1, Proposition (4.2), and Lemma 4.4, we only have

to estimate  $\langle P_\Lambda \rangle^{1/|\Lambda|}$  and  $\langle P_\Lambda^{<\delta} \rangle^{1/|\Lambda|}$ . We choose  $\delta = S - \varepsilon/2$  (see Appendix B).

**Lemma 4.7.** Let  $\sigma$  and  $d_1$  be defined as in Theorem 4.6. Then

$$\langle P_\Lambda \rangle^{1/|\Lambda|} \leq (2S + 1) \exp(-\beta^{1/4}) + \sigma^{d_1} \quad (4.29)$$

*Proof.* Following Ref. 21 we put

$$\begin{aligned} \langle P_\Lambda \rangle &= Z_\Lambda^{-1} \left\{ \int_0^{\Delta|\Lambda|} e^{-\beta e} \text{Tr}[P_\Lambda E_\Lambda(de)] \right. \\ &\quad \left. + \int_{\Delta|\Lambda|}^\infty e^{-\beta e} \text{Tr}[P_\Lambda E_\Lambda(de)] \right\} \leq I_\Lambda + J_\Lambda \end{aligned} \quad (4.30)$$

where

$$I_\Lambda = Z_\Lambda^{-1} \sum'_\Delta e^{-\beta e_i} (\phi_i, P_\Lambda \phi_i) \quad (4.31)$$

and

$$J_\Lambda = e^{-\beta\Delta|\Lambda|} \text{Tr}(\mathbb{1})/Z_\Lambda \quad (4.32)$$

We explain the notation.  $E_\Lambda$  is the spectral measure of  $H_\Lambda^{\text{kin}}$ ,  $\Delta$  is a positive number to be chosen shortly,  $Z_\Lambda = \text{Tr} \exp(-\beta H_\Lambda^{\text{kin}})$ , and  $\sum'_\Delta$  denotes a sum over all (orthonormal) eigenfunctions of  $H_\Lambda^{\text{kin}}$  with eigenvalues  $e_i < \Delta|\Lambda|$ . Since  $e_0 = 0$ ,  $Z_\Lambda \geq 1$ . Moreover,  $\text{Tr} \mathbb{1} = (2S + 1)^{|\Lambda|}$ . Choosing  $\Delta = \beta^{-3/4}$  we obtain

$$J_\Lambda^{1/|\Lambda|} \leq (2S + 1) \exp(-\beta^{1/4})$$

Because

$$\langle P_\Lambda \rangle^{1/|\Lambda|} \leq (I_\Lambda + J_\Lambda)^{1/|\Lambda|} \leq I_\Lambda^{1/|\Lambda|} + J_\Lambda^{1/|\Lambda|}$$

we are left with estimating  $I_\Lambda^{1/|\Lambda|}$ . This is done by using (4.26) and the exponential localization theorem (Theorem 3.1 and Corollary 3.2 of Ref. 21). The final expression for  $d_1$  is derived in Appendix B. ■

We now finish the argument by giving an estimate for  $\langle P_\Lambda^{<\delta} \rangle$ .

**Lemma 4.8.** Define  $\sigma$  and  $d_2$  as in Theorem 4.6. Then

$$\langle P_\Lambda^{<\delta} \rangle^{1/|\Lambda|} \leq (2S + 1) \exp(-\beta^{1/4}) + \sigma^{d_2} \quad (4.33)$$

*Proof.* We proceed as in the proof of the previous lemma. The expression for  $d_2$  is given in Appendix B. ■

The previous results have been derived neglecting  $C_\Lambda$  in (4.21). We now present an argument to justify this procedure. Let  $H_\Lambda^{\text{kin}}$  still be defined

by (4.23)–(4.25). The true  $H_\Lambda^{\text{kin}}$ , which is given by (4.21), will be denoted henceforth by  $\tilde{H}_\Lambda^{\text{kin}}$ . With this notation,

$$\bar{H}_\Lambda^{\text{kin}} = H_\Lambda^{\text{kin}} + C_\Lambda \quad (4.34)$$

By (4.21) and (4.22)

$$[C_\Lambda, H_\Lambda^{\text{kin}}] = [C_\Lambda, \bar{H}_\Lambda^{\text{kin}}] = 0 \quad (4.35)$$

Let  $\{\phi_i\}$  be the normalized eigenstate of  $H_\Lambda^{\text{kin}}$ , and  $\{e_i\}$  the corresponding eigenvalues, as in (4.30)–(4.32). By (4.35) the  $\phi_i$  are also eigenstates of  $C_\Lambda$  with eigenvalues we call  $f_i$ :

$$C_\Lambda \phi_i = f_i \phi_i, \quad f_i \leq 0 \quad (4.36)$$

We may now write as in (4.30)–(4.32)

$$\langle P_\Lambda \rangle_{\bar{H}_\Lambda^{\text{kin}}} = \tilde{I}_\Lambda + \tilde{J}_\Lambda \quad (4.37)$$

where

$$\tilde{I}_\Lambda = Z_\Lambda^{-1} \sum_{(e_i+f_i) < \Delta|\Lambda|} e^{-\beta(e_i+f_i)} (\phi_i, P_\Lambda \phi_i) \quad (4.38)$$

$$\begin{aligned} \tilde{J}_\Lambda &= Z_\Lambda^{-1} \sum_{(e_i+f_i) \geq \Delta|\Lambda|} e^{-\beta(e_i+f_i)} (\phi_i, P_\Lambda \phi_i) \\ &\leq e^{-\beta\Delta|\Lambda|} \text{Tr} \uparrow \end{aligned} \quad (4.39)$$

We now argue that for low-lying states in the sum (4.38), the contribution of  $f_i$  is  $O(1/S)$  with respect to  $e_i$  and may be neglected for  $S$  sufficiently large. In fact, in Boson language

$$\begin{aligned} H_\Lambda^{\text{kin}} &= \sum_{x,y \in \Lambda} a^+(x) f_S^{1/2}(x) D_\alpha(x,y) f_S^{1/2}(y) a(y) \\ C_\Lambda &= -\frac{Jz}{2S} \sum_{x \in \Lambda} a^+(x) a(x) \end{aligned} \quad (4.40)$$

If  $f_S \sim 1$  in (4.40),

$$H_\Lambda^{\text{kin}} \simeq \sum_{x,y \in \Lambda} a^+(x) D_\alpha(x,y) a(y) \geq (1-\alpha) \sum_{x \in \Lambda} a^+(x) a(x)$$

which “dominates”  $C_\Lambda$  for  $S$  sufficiently large. Alternatively, the low-lying eigenvalues of  $A_\Lambda$  [given by (4.24), and which dominates  $B_\Lambda$  by (4.26)], are  $O(1)$  while the corresponding  $f_i$  in (4.36) are  $O(1/S)$ . A rigorous proof of this approximation depends, however, on more information about the spectrum of  $H_\Lambda^{\text{kin}}$  on  $\mathfrak{H}_\Lambda$ .

## 5. CONCLUSION

Throughout this paper we have worked in *configuration* space. This is of particular relevance to applications in random systems,<sup>(6)</sup> where a (classical) ground state may be known, but translational invariance of the Hamiltonian fails completely. In Sections 2 and 3 we could dispense with translational invariance altogether. On the other hand, in Section 4, we needed both translational invariance and nearest-neighbor interactions so as to take advantage of reflection positivity.

Even for  $\alpha < 1$  the approximation discussed at the end of Section 4—however plausible—still has to be justified rigorously. In addition, it must be kept in mind that we finally wish estimates in the limit  $\alpha \rightarrow 1$  (or, alternatively, for  $\alpha = 1$  and in the limit of zero external field). These difficulties seem to be much deeper, and in the case of the kinematical interaction are related to those encountered in Appendix A. Nevertheless, even under the above limitations, Theorem 4.6 indicates an interesting feature. The point is that we may scale the local spin operators  $\mathbf{S}(x)$  in two different ways: by  $S^{-1}$  to obtain the classical limit,<sup>(21,17)</sup> and by  $S^{-1/2}$  to obtain the spin wave limit. The latter is expected to be suitable for studying low-temperature excitations. Indeed, our estimates in Section 4 become accurate if  $S$  is large enough and the temperature is low enough, i.e., the inverse temperature  $\beta$  is high enough. Surprisingly, the choice of  $\beta$  depends on  $S$ . This is indicative of an asymptotic (in contrast to convergent) expansion, whose form is suggested by Theorem 4.6.

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## APPENDIX A

In this appendix we show that, in contrast to Dyson's suggestion [Ref. 2, Eq. (47)], there is *no* energy gap between the physical ground state and the *improper* Hilbert space. Since in Dyson's argument the external magnetic field does not play any role, we will put  $h = 0$  (in Dyson's notation,  $L = 0$ ). Throughout what follows we assume a translation-invariant, nearest-neighbor, ferromagnetic Heisenberg model with ground-state energy  $E_0$ .

Let  $g$  be a subset of  $\mathcal{A}$ . To each  $x$  in  $g$  we assign, as in Ref. 2, a number  $M(x) \geq 2S + 1$ . Let  $\mathcal{S}_M$  be the subspace of  $\mathcal{F}_\mathcal{A}$  consisting of the linear span of states  $\{|m(x)\rangle\}$  with  $m(x) = M(x)$  if  $x$  is in  $g$  and  $m(x) \leq 2S$  if  $x$  belongs

to  $\bar{g} = \Lambda \setminus g$ ; cf. Eq. (3.15). In spin language the restriction of the Dyson Hamiltonian  $\mathcal{H}_{D,\Lambda}$  (Section 3.3) to  $\mathcal{L}_M$  may be written

$$H_M = E_0 + \frac{1}{2}J\Sigma_1[S^2 - \mathbf{S}(x)\mathbf{S}(x + \delta)] \\ + \frac{1}{2}J\Sigma_2M(x)[S - S_3(x + \delta)] \quad (\text{A.1})$$

This is Dyson's equation (36) in Ref. 2.  $\Sigma_1$  denotes a sum over pairs  $\langle x, x + \delta \rangle$  of nearest neighbors which are *both* in  $\bar{g}$ , and  $\Sigma_2$  is a sum over nearest neighbors  $x$  and  $x + \delta$  with  $x$  in  $g$  and  $x + \delta$  in  $\bar{g}$ .

Now let  $g$  consist of one point, and take  $m(x) = 2S$  for all  $x$  in  $\bar{g}$ , i.e.,  $\sigma(x) = +S$ . Then we have obtained an eigenstate of  $H_M$  with eigenvalue  $E_0$ . In fact, a host of such states exist, even with  $|g| = O(|\Lambda|)$ . To see this, decompose  $\Lambda$  into two sublattices  $g$  and  $\bar{g}$  such that all points in  $g$  and  $\bar{g}$  are nearest neighbors, and let  $m(x) = 2S$  for all  $x$  in  $\bar{g}$ . Then the first sum in (A.1) is empty, and any improper state consistent with the above prescription is an eigenstate of  $\Sigma_2$  with eigenvalue  $E_0$ .

## APPENDIX B

We now provide the estimates for  $d_1$  and  $d_2$  used in the main text. For the sake of definiteness we take  $\nu = 3$ , and follow the notation of Ref. 21, which does not always agree with the rest of this paper. Let  $P_\Lambda$  be a projection onto eigenvectors  $\psi$  of  $A_\Lambda$  with eigenvalues exceeding  $\rho = n\Delta|\Lambda|$ , for some positive  $\Delta$  and  $n > 1$ , and let  $P_\rho$  project onto *all* the eigenstates of  $A_\Lambda$  with eigenvalues in  $[\rho, \infty)$ . Moreover, define  $d$  by the condition

$$(1 - P_\rho)[B_\Lambda(A_\Lambda - \lambda)^{-1}]^d \psi \neq 0 \\ (1 - P_\rho)[B_\Lambda(A_\Lambda - \lambda)^{-1}]^j \Psi = 0, \quad j = 0, 1, \dots, d - 1 \quad (\text{B.1})$$

where  $\psi$  is an arbitrary normalized vector in the range of  $P_\Lambda$ :  $P_\Lambda \psi = \psi$  and  $\lambda < \rho$ . Denote by  $E_{\text{gap}}$  the difference between the minimal  $A_\Lambda$  energy of any state in  $P_\Lambda \mathfrak{H}$  and  $\rho$ :

$$E_{\text{gap}} = \inf \text{spec}\{(P_\Lambda A_\Lambda P_\Lambda) - \rho\} > 0 \quad (\text{B.2})$$

Then  $d$  is the number of times  $B_\Lambda$  may be applied to  $\psi$  without lowering the  $A_\Lambda$ -energy by more than  $E_{\text{gap}}$ . In models with a ferromagnetic ground state an estimate for  $d$  may be obtained in the following way.

Eigenstates of  $A_\Lambda$  in  $(1 - P_\rho)\mathfrak{H}$  are "near" the ground state. Let  $l \geq 2$  be an integer such that  $|\Lambda|^{1/3}/l$  is also an integer, and decompose  $\Lambda$  into  $|\Lambda|/l^3$  disjoint congruent cubes  $c$ , with sides of length  $l$ . Let  $\phi$  be an eigenvector of  $\{S^3(x), x \in \Lambda\}$ . For  $\phi$ , a *perfect* cube is defined to be a cube  $c = c_\phi$  such that



$S_3(x)\phi = -S\phi$  for all  $x$  in  $c_\phi$ . Otherwise the cube is called *imperfect*. Suppose the  $A_\Lambda$ -energy of  $\phi$  is smaller than  $\rho$ . We must answer two questions:<sup>(21)</sup>

(a) What is the minimum number of perfect cubes necessary to obtain a state with such a low  $A_\Lambda$  energy?

(b) How many times must  $B_\Lambda$  be applied to convert an imperfect cube into a perfect one?

Turning to (a), we set the  $A_\Lambda$  energy of a perfect cube equal to zero. Then the  $A_\Lambda$  energy of an imperfect cube is positive. Its minimal  $A_\Lambda$  energy is greater than or equal to the energy obtained in a configuration where at one site, say  $x_0$ ,  $\sigma_3(x_0) > -S$  and  $\sigma_3(x) = -S$  at all other sites  $x \neq x_0$ , i.e.,

$$\min_{\sigma(x) > -S} \left( \frac{Jz}{2S} \{S(S+1) - \sigma(x)[\sigma(x) - 1]\} \right) = Jz \quad (\text{B.3})$$

See also Eqs. (4.18)–(4.20).  $A_\Lambda$  is diagonal with respect to the usual basis of eigenvectors of  $S_3(x)$ , characterized by the eigenvalues  $\sigma(x)$ ,  $x \in \Lambda$ . The minimal number  $N$  of perfect cubes for a state  $\phi$  with  $A_\Lambda$ -energy  $< \rho$  then satisfies the inequality

$$(|\Lambda|/l^3 - N)Jz \leq n\Delta |\Lambda|$$

so that

$$N \geq |\Lambda| \left( l^{-3} - \frac{n\Delta}{Jz} \right) \quad (\text{B.4})$$

Since  $l \geq 2$ ,  $n\Delta < Jz/16$ .

The rest of the argument is now identical to Ref. 21, p. 260. We obtain, with  $\Delta = \beta^{-3/4}$  and  $n = (1 + \alpha)/(1 - \alpha)$ ,  $I_\Lambda \leq \sigma^{d'_1}$  and

$$d'_1 \geq \left\{ \frac{S|\Lambda|}{32} \left[ \frac{Jz(1-\alpha)}{2(1+\alpha)} \right]^{1/3} \beta^{1/4} \right\}_+ \quad (\text{B.5})$$

Using (4.25) we finally get (4.24) and  $d_1$ .

To estimate  $d_2$ , we define a cube  $c_\phi$  to be *perfect* for an eigenstate  $\phi$  of  $\{S_3(x); x \in \Lambda\}$ , with  $S_3(x)\phi = \sigma(x)\phi$ , by the requirement  $\sigma(x) < -\lambda S$  for all  $x$  in  $c_\phi$ . Here  $1 - 1/S < \lambda < 1 - 1/(2S)$ . Then it is easy to see that the minimal  $A_\Lambda$  energy of an imperfect cube is given by

$$\begin{aligned} \min_{\sigma(x) > -\lambda S} \left( \frac{Jz}{2S} \{S(S+1) - \sigma(x)[\sigma(x) - 1]\} \right) \\ = \frac{Jz}{2} (1 - \lambda)[S(1 + \lambda) + 1] \equiv \Gamma \end{aligned} \quad (\text{B.6})$$

The minimal number  $N$  of perfect cubes for a state  $\phi$  of  $A_\Lambda$  energy  $\langle \rho \rangle$  satisfies the inequality

$$(|A|/l^3 - N)\Gamma \leq n\Delta |A|$$

so that

$$N \geq |A| (l^{-3} - n\Delta/\Gamma) \quad (\text{B.7})$$

Since  $l \geq 2$ ,  $n\Delta < \Gamma/16$ .

If we want to get a perfect cube by applying  $B_\Lambda$  to a vector  $\psi$  in the range of  $P_\Lambda^{\leq \delta}$ , we have to apply  $B_\Lambda$  at least  $m$  times, where

$$m \geq (\lambda S - \delta)l^4/8 \quad (\text{B.8})$$

Equation (B.8) follows from an argument similar to Ref. 21, p. 260:  $l^3$  spins in a cube must be lowered at least from  $\sigma_3(x) = -\delta$  to  $\sigma_3(x) = -\lambda S$ , i.e.,  $\sigma_3(x)$  must change by at least  $(\lambda S - \delta)$ . Choosing  $\lambda = 1 - \varepsilon/4S$ , and  $\delta = S - \varepsilon/2$ , and taking  $n$  and  $\Delta$  as before, we find

$$d'_2 \geq \left\{ \frac{\varepsilon |A|}{64} \left( \frac{1 - \alpha}{2(1 + \alpha)} \Gamma \right)^{1/3} \beta^{1/4} \right\}_+ \quad (\text{B.9})$$

and

$$\Gamma = \frac{Jz\varepsilon}{4} \left( 1 + \frac{1}{2S} - \frac{\varepsilon}{8S} \right) \quad (\text{B.10})$$

Notice that the conditions  $2 < \varepsilon < 4$  assumed on  $\varepsilon$  are precisely consistent with the inequalities  $1 - 1/S < \lambda < 1 - 1/(2S)$  which were previously required.

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