Universality, low-temperature properties, and finite-size scaling in quantum antiferromagnets

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The behavior of ordered quantum Heisenberg antiferromagnets is analyzed from the nonlinear σ model in two and three dimensions. Many thermodynamic and dynamic properties are found to be universal at low temperatures and small magnetic fields. Finite-size effects are also investigated in detail; the results should be useful for analyzing numerical work on two-dimensional (2D) quantum antiferromagnets. The *X-Y* phase transition in 2D which is induced by a magnetic field is discussed. Applications to the ordered phase of solid ^{3}He are also given.

I. INTRODUCTION

During the past decade, two antiferromagnets have been discovered which are both extremely isotropic and have strong quantum fluctuations in their ground states. In one of these systems, solid ^{3}He,[1,2] three-dimensional (3D) nuclear antiferromagnetism occurs only below 1 mK, while in the quasi-two-dimensional $LaCu_2O_4$, the characteristic temperature for the 2D magnetism is above room temperature.[3,4] Nevertheless, both systems consist of $S=\frac{1}{2}$ spins coupled by short-range exchange, and both systems show a suppression of the staggered moment in the ground state down to $\sim 60\%$ of the Néel value.[2,3] This suppression is indicative of the strong quantum fluctuations. In the case of ^{3}He these are enhanced by frustration in the interactions which leads to a complicated ordered state and in $LaCuO_2$ they are due to the strong 2D quantum fluctuations caused by the small number of nearest neighbors. Because of the strong quantum fluctuations, analytic calculations (e.g., spin-wave expansions) are difficult and, as evidenced by the recent flurry of work on the 2D spin-$\frac{1}{2}$ system,[5,6] reliable interpretation of numerical calculations can be tricky.

In this paper, we show that in any ordered quantum antiferromagnet (which leaves one of the spin symmetries unbroken) the leading low-temperature, small magnetic field and finite-size corrections are *universal* depending only on the dimension and the basic energy and length scales which are set by properties of the ground state. The results we obtain should be useful both for analyzing experiments on solid ^{3}He and for analyzing numerical calculations on 2D quantum antiferromagnets.

The basic observation, which had already been used in solid ^{3}He,[7,8] and has come to prominence recently in connection with the copper-oxide superconductors, is that at long wavelengths and low frequencies, the dominant fluctuations in an ordered antiferromagnet are controlled by the quantum nonlinear σ model[9–11] with imaginary-time action

$$S=\frac{1}{2\hbar}\int d^dx\int_0^{\beta\hbar}d\tau\left[\Upsilon(\nabla\hat{\mathbf{n}})^2+\chi\left[\frac{\partial\hat{\mathbf{n}}}{\partial\tau}-i\hat{\mathbf{n}}\times\mathbf{H}\right]^2\right] \tag{1.1}$$

where Υ is the spin-wave stiffness, χ is the (transverse) susceptibility, and $\beta=1/T$. We have normalized the field so that the Larmor precession frequency is H. The unit vector $\hat{\mathbf{n}}$ describes the direction of the local staggered magnetization.

At $T=0$ and $H=0$ in dimensions $d>1$, the fully ordered antiferromagnetic fixed point is stable to small fluctuations. Thus as long as the system is in an antiferromagnetic phase, at long length scales at $H=T=0$, it will renormalize towards this fixed point. In the process, other irrelevant operators which can be added to S will renormalize Υ and χ in a nonuniversal manner as they flow away leaving, at long length and time scales, only the least-irrelevant operators (i.e., $1/\Upsilon$ and $1/\chi$ with eigenvalue $1-d$) which appear in Eq. (1.1). The long-wavelength low-frequency fluctuations involve only the final approach to the ordered fixed point and will thus be controlled by the fully renormalized, i.e., physical values of Υ and χ. All physical quantities which we will calculate thus involve these, not the "bare" values. So too, will the behavior for small T and small H, although for any $H\neq 0$, the system flows towards the *X-Y* ordered fixed point while for $T>0$ in $d\leq 2$, it eventually flows to infinite temperature. Thus, care must be exercised for $T,H\neq 0$ in determining which quantities are universal.

Energy, length, and time scales are set by Υ, χ, and $\hbar$, and, if measured in these units, many quantities will just be universal constants.

For definiteness, we consider a hypercube of linear size L with periodic boundary conditions, at temperature T. The free energy can be obtained from the partition function

$$Z=\mathrm{Tr}e^{-S} \text{ via } F=-T\ln Z \ .$$

In the limit $T\to 0$, $H\to 0$, and $L\to\infty$, the free energy per unit volume is just the (nonuniversal) ground-state energy density, ε_0. The corrections to this due to the fluctuations described by Eq. (1.1) (with the cutoff $\to\infty$) have the form

$$\frac{\Delta F}{T}\equiv\frac{F}{T}-\frac{\varepsilon_0L^d}{T}+\frac{1}{2}\frac{\chi H^2L^d}{T}=\tilde{\Sigma}\left[\frac{L}{\xi_0},\frac{T\xi_0}{\hbar c},\frac{H\xi_0}{c}\right] , \tag{1.2}$$

where the length scale

$$\xi_0 \equiv \left[\frac{\hbar^2}{\Upsilon\chi} \right]^{1/2(d-2)} , \tag{1.3}$$

the velocity scale c is the zero-temperature spin-wave velocity

$$c = \sqrt{\Upsilon/\chi} , \tag{1.4}$$

and we have subtracted in (1.2) the magnetic free energy associated with the *linear* susceptibility.

The length ξ_0 sets the scale of the nonlinearities: on scales $\leq \xi_0$ the fluctuations will be strongly nonlinear while on scales $> \xi_0$ they will be approximately linear.

When $T \gtrsim \xi_0$ in $d > 2$, the system will presumably disorder, although this may be accompanied by the breakdown of the nonlinear σ-model representation.[12] In $d = 2$, it will be disordered for all T with

$$\xi = K\xi_0 e^{2\pi\hbar c/T\xi_0} = K\xi_0 e^{2\pi\Upsilon/T} , \tag{1.5}$$

with K a universal constant. The *absence* of a nontrivial power of T in Eq. (1.5) is due to the cancellation of the two-loop term in the thermal β function with the factor of $1/T$ arising from the quantum-to-thermal crossover (see detailed discussion in Ref. 9).

In principle, Eq. (1.2) is valid for all ranges of the parameters provided all lengths are much larger than the microscopic scale a, whose inverse gives a momentum cutoff. However, in practice, there will always be other irrelevant operators whose strength is characterized by other length scales ξ_1, ξ_2, etc., and the fluctuations will only be described by the nonlinear σ model, for L, T^{-1}, and H^{-1} much larger than these other scales. Since ξ_0 will typically be of order a (except near critical points), these scales can all be of the same order. We will thus restrict ourselves to the behavior for asymptotically long scales for which Eq. (1.1) will always be valid provided the system is ordered. This yields

$$\frac{\Delta F}{T} = \Sigma \left[\frac{TL}{\hbar c}, \frac{HL}{c} \right] , \tag{1.6}$$

the function Σ is obtained *almost entirely from linear fluctuations.*

We will find that in the small-volume limit with $TL/\hbar c \ll 1$, a different scaling form is needed which includes some nonlinear fluctuations. The nonlinear fluctuations actually give rise to a contribution to $\Delta F/T$ for $TL \sim 1$, which does not scale as simply as Eq. (1.6). However the nonscaling part of this term drops out of physical observables like the energy and magnetization. In addition, logarithmic dependence on the cutoff will appear in $d = 3$.

The remainder of this paper is organized as follows. In Sec. II the thermodynamic properties at low temperatures and small magnetic fields are analyzed, and in Sec. III the scaling of the transition temperature in a magnetic field in two dimensions is discussed. Finite-size effects, useful for the analysis of numerical calculations in two dimensions, are investigated in Sec. IV. In Sec. V, corrections to scaling are discussed briefly and implications drawn for analysis of numerical calculations. In Sec. VI, the present results are related to other problems. Finally, in Sec. VII, applications to solid ^{3}He and dynamic measurements are mentioned.

II. INFINITE SYSTEMS

We first consider the thermodynamic behavior in the limit $L \to \infty$, where the effects of the nonlinear fluctuations do not occur. In this limit the first fluctuation correction to the free energy can be evaluated straightforwardly. We expand Eq. (1.1) in spin-wave modes about $\hat{\mathbf{n}} = \hat{\mathbf{z}}$ with a magnetic field in the x direction. At this order, the Jacobian can be ignored and we have in terms of $\boldsymbol{\pi} \equiv (n_x, n_y)$, the linearized action

$$S_L \approx \frac{1}{2} d^d x \int_0^\beta d\tau \left[-\chi H^2 + \chi H^2 \pi_x^2 + \chi \left[\frac{\partial \boldsymbol{\pi}}{\partial t} \right]^2 + \Upsilon (\nabla \boldsymbol{\pi})^2 \right] , \tag{2.1}$$

(dropping $\hbar$'s) yielding, on integrating out the π's,

$$\frac{\Delta F}{T} = V \int_q \left[\sum_{\omega_n} \frac{1}{2} \{ \ln(\chi\omega_n^2 + \Upsilon q^2) + \ln[\chi(\omega_n^2 + H^2) + \Upsilon q^2] \} - \frac{1}{T} \int_\omega \left[\ln(\chi\omega^2 + \Upsilon q^2) - \frac{\frac{1}{2}\chi H^2}{\chi\omega^2 + \Upsilon q^2} \right] \right] , \tag{2.2}$$

where the sum over ω_n runs over $\omega_n = 2\pi n/\beta$ and V is the volume. This yields

$$\Delta f \equiv \Delta F/V = T \int_q \ln(1 - e^{-\beta c q}) + \ln[1 - e^{-\beta (H^2 + c^2 q^2)}]^{1/2} + \frac{1}{2} \int_q \left[(H^2 + c^2 q^2)^{1/2} - cq - \frac{1}{2} \frac{H^2}{cq} \right] , \tag{2.3}$$

where the second term is just the change in the zero-point energy density of the π_x modes due to the field, less the fluctuation contribution to $-1/2\chi H^2$. In the limit of large L, we thus obtain the scaling function

$$\lim_{L\to\infty} \Sigma \left[\frac{TL}{c}, \frac{HL}{c}\right] \approx \left[\frac{TL}{c}\right]^d \sigma\left[\frac{H}{T}\right] , \tag{2.4}$$

where

$$\sigma(h)=\tfrac{1}{2}\sigma(0)+\int_p \ln[1-e^{-(h^2+p^2)}]^{1/2} + \frac{h^{d+1}}{2}\int_p \left[(1+p^2)^{1/2}-p-\frac{1}{2}\frac{1}{p}\right] , \tag{2.5a}$$

with

$$\sigma(0)=\frac{-4\zeta(d+1)\pi^{d/2}\Gamma(d)}{\Gamma(d/2)(2\pi)^d} . \tag{2.5b}$$

For $d \geq 3$ the last term is divergent at large p. However, in this regime, the dominant nonlinear magnetic energy will be the analytic H^4 term which has been neglected and which involves ξ_0 and the other irrelevant length scales. We will not consider $d>3$ further.

For $d=3$, the integral in Eq. (2.5) is logarithmically divergent yielding $T=0$ the energy density

$$\varepsilon_0(H)=\varepsilon_0-\tfrac{1}{2}\chi H^2-\frac{1}{32\pi^2}\frac{H^4}{c^3}\ln\left[\frac{c}{\xi_0 H}\right] , \tag{2.6}$$

since the cutoff will be of order ξ_0. In $1<d<3$, the function $\sigma(h)$ is well defined and we have in $d=2$ the ground-state energy density

$$\varepsilon_0(H)=\varepsilon_0-\tfrac{1}{2}\chi H^2-\frac{|H|^3}{12\pi c^2} , \tag{2.7}$$

yielding a *divergent nonlinear susceptibility for* $d \leq 3$.

At fixed field and low temperature, we recover the usual T^d specific heat with two modes contributing for $H=0$, but only one for $H\neq 0$, the other obtaining a gap due to the field. We may also evaluate the temperature-dependent magnetization:

$$m(H,T)=\frac{-\partial f}{\partial H}=-\left[\frac{T}{c}\right]^d \sigma'\left[\frac{H}{T}\right]+\chi H , \tag{2.8}$$

where primes on σ denote differentiation. For $T \ll H$,

$$m(H,T)=m(H,T=0)+O(e^{-H/T}) , \tag{2.9}$$

while the zero-field susceptibility $\chi(T)=\partial m/\partial H|_{H=0}$ has a correction

$$\chi(T)=\chi-\frac{T^{d-1}}{c^d}\sigma''(0) , \tag{2.10}$$

where

$$\sigma''(0)=\frac{\pi^{d/2}2}{\Gamma(d/2)(2\pi)^d}\zeta(d-1)\Gamma(d-1) =\frac{1}{12} \text{ in } d=3 . \tag{2.11}$$

For $d=2$, $\sigma''(h)$ diverges logarithmically as $h \to 0$, this divergence is associated with the instability of the ordered phase to thermal fluctuations for $d \leq 2$. If the integral over q in Eq. (2.3) is cut off by the correlation length

$$\xi(T) \sim \xi_0 e^{2\pi\Upsilon/T} \text{ for } d=2 , \tag{2.12}$$

or

$$\xi(T) \sim \left[\frac{\Upsilon}{T}\right]^{1/2-d} \text{ for } d<2 , \tag{2.13}$$

then we would obtain a correction to $\chi(T)$ which is of the same order as χ. This is clearly not a sensible procedure. A reasonable guess is, however, that for $1<d\leq 2$, the absence of order for $T>0$ implies that as $T\to 0$ the linear susceptibility will be an angular average of the longitudinal and transverse susceptibilities at $T=0$. Since $\chi_{\parallel}(T=0)=0$, (defined from the ω, $q\to 0$ limit of the response function), this yields

$$\chi(T\to 0)=\tfrac{2}{3}\chi \tag{2.14}$$

for $d \leq 2$. It is not obvious how to obtain corrections to this result, since both the "longitudinal" and "transverse" parts will enter.

Returning to $d>2$, it is useful to note that the linear susceptibility could also formally be obtained from the $q\to 0$, $\omega\to 0$ limit of the correlation function of $\hat{\mathbf{n}}\times\partial\hat{\mathbf{n}}/\partial\tau$ via

$$\chi^{-1}=T\lim_{\omega_n\to 0}\lim_{q\to 0}\left\langle \int d^dx \int_0^\beta d\tau \left[\hat{\mathbf{n}}\times\frac{\partial\hat{\mathbf{n}}}{\partial\tau}\right](0,0)\left[\hat{\mathbf{n}}\times\frac{\partial\hat{\mathbf{n}}}{\partial\tau}\right](\mathbf{x},\tau)e^{i\omega_n\tau}e^{-iqx}\right\rangle . \tag{2.15}$$

In this way, the T^{d-1} renormalization of χ due to thermal fluctuations [discussed above Eq. (2.10)] appears to be a nonlinear effect which has been calculated to one-loop order, rather than a linear effect. Similarly, one can calculate the temperature dependence of the stiffness at $H=0$ yielding

$$\Upsilon(T)=\Upsilon-\frac{T^{d-1}}{c^{d-2}}\sigma''(0) , \tag{2.16}$$

which, at this order, has the same relative correction as $\chi(T)$. This is due to the absence of dependence on external momentum of the simple one-loop diagram which determines $\Upsilon(T)$ and $\chi(T)$ and is *not* to be expected generally since the finite inverse temperature breaks the Lorentz invariance which existed asymptotically at $T=0$. The hydrodynamic spin-wave velocity for $T>0$ is given by

$$c_h^2=\frac{\Upsilon(T)}{\chi(T)}\ , \tag{2.17}$$

and is thus *independent* of T at order T^{d-1}, but should deviate from $c^2(T=0)$ at higher order.

Note that the temperature dependence of Υ, Eq. (2.16), is *larger* than that for the superfluid density in an X-Y system, whose leading dependence is T^{d+1}. This is a consequence of the curvature of the order-parameter manifold in the Heisenberg case. In the presence of a nonzero applied field, however, the symmetry is reduced to X-Y, and the number of low-frequency spin-wave modes reduced from two to one. In this case, the nonlinearities of the σ model vanish (as readily seen by transforming to angular variables) and thus we expect that the leading singular corrections to $\Upsilon(T)$ and $m(T)$ should also vanish.

Indeed from Eqs. (2.4)–(2.5) this is readily seen to be the case for $m(T)$, since the field-dependent spin-wave contributions to Δf vanish exponentially as $T\to 0$ for $H>0$. In a field, the dominant low-temperature behavior of $m(T)$ will thus *not* be in the scaling function Eq. (2.4) but will be controlled by the irrelevant operators left out of Eq. (1.1). We will then have, for $H\neq 0$,

$$\lim_{T\to 0}\frac{m(T,H)-m(0,H)}{T^{d-1}}=0 \tag{2.18}$$

and

$$\lim_{T\to 0}\frac{\Upsilon(T,H)-\Upsilon(T,0)}{T^{d-1}}=0\ . \tag{2.19}$$

All of the results of this and later sections can be justified by more detailed renormalization group calculations whereby the last stage of the flow at long-length scales yields the long-length, low-T, low-H behavior in terms of the fully renormalized physical values of Υ and χ. The corrections which arise from irrelevant operators are discussed in Sec. V.

III. TWO DIMENSIONS IN A MAGNETIC FIELD

A uniform magnetic field on a Heisenberg antiferromagnet acts to break the symmetry down to X-Y; i.e., just the rotation of the order parameter about the field. Thus in two dimensions, we expect a Kosterlitz-Thouless phase transition in any nonzero field, even though there will be no transition *at* the symmetric Heisenberg point at zero field. Because thermal fluctuations are marginal in 2D, the crossover from Heisenberg to X-Y will be very rapid. A simple estimate is that the transition in a field will occur when the length scale associated with the field is of the order of the correlation length $\xi(T)$ in zero field. The length scale associated with the field,

$$\xi_H\equiv\frac{c}{H}\ , \tag{3.1}$$

is just the wavelength above which the linearized spin-wave modes will have a gap due to the field. Thus, we expect that $T_c(H)$ will be given implicitly by

$$\xi[T_c(H)]=C_1\xi_H\ , \tag{3.2}$$

with C_1 some constant. From Eq. (1.5) for $\xi(T)\approx K\xi_0 e^{2\pi\Upsilon/T}$ (Ref. 9) we have,

$$T_c=\Upsilon\frac{2\pi}{\ln\left[\dfrac{C_{xy}\Upsilon}{H}\right]}\ . \tag{3.3}$$

A detailed renormalization group calculation yields exactly Eq. (3.3) with $C_{xy}=C_1/K$ a *universal,* although hard to calculate, constant which depends *both* on the quantum-to-classical Heisenberg crossover calculated by Chakravarty *et al.*[9] (which yields $K\approx\frac{1}{2}$) and on the crossover from *classical* Heisenberg to X-Y. A naive estimate, using the universal value of $\rho_s(T_c)/T_c=2/\pi$ for the Kosterlitz-Thouless transition, suggests that C_1 in Eq. (3.2) is likely to be quite large so that a larger field than might have been expected is needed to yield a given T_c. However, this estimate is definitely not reliable and a detailed numerical calculation would be needed to yield the correct constant, C_{xy}. It is plausible that if C_{xy} is not too large, the antiferromagnetic transition temperature in $LaCu_2O_4$ could be raised significantly by the application of a large field. This possibility certainly merits further investigation.

IV. FINITE-SIZE EFFECTS

We now turn to the calculation of finite-size corrections to the free energy in a system of volume V. We first consider zero temperature for which there are fewer subtleties. A naive calculation of the zero-temperature finite-size correction to the free energy simply includes the change in zero-point energy of the two linear spin-wave modes:

$$\Delta E_0=2\int_\omega\left[\sum_q-V\int_q\right]\frac{1}{2}\ln(\chi\omega^2+\Upsilon q^2)$$
$$=2\left[\sum_q-V\int_q\right]\frac{1}{2}cq\ , \tag{4.1}$$

where the factor of 2 is for the two modes and the $\sum_q$ is over allowed wave vectors, i.e., for a hypercubic system with periodic boundary conditions,

$$\mathbf{q}=\frac{2\pi}{L}\mathbf{n}\ , \tag{4.2}$$

with $\mathbf{n}$ an integer vector.

From the d-dimensional Poisson summation formula we have, for any well-behaved function $g(\mathbf{q})$,

$$\left[\sum_{\mathbf{q}}-V\int_q\right]g(\mathbf{q})=V\sum_{\mathbf{m}\neq 0}\hat{g}(\mathbf{m}L)\ , \tag{4.3}$$

where $\mathbf{m}$ is an integer vector, and

$$\hat{g}(\mathbf{R})=\int_q g(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{R}} \tag{4.4}$$

is the Fourier transform of g. In d dimensions the Fourier transform of $|q|$ is

$$\mathcal{F}(|q|)=\frac{-(d-1)!A_d}{(2\pi)^d R^{d+1}} , \tag{4.5}$$

where $A_d=\pi^{d/2}2/\Gamma(d/2)$ is the surface area of a d-dimensional unit sphere. We thus find that for a hypercubic system at $T=0$,

$$\Delta E_0=\frac{-\hbar c}{L}\frac{(d-1)!}{2^{d-1}\pi^{d/2}\Gamma(d/2)}\sum_{\mathbf{m}\neq 0}\frac{1}{|\mathbf{m}|^{d+1}} . \tag{4.6}$$

We can evaluate the sum numerically to yield for a square system in $d=2$,

$$\Delta E_0=\frac{-\hbar c}{L}(1.438) . \tag{4.7}$$

For a system with skewed periodic boundary conditions on a hyperparallelogram with basis vectors $\mathbf{a}_1$, $\mathbf{a}_2, \ldots, \mathbf{a}_d$, Eq. (4.6) is replaced by

$$\Delta E_0=\frac{-\hbar c}{L}\frac{(d-1)!}{2^{d-1}\pi^{d/2}\Gamma(d/2)}V\sum_{\mathbf{m}\neq 0}\frac{1}{|\sum_j m_j\mathbf{a}_j|^{d+1}} . \tag{4.8}$$

We will see below, that these naive, linear spin-wave calculations do, in fact, yield the correct results for zero temperature, although the effects of the uniform mode (i.e., $q=0$) have not properly been taken into account.

A. Nonzero temperature

At nonzero temperature, the behavior is rather more subtle due to the effects of spatially uniform rotations of the order parameter as a function of imaginary time. There are three regimes of temperature:

(i) very low temperature,

$$T\sim\frac{1}{V\chi}\ll\frac{c}{L} , \tag{4.9}$$

(ii) low temperature,

$$T\sim\frac{c}{L} , \tag{4.10}$$

and

(iii) intermediate temperature,

$$\begin{aligned} &T\sim\Upsilon\xi_0^{d-2} \quad \text{for } d>2 , \\ &T\gtrsim\frac{\Upsilon}{\ln(L/\xi_0)} \quad \text{for } d=2 , \\ &T\gtrsim\Upsilon L^{d-2} \quad \text{for } 1<d<2 . \end{aligned} \tag{4.11}$$

Note that in one dimension, there is no regime (i) since $V\propto L$. This is related to the source of the subtleties in one dimension which cause the system to be disordered or quasiordered and the correct long-wavelength description needs to include an extra topological term.[10,11] For the scaling behavior discussed in the Introduction, we are interested in regime (ii), nevertheless, it is necessary to analyze the behavior in regime (i) in order to obtain the small TL/c limit of the scaling functions in regime (ii). Indeed, we will find that there is a slight modification of the scaling form for the free energy Eq. (1.6) due to the fluctuations in regime (i).

It is useful to divide the fluctuations into uniform ($q=0$) and nonuniform ($q\neq 0$) components. In all of the regimes the contribution to the fluctuations of $\hat{\mathbf{n}}(\mathbf{x},\tau)$ from the nonuniform thermal fluctuations will be small as can readily be seen by calculating the linear spin-wave contribution to

$$\langle[\hat{\mathbf{n}}(0,\tau)-\hat{\mathbf{n}}(\mathbf{x},\tau)]^2\rangle_T\approx V\sum_{\mathbf{q}}2(1-e^{i\mathbf{q}\cdot\mathbf{x}})\frac{1}{\sqrt{\Upsilon\chi}\,q}\frac{1}{e^{\beta cq}-1} , \tag{4.12}$$

where the subscript T denotes the thermal contribution to the fluctuations only. Since the sum in Eq. (4.12) has no contribution from $\mathbf{q}=\mathbf{0}$, it will be small, even for $|\mathbf{x}|\sim L/2$, provided that the contribution from other wavelengths is not too large: this is just the condition for *not* being in regime (iii). In regimes (i) and (ii) the nonlinearities in the nonuniform modes, which are controlled by the size of the fluctuations in $\hat{\mathbf{n}}$, will therefore be small. At $q=0$, on the other hand, the absence of stiffness makes the linearized fluctuations divergent and we need to treat the overall rotation of the order parameter as a collective coordinate. Indeed, in regime (i) the contribution from all the nonuniform excitations to the thermal free energy is small because of the exponential suppression factors.

B. Regime (i): Very low temperatures

In this regime,

$$T\ll\frac{c}{L} ,$$

and we need thus only consider the uniform notations of the order parameter in imaginary time. The controlling action for this is simply

$$S_U=\frac{V}{2}\int_0^\beta d\tau\,\chi\left[\frac{\partial\hat{\mathbf{N}}}{\partial\tau}-i\hat{\mathbf{N}}\times\mathbf{H}\right]^2 , \tag{4.13}$$

where $\hat{\mathbf{N}}$ is a unit vector which describes the orientation of the spatial average of the order parameter. It should be apparent that Eq. (4.13) is just the action for a quantum rotor with Hamiltonian

$$\hat{\mathcal{H}}_u=\tfrac{1}{2}(\chi V)^{-1}S^2-\mathbf{H}\cdot\mathbf{S} , \tag{4.14}$$

where we have dropped a constant term arising from the choice of the normalization of the functional integral which defines the partition function. The contribution of the uniform modes to the free energy, ΔF_u can now be written simply by using the quantization condition that the total spin S, and S_z are both integers. This arises simply from the general structure of the eigenvalues of the differential imaginary time transfer operator described by Eq. (4.14), and *no* reference to the underlying microscopic spins is needed here.[13] (Note, however, that with nonfrustrating periodic boundary conditions, the total spin is in any case expected to be an integer for any value of the microscopic elementary spin.) We thus have

$$\Delta F_u = -T\ln Z_u \ , \tag{4.15}$$

where the partition function

$$Z_u = \sum_{S=0}^{\infty} e^{-S(S+1)/2\chi VT} \left[\frac{\sinh[(S+\frac{1}{2})H/T]}{\sinh(\frac{1}{2}H/T)} \right] . \tag{4.16}$$

In *zero magnetic field,* the characteristic temperature scale is simply $1/\chi V$ [as claimed for regime (iii)]; this is just the energy scale for excitation from a singlet to a triplet state. For $T \gg 1/\chi V$, (but still $\ll 1/L$) the sum over S can be replaced by an integral yielding

$$\Delta F_u \approx -T\ln(2\chi VT) \ . \tag{4.17}$$

For $T \ll 1/\chi V$ on the other hand, $\Delta F_u \approx -3Te^{-1/\chi VT}$, reflecting the correction due to the $S=1$ state. It is intriguing to note that the expression, Eq. (4.17), is a real physical manifestation of the logarithmic size dependence of the free energy of a *classical* Heisenberg model.

In *nonzero magnetic field* there are several regimes: for $H \gg (T/\chi V)^{1/2}$, the large S_z and S states will dominate for $T \gg 1/\chi V$ yielding

$$\Delta F_u \approx -\frac{H^2\chi V}{2} - T\ln\sqrt{2\pi\chi VT} + T\ln(1-e^{-H/T}) \ , \tag{4.18}$$

which, if H is now formally taken to be $\ll T$, yields the zero-temperature transverse magnetic energy term plus a field independent part which differs from Eq. (4.17). This is due to the freezing of the direction of $\hat{N}$ perpendicular to $\mathbf{H}$ in this range of fields.

Conversely, for $H \ll (T/\chi V)^{1/2}$ but still $T \gg 1/\chi V$,

$$\Delta F_u \approx -\frac{2}{3}\frac{H^2\chi V}{2} - T\ln(2\chi VT) \ , \tag{4.19}$$

with the field-independent term from Eq. (4.17) and a magnetic free energy which reflects the mean-square projection of $\frac{2}{3}$ of $\hat{\mathbf{N}}\perp\mathbf{H}$, since in this regime, $\hat{\mathbf{N}}$ will fluctuate in all directions. This is a trivial version of the effect in an infinite system in $d \le 2$ discussed in Sec. II. Note that here we have not subtracted the $-1/2\chi H^2 V$ function as was done in Secs. I and II.

We now turn to an analysis of regime (ii) after observing that with $T \sim c/L$, the uniform modes yield a contribution to ΔF, Eq. (4.17), which is of the scaling form of Eq. (1.6) except for the logarithmic factor. If we calculate the energy, however, Eq. (4.17) yields a term without the logarithm, and hence of the appropriate scaling form expected for regime (ii).

C. Regime (ii): Low temperature

This is the main regime we are concerned with. It is defined by

$$T \sim c/L \ .$$

For simplicity we will restrict consideration to zero magnetic field. As argued above, in this regime the fluctuations are predominantly linear in character with the exception of the $q=0$, uniform modes. It is thus straightfoward to calculate the finite-size correction to the free energy by combining the contributions from the $q=0$ and $q\neq 0$ modes, and from zero and positive temperatures. The total free-energy correction is

$$\Delta F = \Delta E_0 + \Delta F_u + \Delta F_{NT} \ , \tag{4.20}$$

where ΔE_0 is the finite-size correction at zero temperature calculated above, ΔF_u is the finite-temperature contribution of the uniform modes given by Eq. (4.17), and ΔF_{NT} is the finite-temperature correction due to the nonuniform modes. The nonuniform thermal correction to the free energy can formally be written as

$$\Delta F_{NT} = \sum_{q\neq 0} \left[T\sum_{\omega} - \int_{\omega} \right] \ln(\omega^2 + c^2q^2) \ , \tag{4.21}$$

[where we have changed from $\ln(\chi\omega^2 + \Upsilon q^2)$ to $\ln(\omega^2+c^2q^2)$ which yields two cancelling terms]. (Note that in all expressions such as Eq. (4.21), care must be taken with the ultraviolet cutoffs in ω and q. However, since the singular terms of interest all come from long wavelengths and low frequencies, the detailed form of the cutoff should not matter. A simple lattice discretization of Eq. (1.1) with spatial lattice constant a and temporal lattice constant δ with a factor of $\chi a^d/2\pi\delta$ in the functional integral for each space-time lattice point yields simple limits independent of a and δ. All $\ln\omega$ are then really $\ln\omega\delta$ etc., with the δ-dependent parts cancelling in final results). The frequency sum and integration in Eq. (4.21) yield

$$\Delta F_{NT} = T\sum_{q\neq 0} 2\ln(1-e^{\beta cq}) \ , \tag{4.22}$$

which is convenient for evaluating the limit $T \gg c/L$ of the scaling function. In this limit, the dominant term is just the L^dT^{d+1} bulk thermal free energy given by the $H=0$ limit of Eq. (2.4). The leading finite-size correction arises from the $\ln q$ singularity of the summand in Eq. (4.22); this yields a correction of relative order $(c/TL)^d$ implying

$$\Delta F_{NT} \approx \sigma(0)T^{d+1}\left[\frac{L}{c}\right]^d + O(T) \ . \tag{4.23}$$

for $T \gg c/L$, with $\sigma(0)$ given by Eq. (2.5b). The contribution from the uniform modes, ΔF_u, is of order $T\ln T$ in this regime and hence dominates over ΔF_{NT} and ΔE_0 since the latter is of order $1/L$. Therefore, we have,

$$\Delta F \approx \sigma(0)T^{d+1}\left[\frac{L}{c}\right]^d - T\ln T + O(T) \ , \tag{4.24}$$

for $T \gg c/L$. Because of the $T\ln T$ term, the *energy* at positive temperatures has a positive size-independent finite-size correction,

$$E(T)-\epsilon_0 L^d \approx -d\sigma(0)T^{d+1}\left[\frac{L}{c}\right]^d + T + O(c/L)\ , \tag{4.25}$$

which dominates over the zero-temperature finite-size correction in this limit.

In order to obtain useful expressions valid for general $T \sim c/L$, some care is needed in treating both the small and large q and ω limits of the sums in Eq. (4.21), because of the logarithmic behavior.

We first rewrite the various contributions to ΔF in a form more symmetric in q and ω, separating out just the $q=0$ components both at positive and zero temperatures:

$$\Delta F = T\Phi - \Delta F_c + \Delta F_u\ , \tag{4.26}$$

where

$$\Phi = \sum_{Q\neq 0} \ln Q^2 - \Omega \int_Q \ln Q^2\ , \tag{4.27}$$

with

$$Q \equiv (\omega, c\mathbf{q})\ , \tag{4.28}$$

$$\Omega = \frac{V}{Tc^d}\ , \tag{4.29}$$

the space-time volume; and with

$$\Delta F_c = \left[T\sum_{\omega\neq 0} - \int_\omega\right] \ln\omega^2 = -2T\ln T\ , \tag{4.30}$$

giving the linearized approximation to the contribution from the $q=0$, $\omega\neq 0$ modes which are included in Φ, and are hence overcounted since the $q=0$ contribution is included in the uniform contribution ΔF_u which was calculated earlier. We can now evaluate Φ by the standard procedure of dividing $\ln Q^2$ into a part which decays rapidly for large Q and a part which is smooth near $Q=0$ so that its Fourier transform will decay rapidly. We restrict our specific considerations to two dimensions, but for a general parallelogram shape. A convenient choice in 2D is

$$\ln Q^2 = g_>(Q) + g_<(Q)\ , \tag{4.31}$$

with

$$g_>(Q) = -\mathrm{Ei}(\alpha^2 Q^2)\ , \tag{4.32}$$

in terms of the exponential integral function

$$\mathrm{Ei}(x) \equiv \int_x^\infty \frac{e^{-t}}{t} dt\ , \tag{4.33}$$

which decays rapidly for large x. The function $g_<(Q)$ is smooth for small Q with $g_<(0) = -\ln\alpha^2 - \gamma$ with $\gamma \approx 0.577$, Euler's constant. The arbitrary parameter α will later be chosen in a convenient manner.

The Fourier transform of $g_<(Q)$ is

$$\hat{g}_<(R) = \frac{-1}{2\pi R^3}\left[\mathrm{erfc}\left[\frac{R}{2\alpha}\right] + \frac{2}{\sqrt{\pi}}\frac{R}{2\alpha}e^{-(R/2\alpha)^2}\right]\ , \tag{4.34}$$

where

$$\mathrm{erfc}(x) \equiv \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-t^2} dt \tag{4.35}$$

is the complementary error function; $\hat{g}_<(R)$ hence decays as $e^{-(R/2\alpha)^2}$ for large R. We may now make use of the Poisson summation formula

$$\sum_Q g(Q) = \Omega \sum_R \hat{g}(R)\ , \tag{4.36}$$

with the sum on R running over the space-time reciprocal lattice of $\{Q\}$. Care is needed to properly subtract the $Q=0$ and $R=0$ terms from Eq. (4.36). The latter can be done by including a factor $e^{iQ\epsilon}$ and taking ϵ to zero at the end. We generally have, for singular sums such as the one needed,

$$\left[\sum_{Q\neq 0} - \Omega\int_Q\right] g(Q) = \sum_{Q\neq 0} g_>(Q) - g_<(0) + \Omega\sum_{R\neq 0}\hat{g}_<(R) + \Omega\hat{g}'_<(0)\ , \tag{4.37}$$

where

$$\hat{g}'_<(0) = \lim_{\epsilon\to 0}\left[\hat{g}_<(\epsilon) - \int_Q g(Q)e^{iQ\epsilon}\right]\ . \tag{4.38}$$

With $g(Q) = \ln Q^2$ and the choice for $g_<$ and $g_>$ given above, Eq. (4.32), we have, in two dimensions,

$$\hat{g}'_<(0) = \frac{1}{12\pi^{3/2}\alpha^3}\ , \tag{4.39}$$

whence

$$\Phi = \sum_{Q\neq 0}[-\mathrm{Ei}(\alpha^2 Q^2)] + \ln\alpha^2 + \gamma + \Omega\sum_{R\neq 0}\left[-\frac{1}{2\pi R^3}\left[\mathrm{erfc}(R/2\alpha) + \frac{2}{\sqrt{\pi}}\frac{R}{2\alpha}e^{-(R/2\alpha)^2}\right]\right] + \frac{\Omega}{12\pi^{3/2}\alpha^3}\ . \tag{4.40}$$

Since Φ is independent of α, we can choose α to make the sums converge most rapidly. If $1/T$ and all L/c are of the same order, the best choice is

$$\alpha = \frac{1}{T\sqrt{4\pi}}\ , \tag{4.41}$$

and the sums in Eq. (4.40) both converge as Gaussians and can be easily evaluated numerically. For a rectangular system with sides $\mathbf{a}_1$ and $\mathbf{a}_2$ with periodic boundary conditions, the real-space sum in Eq. (4.40) is over

$$R = (n\beta, m_1\mathbf{a}_1 + m_2\mathbf{a}_2)\ , \tag{4.42}$$

and that over Q just the lattice reciprocal to $\{R\}$.

In regime (ii) we thus have, collecting terms from Eq. (4.17), (4.30), and (4.40),

$$\Delta F = T[\Phi(\alpha) - \ln\alpha^2] - T\ln\left[\frac{2\chi V}{\alpha^2 T}\right], \tag{4.43}$$

where we have combined terms so that only dimensionless numbers appear in arguments of logs, the $\ln\alpha^2$ term just cancelling that in Eq. (4.40).

Note that the factor $\chi V/T = \Omega(\chi c^d)$ is just the space-time "volume" times the susceptibility in units in which $c=1$. Thus, we see that the expression Eq. (4.43) is explicitly Lorentz invariant, as it should be, since Φ is a function only of ratios of times. As mentioned earlier, the logarithmic factor in Eq. (4.43) is analogous to that appearing for a classical system; in the classical case it is arbitrary. Here, however, because of the underlying quantum nature of the problem, this term is *not* arbitrary, the only arbitrariness being the overall constant ground-state energy density.

It is straightforward, although somewhat tedious, to check that the previous limits of $T \ll c/L$ (i.e., the finite-size corrections to the ground state) and $T \gg c/L$ (i.e., the bulk specific heat) can be extracted from Eqs. (4.40) and (4.43); it is easiest to choose a different value of α to obtain these limits analytically.

V. CORRECTIONS TO SCALING AND ANALYSIS OF NUMERICAL RESULTS

So far, we have primarily been concerned with the leading corrections to the ordered fixed point which are controlled by the linear spin-wave fluctuations with renormalization group eigenvalue $\lambda_0 = 1-d$, i.e., the leading irrelevant operator. Other quantities will also have leading corrections controlled by this operator. For example, the finite-size susceptibility will have a correction of order $1/L^{d-1}$ at zero temperature as expected from the scaling form for the free energy Eq. (1.6) as a function of H, T, and L.

A natural expectation is that a second-order correction to the free energy would appear whose magnitude relative to the simple scaling corrections would be smaller by $(1/L)^{d-1}$, or some dimensionally similar combination of T and L. This could just arise from higher-order terms in an expansion in terms of the leading irrelevant operator. However, an examination of possible corrections to the free energy shows that all such $1/L^{d-1}$ corrections will be cancelled by terms arising from the Jacobian of the transformation from $\hat{\mathbf{n}}$ to $\boldsymbol{\pi}$ since no nontrivial two-loop diagrams in the free energy exist. The first nontrivial singular corrections will come from the three-loop "watermelon" diagrams yielding a correction to, for example, the ground-state energy of order

$$\Delta E_0 \sim \frac{1}{L}\left[\frac{1}{L^{2(d-1)}}\right]. \tag{5.1}$$

In addition, there will be corrections due to more strongly irrelevant operators. The leading such operators which can appear in the action are $(\nabla\hat{\mathbf{n}})^4$ and magnitude fluctuations of $\hat{\mathbf{n}}$ away from unity. The latter can be integrated out to yield the former; the eigenvalue of both leading corrections is simply

$$\lambda_1 = -d-1 . \tag{5.2}$$

The corrections due to $(\nabla\hat{\mathbf{n}})^4$ are thus down by two powers of length yielding, for example, T^{d+3} contributions to the bulk free-energy density arising from analytic corrections to the spin-wave dispersion: $\omega \approx cq + O(q^3)$. The correction to the ground-state energy will similarly be

$$\Delta E_0 \sim \frac{1}{L}\left[\frac{1}{L^2}\right]. \tag{5.3}$$

In two dimensions, the nonlinear singular corrections, Eq. (5.1) and the analytic corrections from $(\nabla\hat{\mathbf{n}})^4$, Eq. (5.3), are thus both of order $1/L^3$. *No $1/L^2$ terms exist,* nor, for that matter, do any terms in the free energy exist with any combination of H, T, and $1/L$ of this order.

A. Analysis of Numerical Results

We conclude this section with some brief comments on analysis of numerical calculations on 2D antiferromagnets.[5,6] Firstly, it is clear that extracting χ from finite-size exact diagonalization should be straightforward via, at $T=0$,

$$\Delta E_0(S) - \Delta E_0(S=0) = -\frac{\chi VS(S+1)}{2} \tag{5.4}$$

for small total spin S. For larger total spin, $S \sim sV$ with s small but of order unity, the singular corrections to the ground-state energy density in a field, Eq. (3.7), may be useful for extracting the spin-wave velocity, c. However, this intermediate region may be hard to extract useful information from numerically. Caution must be exercised concerning the corrections to scaling, as discussed above. In particular, the $1/L$ correction to $\chi(L)$ will complicate the analysis, although this correction is also universal and could be useful.

From the finite-size corrections to the ground state energy, Eq. (4.7), one can extract c directly. In this case, the corrections will only be at relative order $1/L^2$ so they should be controllable.

In finite-temperature Monte Carlo simulations, it should be apparent that it is best to work at temperatures $T \sim c/L$ since the most information is available in this regime, i.e., both c, as well as the quantities measured directly. Care must be taken to include the $O(T)$ correction to the energy in Eq. (4.24), if extraction of c from the specific heat with $T > c/L$ is attempted.

A combination of numerical techniques combined with careful analysis of the finite-size effects should yield real consistency checks for the hypothesis that a given system is an ordered antiferromagnet, unless the system is rather close to a zero-temperature critical point.

VI. COMPARISON WITH SCALING AT A CRITICAL POINT, DISCUSSION, AND FURTHER RESULTS

The finite-size scaling behavior found here is similar to that expected in general at a $(d+1)$ dimensional quantum critical point with β playing the role of the finite size in the time direction. The singular part of the action in the correlation volume thus plays the role of the singular part of the free energy at a finite-temperature critical point. Thus, from hyperscaling, we expect the singular part of the *action* in a space-time volume to be of order unity (i.e., $\hbar$). With β scaled by the spin-wave velocity to make the system isotropic we expect with $H=0$,

$$S_{\text{sing}}=\beta\Delta F\approx\Sigma_0\left[\frac{L}{\beta c}\right] \tag{6.1}$$

as from Eq. (1.6). In fact, however, the contribution from the uniform modes yields a weakly nonscaling contribution to S_{sing}, with a $\ln T$ dependence. This is analogous to that which occurs at conventional critical points when some exponents are integers, for example the logarithmic specific heat in the 2D Ising model.

It is important to note, however, that at *any* zero-temperature critical point at which hyperscaling holds and the dynamic exponent z, which relates the scaling of space and time, is equal to unity, with the system being "Lorentz invariant" at the critical point, one expects the singular part of the action to scale as in Eq. (6.1).[14] All such critical points will thus have the same finite-size scaling behavior but with *different* scaling functions which will generally *not* include logarithmic pieces, except when some exponents are integers.

A. Staggered susceptibility

One of the ways in which the trivial ordered fixed point analyzed here differs from nontrivial critical points is in the scaling of the order-parameter susceptibility: i.e., the staggered susceptibility, χ_s. The staggered susceptibility in a volume V is expected generally to scale as[13]

$$\chi_s\propto\frac{1}{V}\frac{(m_sV)^2}{T}\sim\frac{V}{T}m_s^2\ , \tag{6.2}$$

where m_s is the staggered magnetization density. In general, at a critical point m_s will decrease with size as $L^{-\beta\nu}$. In our case, on the other hand, it is size independent by the assumption of long-range order so that $\chi_s\sim V/T\sim\Omega$, i.e., a trivial scaling with the space-time volume. (ME) Fisher and Privman[13] have carried out a detailed analysis of the finite-size scaling behavior of the susceptibility of $O(n)$ ferromagnets in their ordered phase. Their results can be applied directly to the scaling of the staggered susceptibility in the $n=3$ quantum antiferromagnets of interest here by taking one of the lengths to be c/T (they evaluate the strongly anisotropic limit $T\ll c/L$ as well as the isotropic limit $T\sim c/L$ in a staggered field). We will not reproduce Fisher and Privman's[13] results here. Note only that for the staggered susceptibility, as for the free energy, one must separate the uniform and the nonuniform spin-wave contributions which each dominate in different regimes.

B. One dimension

In one dimension, all of the analysis presented here breaks down since the long-wavelength behavior of quantum antiferromagnets is *not* controlled by the simple nonlinear σ-model fixed point which is unstable to nonlinear spin-wave fluctuations. However as shown by Haldane and Affleck,[10,11] for $\frac{1}{2}$ integer spins the system is still (at least in some ranges of parameters) controlled by a marginally stable Lorentz-invariant fixed point of the nonlinear σ model with an additional topological term. This yields nontrivial power-law decays of correlations as found in the Bethe-Ansatz solution of the spin-$\frac{1}{2}$ nearest-neighbor antiferromagnetic chain. Affleck[11] has examined the finite-size corrections to the ground-state energy and finds, in a system of size L, $O(1/L)$ corrections to the total energy. In addition, a linear specific heat at positive temperature is found which, when scaled by the long-wavelength spin-wave velocity, is simply related to the finite-size correction to the ground-state energy, as expected by the asymptotic Lorentz invariance. Although the form of the finite-size and finite-β corrections are thus the same in 1D as found here for $d>1$, the coefficients in 1D are entirely nontrivial, since they are related to the central charge of the corresponding conformal field theory.[11]

VII. SOLID ^{3}He AND DYNAMICS

We have seen that the thermodynamic behavior of quantum antiferromagnets at low temperatures and small magnetic fields should be universal. This also applies in systems with tetragonal or orthorhombic symmetry, such as the tetragonal ordered phase of solid ^{3}He. The only adjustment necessary is to rescale the lengths in each direction by the anisotropy in the spin wave velocities.

In solid ^{3}He, the transitions out of the low-field ordered phase, as either the temperature or magnetic field are raised, are both strongly first order.[2] Thus it is likely that the thermodynamics of the entire ordered phase is determined solely by the universal nonlinear σ-model fluctuations analyzed here. The susceptibility at low temperature can be measured directly, and the appropriate combination of spin-wave velocities determined from the T^3 specific heat. All the other universal properties can then be derived from these two, particularly $M(H,T)$ from Eq. (2.8). (Note that the leading T^5 correction to the specific heat will have both a universal and nonuniversal component). If the low-field thermodynamic properties do *not* agree with the results presented here, it suggests that the inference that the ordered phase breaks only two of the spin symmetries should be reexamined. A helicoidal phase with a more complicated order parameter and thus different low-T thermodynamics, has not yet been directly excluded by experiments.

In addition to the universality of the thermodynamic properties, dynamic properties which depend on the long-wavelength spin waves will also be universal. In particular, in the presence of the weak nuclear dipolar spin anisotropy, the temperature dependence of the NMR mode measured experimentally will be universal. This has been independently pointed out by Grishchuk and Marchenko[7] and the result is in good agreement with experiments of Osheroff.[15]

A. Spin-wave scattering

Properties which depend on the scattering of long-wavelength spin waves can also be derived as universal functions of Υ and χ. The matrix elements for scattering of, say, two-wavelength spin waves can be derived by canonically quantizing the spin waves from the long-wavelength Lagrangian, Eq. (1.1), *after* having integrated out the short-wavelength quantum fluctuations. The remaining nonlinearities will be weak for $d>1$ and can thus be treated perturbatively. The matrix elements from the nonlinear σ model will just be *universal* constants times powers of the macroscopic Υ and χ with wave-vector and angular-dependent factors which have simple forms. The angular dependence of the four spin-wave matrix elements were shown, some time ago, to have simple forms to all orders in perturbation theory in powers of $1/S$ by a complicated calculation of Kumar *et al.*,[16] they did not, however, realize that the coefficients were universal. The angular dependence can, in fact, be derived in general in a few lines directly from the nonlinear σ-model representation. The universality of spin-wave-scattering processes has various experimental consequences for solid ^3He, for example, in determining the linewidths of the NMR modes in the presence of weak anisotropy, and various hydrodynamic relaxation processes. These will not be discussed in detail here. We should note, however, that processes which depend on nonlinearities in the dispersion of spin waves will not be universal, but rather controlled by corrections such as those due to the $(\nabla\hat{\mathbf{n}})^4$ terms in the action.

Note added: After this work was complete, unpublished work by Neuberger and Ziman[17] was received, which also considers finite-size corrections to ground-state properties.

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