Correlated-basis-function analysis of the transverse Ising model

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Correlated-basis-function (CBF) theory, which has provided a firm foundation for *ab initio* calculations of the properties of quantum fluids such as liquid ^{4}He, is adapted and applied at the Jastrow-Feenberg variational level to give an optimized description of the structure and of the elementary excitations of the Ising-spin model in a transverse magnetic field. A set of trial wave functions of Hartree-Jastrow form is assumed to describe the spatial correlations present in the ordered as well as the disordered ground states, and the Feynman *Ansatz* is consistently adopted to represent the elementary magnon states. The CBF analysis of the spin system employs the hypernetted-chain (HNC) formalism for a substitutional binary mixture of bosons and derives HNC equations for the spatial distribution functions which determine the ground-state energy expectation value. Functional variation of this quantity with respect to the magnetic order parameter and the trial states leads to two Euler-Lagrange equations, which may be interpreted as a renormalized Hartree equation for the optimal magnetization and as a paired-magnon equation for the magnetic correlation function that is analogous to the familiar paired-phonon equation for conventional quantum fluids. Numerical calculations are based on simple cubic lattices and an optimized nearest-neighbor *Ansatz* for the generating pseudopotential. Results are reported on the order parameter, the energy per lattice site, the transverse magnetization, and the magnon excitation energies as functions of the coupling parameter $0 \leqslant \lambda \leqslant \infty$ measuring the strength of the transverse magnetic field. We also present numerical results on the magnetic correlation function, the static structure function, and the correlation length. The system exhibits a second-order phase transition at a critical value λ_c of the coupling strength. Our numerical calculations of the optimal order parameter yields $\lambda_c \simeq 5.17$ for a simple cubic lattice and $\lambda_c \simeq 3.12$ for a square planar lattice. The calculated data are in very good agreement with results derived from perturbation expansions in conjunction with Padé techniques.

I. INTRODUCTION

Correlated-basis-function (CBF) theory[1–6] provides a powerful and efficient *ab initio* treatment of the ground and excited states of strongly correlated quantum fluids. It has been successfully applied to homogeneous and inhomogeneous Bose and Fermi systems such as liquid helium,[5,7,8] helium mixtures,[9,10] interfaces,[11] planar surfaces,[12,13] and helium films with or without a supporting substrate[14,15] and helium droplets.[16] The semianalytic theory gives valuable insight into the correlated structure of the ground state and its stability and permits, notably, a quantitative analysis of the elementary excitations of a correlated many-body system.

Usually, CBF theory is employed in conjunction with the hypernetted-chain (HNC) classification scheme and has therefore close relations with the diagrammatic parquet approach.[17,18] Further, CBF theory may be used to improve systematically the density-functional models[19] often adopted in theoretical studies of problems in condensed matter physics.[20]

It is our present aim to extend the application of CBF theory to an adequate formal and numerical study of correlation effects in crystalline materials that may underlie structural phase transitions of second order or may generate anomalies in the elementary excitation modes of these systems. Such an analysis may be based, initially, on sufficiently simple Hamiltonian models characterized by one- or two-dimensional order parameters for certain classes of magnetic, ferroelectric,[21–24] or ferroelastic materials[25] or of alloys.[26] We are primarily interested in exploring, qualitatively and quantitatively, the properties of these systems or models in an intermediate region of their phase spaces where a molecular-field approximation is not sufficiently accurate but theories of the fine structure of phase transitions very close to the critical point[26–28] do not yet apply. Investigations of this nature are certainly of interest since anomalous features in this range of phase space may signal the possibility of structural transitions. A sophisticated many-body theory of correlations such as the CBF approach has the potential to realize these objectives and to provide insight into the physical problems. It has been already applied to explore the vibrational modes in quantum solids[29,30] the mass gap of the elementary excitations in a lattice gauge model of quantum field theory,[31,32] and the properties of the Hubbard model.[33,34] However, a systematic study of lattices or models of solids within CBF theory is still lacking. We therefore concentrate at present on one of the simplest models that exhibits a second-order phase transition, the Ising model[35,36] in a transverse magnetic field.[21] This spin-lattice system has been extensively studied[37–39] and its known properties may be used to test the quality of the approximations in each systematic step within the CBF approach before we proceed to more complex lattice systems. We note that the transverse Ising model provides, despite its simplicity, a useful description of insulating magnetic systems, order-disorder ferroelectrics, cooperative Jahn-Teller systems, and other systems with pseudospin-phonon interactions.[21,22,24,39,40] Moreover, in two spatial dimensions the model is dual to the $Z(2)$ lattice gauge model in the uncharged sector of states.[41] The transverse Ising system therefore provides information on the

structure of the field vacuum and on the mass of the vacuum excitations.[42–45]

CBF theory begins with an appropriate formulation of the expectation value of the ground-state energy of the spin-lattice model with respect to a set of trial many-body states. In a first step we assume these states to be of Hartree-Jastrow form.[46] To evaluate the associated spatial distribution function and the transverse magnetization that enter the energy expectation value we equivalently describe the infinitely extended lattice as a substitutional binary mixture of two types of bosons.[25] The results of Ref. 47 may be utilized to perform a hypernetted-chain (HNC) analysis of the corresponding partial distribution functions and to extract a set of HNC equations for the magnetic correlation function. We may also use this formalism to evaluate the transverse magnetization in terms of the magnetic order parameter and the spin-exchange strength. In the disordered phase this strength may be expressed in terms of the nodal and nonnodal components of the spatial distribution function. To evaluate the exchange strength associated with an ordered state a second set of HNC equations for a modified spatial distribution function is needed. This function describes the additional correlation effects that are induced by the condensation of paramagnons into the degenerate ordered state. The solutions of these HNC equations may be employed to evaluate the excitation energies of the elementary excitations of the ordered states and the disordered states, in Feynman approximation.[48]

The CBF analysis on the variational level may be completed by a systematic optimization procedure for constructing the best wave function of Hartree-Jastrow type. Two Euler-Lagrange equations are derived by utilizing the minimum principle for the ground-state energy.[3] These equations can be interpreted as a renormalized Hartree equation for the optimal magnetization if the system is ordered, and as a paired-magnon equation that determines the optimal spatial distribution function of the spin system. The latter equation is the analog of the paired-phonon equation[3] familiar from the CBF theory of liquid ^{4}He.

Numerical calculations within the CBF formalism developed here are performed on the order parameter, the transverse magnetization, the ground-state energy, the spatial distribution function, and the magnon energies. These calculations are based on an optimized nearest-neighbor *Ansatz* for the pseudopotential defining the correlated wave function of Jastrow type that describes the ground state of Ising spins on a simple cubic lattice. The results for these physical quantities as functions of the applied external field are compared with available results obtained by series-expansion techniques.[38,39]

Section II provides the necessary information on the transverse Ising model and the set of correlated basis functions adopted. Section III describes the binary mixture formalism that is employed to analyze the energy functional, the distribution functions, and the transverse magnetization. The next two sections report on the results of the formal CBF analysis of the disordered phase of the model (Sec. IV), and of the ordered phase (Sec. V). The renormalized Hartree equation and the paired-magnon condition are developed in Sec. VI. The numerical results on various physical quantities that describe the properties of the spin-lattice model are reported and discussed in Sec. VII. This section concludes with a discussion of future improvements within CBF theory and application of the theory to more complex models of crystalline materials. The Appendix summarizes the HNC analysis of the modified spatial distribution function that is needed for the evaluation of the transverse magnetization in the ordered phase.

II. THE ENERGY FUNCTIONAL

The Ising model in a transverse magnetic field is described by the Hamiltonian[38,39]

$$\mathscr{H}=\frac{1}{2}\sum_{i,j}^{N}\Delta_{ij}\sigma_i^x\sigma_j^x+\lambda\sum_{i}^{N}(1-\sigma_i^z), \tag{1}$$

defined on a D-dimensional simple hypercubic lattice with N lattice points and periodic boundary conditions. The spin at site i ($i=1,2,\ldots,N$) is represented by the x and z components of the Pauli operator, σ_i^x and σ_i^z, respectively. The potential Δ_{ij} characterizes the spin-spin interaction that depends on the relative distance $|\mathbf{n}|=|\mathbf{r}_i-\mathbf{r}_j|$ between the lattice points i and j. The transverse field is measured by the coupling parameter λ ($0\leqslant\lambda\leqslant\infty$). For simplicity, the potential $\Delta_{ij}\equiv\Delta(\mathbf{n})$ is assumed to be of the nearest-neighbor form,

$$\Delta(\mathbf{n})=\begin{cases}2D, & \mathbf{n}=\mathbf{0},\\ -1, & \text{for nearest neighbors},\\ 0, & \text{otherwise.}\end{cases} \tag{2}$$

At zero temperature the model exhibits an ordered (ferromagnetic) phase at a coupling parameter $0\leqslant\lambda<\lambda_c$ and a disordered (paramagnetic) phase at $\lambda_c<\lambda\leqslant\infty$. A second-order phase transition occurs at the critical-field strength $\lambda=\lambda_c$. The order in the ferromagnetic phase is measured by the magnetization in the x direction,

$$M=\frac{\langle\Psi|\sigma_i^x|\Psi\rangle}{\langle\Psi|\Psi\rangle}. \tag{3}$$

The ground state $|\Psi\rangle$ has the symmetry of the Hamiltonian (1) at $M=0$, while the reflection symmetry of the Hamiltonian (with respect to the operation $x\rightarrow -x$) is broken in the ordered phase, where $M\neq 0$.

Within CBF theory[1–3] the analysis begins with the evaluation of the expectation value of the ground-state energy per lattice site,

$$\frac{E}{N}=\frac{\langle\Psi|\mathscr{H}|\Psi\rangle}{N\langle\Psi|\Psi\rangle}, \tag{4}$$

with respect to a suitable set of correlated trial wave functions Ψ. Defining the spatial distribution function

$$g(\mathbf{n})=\frac{\langle\Psi|\sigma_i^x\sigma_j^x|\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{5}$$

and the transverse magnetization

$$A=\frac{\langle\Psi|\sigma_i^z|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \tag{6}$$

we may write the expectation value (4) in the form

$$\frac{E}{N}=\frac{1}{2}\sum_{\mathbf{n}}\Delta(\mathbf{n})g(\mathbf{n})+\lambda(1-A), \tag{7}$$

where the sum extends over N lattice points. The distribution function (5) is short ranged in the disordered phase and exhibits long-range spatial order in the ferromagnetic phase of the infinitely extended lattice, with $g(\mathbf{n})=M^2$ as $|\mathbf{n}|\rightarrow\infty$. We therefore decompose this function according to

$$g(\mathbf{n})=\delta_{\mathbf{n0}}+(1-\delta_{\mathbf{n0}})M^2+(1-M^2)G(\mathbf{n}). \tag{8}$$

The correlation function $G(\mathbf{n})$ vanishes at $\mathbf{n}=\mathbf{0}$ and in the asymptotic region $|\mathbf{n}|\rightarrow\infty$. In the molecular-field approximation, which ignores the effects of spatial correlations, the function $G(\mathbf{n})$ vanishes identically.

To separate kinematic and dynamic effects in the transverse magnetization we cast expression (6) into the factorized form

$$A=(1-M^2)^{1/2}n_{12}. \tag{9}$$

In the mean-field approximation the spin-exchange strength n_{12} is unity, but it is smaller than unity if the spatial correlations are properly incorporated.

In terms of the quantities M, n_{12}, and $G(\mathbf{n})$, the energy functional reads, explicitly,

$$\frac{E}{N}=(1-M^2)\left\{D+\frac{1}{2}\sum_{\mathbf{n}}\Delta(\mathbf{n})G(\mathbf{n})\right\}+\lambda\{1-(1-M^2)^{1/2}n_{12}\}. \tag{10}$$

In the mean-field approximation, expression (10) is reduced to a simple function of the magnetization M. In this case the energy is minimal for

$$M^2=1-\left(\frac{\lambda}{2D}\right)^2 \tag{11}$$

in the ordered state, implying the familiar result $\lambda_c=2D$ for the critical coupling parameter.

CBF theory provides a systematic and efficient scheme for evaluating the optimal magnetizations M and A and the optimal spatial correlation function $G(\mathbf{n})$ associated with a set of suitably correlated many-body wave functions. In analogy to the established CBF treatment of conventional quantum fluids,[3–6] we adopt a correlated many-body ground state of Hartree-Jastrow type,[12,46]

$$|\Psi\rangle=\exp\{MU_M+U\}|0\rangle, \tag{12}$$

with

$$U=\frac{1}{2}\sum_{i<j}^{N}u(\mathbf{r}_{ij})\sigma_i^x\sigma_j^x, \tag{13}$$

$$U_M=\sum_{i}^{N}u_1(\mathbf{r}_i)\sigma_i^x+\frac{1}{4}\sum_{i<j}^{N}u_M(\mathbf{r}_{ij})(\sigma_i^x+\sigma_j^x). \tag{14}$$

The reference state $|0\rangle$ is represented by a symmetric product of N single-spin states with spin component $\sigma^z=+1$. For a translationally invariant system the single-spin quantity $u_1(\mathbf{r}_i)$ is independent of the lattice point i and the pseudopotentials $u(\mathbf{r}_{ij})$ and $u_M(\mathbf{r}_{ij})$ depend only on the relative distance $|\mathbf{n}|$ ($\mathbf{n}\equiv\mathbf{r}_{ij}\equiv\mathbf{r}_i-\mathbf{r}_j$). In the disordered phase, the state (12) is determined by the *Ansatz* (13) and the component (14) is not needed. The latter portion contributes to the correlations present in the ordered state and accounts for the symmetry breaking. Reflection at a mirror plane normal to the x axis transforms the quantity (14) to $(-U_M)$ and reveals a twofold degeneracy of the ordered ground state (characterized by the magnetizations M and $-M$). We note that the component $u_M(\mathbf{n})$ is not independent of the pseudopotential $u(\mathbf{n})$. Their relationship will be analyzed in the following sections. If desirable, the *Ansätze* (13) and (14) may be improved by complementing the pair potentials by pseudopotentials of triplet form.[49]

We next construct the full set of correlated many-body wave functions. In analogy with the density-fluctuation operators employed in the CBF theory of quantum fluids[3] such as liquid ^{4}He, we introduce the excitation operators $\rho_{\mathbf{k}}^x=\sum_i^N e^{i\mathbf{k}\cdot\mathbf{r}_i}\sigma_i^x$ and form the ideal magnon states $|\Psi_{\mathbf{k}}^x\rangle=\rho_{\mathbf{k}}^x|\Psi\rangle$. The excitation energy of the magnons is then evaluated in Feynman approximation,[48]

$$\omega(\mathbf{k})=\frac{\varepsilon}{S(\mathbf{k})}. \tag{15}$$

The static structure function is related to the spatial distribution function by a Fourier transformation,

$$S(\mathbf{k})=1+\sum_{\mathbf{n}}e^{i\mathbf{k}\cdot\mathbf{n}}G(\mathbf{n}). \tag{16}$$

The single-particle energy ε is defined by the expectation value

$$\varepsilon=\frac{\langle\Psi|[\rho_{\mathbf{k}}^x,[\mathscr{H},\rho_{-\mathbf{k}}^x]]|\Psi\rangle}{2N(1-M^2)\langle\Psi|\Psi\rangle}=2\lambda n_{12}(1-M^2)^{-1/2}. \tag{17}$$

In the Hartree approximation, where $G(\mathbf{n})\equiv0$ and $n_{12}=1$, the energy of a magnon is therefore estimated by $\omega(\mathbf{k})\simeq\varepsilon$. In this approximation paramagnons carry the energy $\omega(\mathbf{k})\simeq2\lambda$, while the Hartree energy of ferromagnons is constant, $\omega(\mathbf{k})\simeq4D$. These estimates, however, only provide reasonable results in the weak ($\lambda\rightarrow\infty$) and strong ($\lambda\rightarrow0$) coupling limits. As for the ground-state energy, CBF theory offers a systematic means for the evaluation of correlation effects on the excitation energies at any given value of the coupling parameter λ (see Sec. VII for a detailed discussion).

III. MIXTURE FORMALISM

To evaluate the energy expectation value (10) we have to construct the spatial distribution function $G(\mathbf{n})$ and the spin-exchange strength n_{12} associated with the *Ansätze* (12),(13),(14) as functionals of the pseudopotential $u(\mathbf{n})$ that generates the spatial correlations. To do this we describe the spin-lattice system, more conveniently, as a binary mixture of two types of bosons.[25] The two boson species are characterized by the eigenvalues $(+1)$ and (-1) of the spin operator σ^x and may be called particles and holes, respectively. The partial densities ρ_+ and ρ_- of the two components are determined by the magnetization through $\rho_\pm=\frac{1}{2}(1\pm M)$, i.e., by the expectation values

$$\rho_{\pm}=\frac{\langle\Psi|P_i^{(\pm)}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{18}$$

of the projectors $P_i^{(\pm)}=\frac{1}{2}(1\pm\sigma_i^x)$. Due to the sum rule $P_i^{(+)}+P_i^{(-)}=1$, the total density $\rho=\rho_+ +\rho_-$ of the mixture is unity.

Employing the projectors $P_i^{(\pm)}$, we may rewrite the generator in the exponent of *Ansatz* (12) as

$$\begin{aligned} MU_M+U=u_1M\sum_i^N\,(P_i^{(+)}-P_i^{(-)}) \\ +\frac{1}{2}\sum_{i<j}^N u_{++}(\mathbf{r}_{ij})P_i^{(+)}P_j^{(+)} \\ +\frac{1}{2}\sum_{i<j}^N u_{--}(\mathbf{r}_{ij})P_i^{(-)}P_j^{(-)} \\ +\frac{1}{2}\sum_{i\neq j}^N u_{+-}(\mathbf{r}_{ij})P_i^{(+)}P_j^{(-)}, \end{aligned} \tag{19}$$

having introduced the partial pseudopotentials ($\mathbf{n}\neq 0$),

$$\begin{aligned} u_{++}(\mathbf{n})&=u(\mathbf{n})+Mu_M(\mathbf{n}), \\ u_{+-}(\mathbf{n})&=-u(\mathbf{n}), \\ u_{--}(\mathbf{n})&=u(\mathbf{n})-Mu_M(\mathbf{n}). \end{aligned} \tag{20}$$

Expression (19) has the familiar form corresponding to a Hartree-Jastrow wave function for a homogeneous binary boson mixture.[47] To evaluate the quantities $G(\mathbf{n})$ and n_{12}, we may exploit the HNC analysis of the ground state of such a mixture, given in Ref. 47.

The partial distribution functions characterizing the structure of the binary mixture are[47]

$$\rho_\alpha\rho_\beta g_{\alpha\beta}(\mathbf{n})=(1-\delta_{\mathbf{n0}})\,\frac{\langle\Psi|P_i^{(\alpha)}P_j^{(\beta)}|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \tag{21}$$

where the indices α, β label particles $(+)$ or holes $(-)$. These functions are decomposed into nodal (N) and non-nodal (X) components,

$$g_{\alpha\beta}(\mathbf{n})=1+X_{\alpha\beta}(\mathbf{n})+N_{\alpha\beta}(\mathbf{n}). \tag{22}$$

They are related by a set of HNC equations ($\gamma=+,-$),

$$\begin{aligned} X_{\alpha\beta}(\mathbf{n})=(1-\delta_{\mathbf{n0}})\exp\{u_{\alpha\beta}(\mathbf{n})+N_{\alpha\beta}(\mathbf{n})+E_{\alpha\beta}(\mathbf{n})\} \\ -N_{\alpha\beta}(\mathbf{n})-1, \end{aligned} \tag{23}$$

$$N_{\alpha\beta}(\mathbf{n})=\sum_\gamma\,\rho_\gamma\sum_{\mathbf{m}}\,X_{\alpha\gamma}(\mathbf{n}-\mathbf{m})\{X_{\gamma\beta}(\mathbf{m})+N_{\gamma\beta}(\mathbf{m})\}. \tag{24}$$

For given pseudopotentials $u_{\alpha\beta}(\mathbf{n})$ and elementary quantities $E_{\alpha\beta}(\mathbf{n})$, the HNC equations (23),(24) may be employed to evaluate the distribution functions $g_{\alpha\beta}(\mathbf{n})$. According to the definition (21), the spatial distribution function $G(\mathbf{n})$ can be constructed via any of the relations

$$G(\mathbf{n})=(1-\delta_{\mathbf{n0}})\,\frac{1+M}{1-M}\,\{g_{++}(\mathbf{n})-1\}, \tag{25}$$

$$G(\mathbf{n})=(1-\delta_{\mathbf{n0}})\{1-g_{+-}(\mathbf{n})\}, \tag{26}$$

$$G(\mathbf{n})=(1-\delta_{\mathbf{n0}})\,\frac{1-M}{1+M}\,\{g_{--}(\mathbf{n})-1\}. \tag{27}$$

Since Eqs. (25)–(27) must be simultaneously fulfilled, they constitute, in general, conditions on the partial distribution functions $g_{\alpha\beta}(\mathbf{n})$ and, therewith, on the pseudopotentials (20). These conditions enable us to simplify the HNC equations (23),(24) and to determine the functional dependence of the pseudopotential $u_M(\mathbf{n})$ on the generator $u(\mathbf{n})$ in the ordered state (Secs. IV and V).

Reference 47 provides formal results on the spin-exchange strength [cf. Eq. (33) of Ref. 47] with the mixture formalism,

$$n_{12}=\exp\{D_{12}-\tfrac{1}{2}(D_1+D_2)\}. \tag{28}$$

The quantities D_1 and D_2 appearing in the exponent are explicitly given by the expression

$$\begin{aligned} D_1=\rho_+\sum_{\mathbf{n}}\,X_{++}(\mathbf{n})+\rho_-\sum_{\mathbf{n}}\,X_{+-}(\mathbf{n})-\frac{1}{2}\,\rho_+\sum_{\mathbf{n}}\,N_{++}(\mathbf{n}) \\ \times\{X_{++}(\mathbf{n})+N_{++}(\mathbf{n})\}-\frac{1}{2}\,\rho_-\sum_{\mathbf{n}}\,N_{+-}(\mathbf{n}) \\ \times\{X_{+-}(\mathbf{n})+N_{+-}(\mathbf{n})\}+E_{D_1}. \end{aligned} \tag{29}$$

The quantity D_2 is obtained from Eq. (29) by interchanging the indices $+$ and $-$.

Due to the symmetry of the disordered state the exponential term D_{12} vanishes in the paramagnetic phase. In this case the strength factor n_{12} may be calculated from the solutions of the HNC equations (23),(24).

In the ordered phase, the quantity D_{12} differs from zero and may be evaluated from[47]

$$\begin{aligned} D_{12}=\sum_{\mathbf{n}}\,\{\rho_+X_+(\mathbf{n})+\rho_-X_-(\mathbf{n})\} \\ -\frac{1}{2}\,\rho_+\sum_{\mathbf{n}}\,N_+(\mathbf{n})\{X_+(\mathbf{n})+N_+(\mathbf{n})\} \\ -\frac{1}{2}\,\rho_-\sum_{\mathbf{n}}\,N_-(\mathbf{n})\{X_-(\mathbf{n})+N_-(\mathbf{n})\}+E_{D_{12}}. \end{aligned} \tag{30}$$

This requires the solutions of a second set of HNC equations for a modified distribution function $g_\alpha(\mathbf{n})$ within the binary mixture formalism (see the Appendix).

IV. THE DISORDERED PHASE

The symmetry properties of the paramagnetic phase may be exploited to simplify the HNC equations (23),(24). Specializing to $\rho_+=\rho_-=\frac{1}{2}$ and $g_{++}(\mathbf{n})=g_{--}(\mathbf{n})$ at $M=0$, we work with the sum and the difference of the functions

$g_{++}(\mathbf{n})$ and $g_{+-}(\mathbf{n})$. With Eqs. (25) and (26) we have the relations

$$2G(\mathbf{n})=g_{++}(\mathbf{n})-g_{+-}(\mathbf{n}), \tag{31}$$

$$2(1-\delta_{\mathbf{n0}})=g_{++}(\mathbf{n})+g_{+-}(\mathbf{n}). \tag{32}$$

Introducing the linear superpositions

$$\begin{aligned} X_{++}(\mathbf{n})&=X_{--}(\mathbf{n})=X_0(\mathbf{n})+X(\mathbf{n}),\\ X_{+-}(\mathbf{n})&=X_{-+}(\mathbf{n})=X_0(\mathbf{n})-X(\mathbf{n}), \end{aligned} \tag{33}$$

and

$$\begin{aligned} N_{++}(\mathbf{n})&=N_{--}(\mathbf{n})=N_0(\mathbf{n})+N(\mathbf{n}),\\ N_{+-}(\mathbf{n})&=N_{-+}(\mathbf{n})=N_0(\mathbf{n})-N(\mathbf{n}), \end{aligned} \tag{34}$$

the conditions (31) and (32) can be decoupled,

$$G(\mathbf{n})=X(\mathbf{n})+N(\mathbf{n}), \tag{35}$$

$$0=X_0(\mathbf{n})+N_0(\mathbf{n})+\delta_{\mathbf{n0}}. \tag{36}$$

Employing the decompositions (33),(34) and the relation (36), the set of chain equations (24) collapses into a single equation,

$$N(\mathbf{n})=\sum_{\mathbf{m}} X(\mathbf{n}-\mathbf{m})\{X(\mathbf{m})+N(\mathbf{m})\}. \tag{37}$$

Relation (37) has the form of the familiar chain equation for a one-component system[50] at a density $\rho=1$.

At $M=0$ the hypernet equations (23) reduce to two different equations. With the help of the decompositions (33) and (34), these equations may be reformulated in analogy with the treatment of the chain equations. The consistency condition (32) then permits the explicit construction of the function $N_0(\mathbf{n})$ in terms of the pseudopotential $u(\mathbf{n})$ and the nodal function $N(\mathbf{n})$. Elementary algebraic manipulations yield the result ($\mathbf{n}\neq 0$),

$$\begin{aligned} 2\exp\{-N_0(\mathbf{n})\}=&\exp\{-u(\mathbf{n})-N(\mathbf{n})+E_{+-}(\mathbf{n})\}\\ &+\exp\{u(\mathbf{n})+N(\mathbf{n})+E_{++}(\mathbf{n})\}. \end{aligned} \tag{38}$$

Relation (38) allows us, at $M=0$, to formulate a single hypernet equation associated with the spatial distribution function $G(\mathbf{n})$,

$$X(\mathbf{n})=(1-\delta_{\mathbf{n0}})\tanh\{u(\mathbf{n})+N(\mathbf{n})+E(\mathbf{n})\}-N(\mathbf{n}). \tag{39}$$

The elementary contribution $E(\mathbf{n})$ is defined by the difference $2E(\mathbf{n})=E_{++}(\mathbf{n})-E_{+-}(\mathbf{n})$. Equation (39) constitutes a modified form of hypernet equation for a one-component boson system.[50]

In the disordered state the transverse magnetization (6) or (9) is given by the spin-exchange strength (28) with $D_{12}=0$ and $D_1=D_2$. Expression (29) for the quantity D_1 may be rewritten with the aid of Eqs. (33)–(35), as

$$D_1=-\sum_{\mathbf{n}} N_0(\mathbf{n})-\frac{1}{2}\sum_{\mathbf{n}} N(\mathbf{n})G(\mathbf{n})+E_{D_1}. \tag{40}$$

Finally, we may use Eqs. (38) and (39) to eliminate the function $N_0(\mathbf{n})$ from Eq. (40). The result is

$$D_1=-\frac{1}{2}\sum_{\mathbf{n}} \ln\{1-G^2(\mathbf{n})\}-\frac{1}{2}\sum_{\mathbf{n}} N(\mathbf{n})G(\mathbf{n})+E_D. \tag{41}$$

The HNC equations (37),(39) and the relations (35),(41) provide explicit expressions for the energy expectation value with respect to a disordered state as a functional of the generating pseudopotential $u(\mathbf{n})$.

V. THE ORDERED PHASE

To reformulate the set of HNC equations (23),(24) for the case that the magnetization M differs from zero, we proceed in analogy to the treatment of Sec. IV and generalize the linear superpositions (33),(34). Thus, we introduce

$$\begin{aligned} X_{++}(\mathbf{n})&=X_0(\mathbf{n})+\frac{1-M}{1+M}X(\mathbf{n}),\\ X_{+-}(\mathbf{n})&=X_{-+}(\mathbf{n})=X_0(\mathbf{n})-X(\mathbf{n}),\\ X_{--}(\mathbf{n})&=X_0(\mathbf{n})+\frac{1+M}{1-M}X(\mathbf{n}), \end{aligned} \tag{42}$$

along with similar relations for the nodal functions $N_{\alpha\beta}(\mathbf{n})$. Appealing to the conditions (25)–(27) and the decompositions (42), we may condense the set of three chain equations (24) into the single equation

$$N(\mathbf{n})=\sum_{\mathbf{m}} X(\mathbf{n}-\mathbf{m})\{X(\mathbf{m})+N(\mathbf{m})\} \tag{43}$$

for the distribution function $G(\mathbf{n})=X(\mathbf{n})+N(\mathbf{n})$. Equation (43) holds at any value of the order parameter M and agrees therefore with the result (37) derived in the preceding section. However, at $M\neq 0$ conditions (25)–(27) are only fulfilled if the relation

$$\begin{aligned} (1+M)&\left[\exp\left\{2u(\mathbf{n})+Mu_M(\mathbf{n})+\frac{2}{1+M}N(\mathbf{n})\right.\right.\\ &\left.\left.+E_{++}(\mathbf{n})-E_{+-}(\mathbf{n})\right\}-1\right]\\ =(1-M)&\left[\exp\left\{2u(\mathbf{n})-Mu_M(\mathbf{n})+\frac{2}{1-M}N(\mathbf{n})\right.\right.\\ &\left.\left.+E_{--}(\mathbf{n})-E_{-+}(\mathbf{n})\right\}-1\right] \end{aligned} \tag{44}$$

is satisfied ($\mathbf{n}\neq 0$). For vanishing magnetization, Eq. (44) is identically fulfilled. We may interpret Eq. (44) as an equation defining the pseudopotential $u_M(\mathbf{n})$ of *Ansatz* (14) as a functional of the generator $u(\mathbf{n})$.

In further algebraic manipulations, we solve Eq. (44) for the quantity $u_M(\mathbf{n})$ and insert the result, together with the decompositions (42), into the hypernet equations (23). This enables us to extract an explicit expression for the function $N_0(\mathbf{n})$ in terms of the functions $u(\mathbf{n})$, $N(\mathbf{n})$, $E_{\alpha\beta}(\mathbf{n})$, and the order parameter M,

$$2\exp\{-N_0(\mathbf{n})\}=\{1+[1+(1-M^2)(\cdots)]^{1/2}\}\times\exp\{-u(\mathbf{n})-N(\mathbf{n})+E_{+-}(\mathbf{n})\},\tag{45}$$

with

$$(\cdots)=\exp\{4u(\mathbf{n})+4(1-M^2)^{-1}N(\mathbf{n})+4E(\mathbf{n})\}-1\tag{46}$$

and $4E(\mathbf{n})=E_{++}(\mathbf{n})+E_{--}(\mathbf{n})-2E_{+-}(\mathbf{n})$. This result permits us to replace the hypernet equations (23) by a hypernet equation of the form

$$X(\mathbf{n})=(1-\delta_{\mathbf{n0}})-N(\mathbf{n})-2(1-\delta_{\mathbf{n0}})\times\{1+[1+(1-M^2)(\cdots)]^{1/2}\}^{-1},\tag{47}$$

the bracket term $(\cdots)$ being defined by Eq. (46). Equations (42) and (47) specialize correctly to results (33) and (39), respectively, at vanishing magnetization, $M=0$.

To complete the theoretical analysis of the energy functional (10) we have to derive explicit expressions for the quantities D_{12}, and D_1,D_2 that determine the spin-exchange strength n_{12}. While it is straightforward to express the quantity (29) in terms of the functions $G(\mathbf{n})$ and $N(\mathbf{n})$ via Eqs. (42), we need a modified distribution function $\hat{G}(\mathbf{n})=\hat{X}(\mathbf{n})+\hat{N}(\mathbf{n})$ to evaluate the functional D_{12} at nonzero order parameter M. We may show (see the Appendix) that the nodal and nonnodal components, $\hat{N}(\mathbf{n})$ and $\hat{X}(\mathbf{n})$, respectively, are related by a set of modified HNC equations. These functions together with the quantities $X(\mathbf{n})$ and $N(\mathbf{n})$ suffice to evaluate the functional D_{12}.

The HNC equations associated with the distribution function $\hat{G}(\mathbf{n})$ read

$$\hat{X}(\mathbf{n})=-\hat{N}(\mathbf{n})+(1-\delta_{\mathbf{n0}})M^{-1}\times\frac{\tanh M\{\hat{u}(\mathbf{n})+\hat{N}(\mathbf{n})+\hat{E}(\mathbf{n})\}}{1+M\tanh M\{\hat{u}(\mathbf{n})+\hat{N}(\mathbf{n})+\hat{E}(\mathbf{n})\}},\tag{48}$$

$$\hat{N}(\mathbf{n})=(1-M^2)^{-1}\sum_{\mathbf{m}}G(\mathbf{n}-\mathbf{m})G(\mathbf{m})+\sum_{\mathbf{m}}G(\mathbf{n}-\mathbf{m})\hat{X}(\mathbf{m}).\tag{49}$$

The generating pseudopotential $\hat{u}(\mathbf{n})$ appearing in Eq. (48) is defined by

$$\hat{u}(\mathbf{n})=\frac{1}{4}M^{-1}\left[\ln\left\{1+\frac{1-M}{1+M}G(\mathbf{n})\right\}-\ln\left\{1+\frac{1+M}{1-M}G(\mathbf{n})\right\}\right].\tag{50}$$

The solutions of the HNC equations (43),(47), and (48),(49) provide an explicit expression for the exchange strength (28) where quantities (29) and (30) are given in terms of the distribution functions $G(\mathbf{n})$,$\hat{G}(\mathbf{n})$, the associated nodal portions $N(\mathbf{n})$,$\hat{N}(\mathbf{n})$, and the order parameter M. Thus

$$\ln n_{12}=\frac{1}{2}\sum_{\mathbf{n}}\ln\{1-G(\mathbf{n})\}+\frac{1}{4}\sum_{\mathbf{n}}\ln\left\{1+\frac{1-M}{1+M}G(\mathbf{n})\right\}+\frac{1}{4}\sum_{\mathbf{n}}\ln\left\{1+\frac{1+M}{1-M}G(\mathbf{n})\right\}+\frac{1}{2}(1-M^2)^{-1}\times\sum_{\mathbf{n}}G(\mathbf{n})N(\mathbf{n})-\frac{1}{2}\sum_{\mathbf{n}}\ln\{1-M(1+M)\hat{G}(\mathbf{n})\}-\frac{1}{2}\sum_{\mathbf{n}}\ln\{1+M(1-M)\hat{G}(\mathbf{n})\}-M^2\times\sum_{\mathbf{n}}\hat{N}(\mathbf{n})+\frac{1}{2}M^2\sum_{\mathbf{n}}G(\mathbf{n})\hat{N}(\mathbf{n})-\frac{1}{2}M^2(1-M^2)\times\sum_{\mathbf{n}}\hat{G}(\mathbf{n})\hat{N}(\mathbf{n})+E_{12}.\tag{51}$$

Result (51) specializes correctly to the sum $(D_1+D_2)=2D_1$ that was obtained for the logarithm of the spin-exchange strength at zero magnetization [cf. Eq. (41)].

VI. OPTIMIZATION

To complete the CBF analysis at the variational level we employ the minimum principle for the ground-state energy. The optimal correlated wave function of the type (12)–(14) is determined by the solutions of the Euler-Lagrange equations

$$\frac{\partial E}{\partial M}=0,\tag{52}$$

$$\frac{\delta E}{\delta u(\mathbf{n})}=0.\tag{53}$$

They may be used to calculate the optimal distribution function $G(\mathbf{n})$, the optimal magnetizations M and A, and the optimal magnon energy $\omega(\mathbf{k})$.

Equation (52) may be viewed as a renormalized Hartree equation for the order parameter M of the ferromagnetic state. Equation (52) can be given the explicit form

$$M^2=\left\{1-\frac{\lambda}{2D}n_{12}\frac{1+H_1}{1+H_0}\right\}\left\{1+\frac{\lambda}{2D}n_{12}\frac{1+H_1}{1+H_0}\right\},\tag{54}$$

with the Hartree potentials

$$H_0=\frac{1}{2D}\sum_{\mathbf{n}}\Delta(\mathbf{n})G(\mathbf{n}),\tag{55}$$

$$H_1=2(M^2-1)\frac{\partial\ln n_{12}}{\partial M^2}.\tag{56}$$

An explicit expression for the potential (56) may be derived by taking the derivative of the result (51) with respect to the magnetization M.

Equation (54) yields an implicit condition on the critical coupling parameter,

$$\lambda_c = \frac{2D}{n_{12}} \left(\frac{1+H_0}{1+H_1} \right). \tag{57}$$

The Euler-Lagrange equation (53) is the analog of the paired-phonon equation familiar from the CBF theory of quantum fluids such as liquid helium.[3] We may therefore call Eq. (53) a paired-magnon equation. This equation can be cast into the form

$$\dot{G}(\mathbf{n}) + \tfrac{1}{2}\varepsilon(1-M^2)G(\mathbf{n}) = 0. \tag{58}$$

The function $\dot{G}(\mathbf{n})$ is the derivative $(\partial/\partial\beta)G(\mathbf{n},\beta)|_{\beta=0}$ of a generalized distribution function $G(\mathbf{n},\beta)$ that is generated by a pseudopotential $u(\mathbf{n},\beta)=u(\mathbf{n})+\beta v(\mathbf{n})$. At $\beta=0$ we recover the standard spatial distribution function $G(\mathbf{n})$ generated by the pseudopotential $u(\mathbf{n})$. The quantity $v(\mathbf{n})$ is the Feenberg effective potential[3] associated with the Ising model and the pseudopotential $u(\mathbf{n})$. It can be decomposed into two portions,

$$v(\mathbf{n}) = v^*(\mathbf{n}) + M^2 v_M^*(\mathbf{n}). \tag{59}$$

The component $v_M^*(\mathbf{n})$ contributes only if the system is ordered. It describes the effect that originates from the condensation of paramagnons into the ordered ground state. For the disordered phase the effective potential $v^*(\mathbf{n})$ is explicitly given by

$$v^*(\mathbf{n}) = \Delta(\mathbf{n}) - \frac{\varepsilon}{2}\left\{ N(\mathbf{n}) - \frac{G(\mathbf{n})}{1-G^2(\mathbf{n})} \right\}. \tag{60}$$

It specializes to $v^*(\mathbf{n})=\Delta(\mathbf{n})$ in the weak-coupling limit ($\lambda\to\infty$) since the spins are not correlated in the asymptotic region of the coupling parameter. In the strong-coupling limit ($\lambda\to 0$) the effective potential $v(\mathbf{n})$ vanishes for the same reason.

VII. NUMERICAL RESULTS AND DISCUSSION

In an application of the CBF approach to the transverse Ising model, we perform a restricted optimization based on the one-parameter *Ansatz*

$$u(\mathbf{n}) = \alpha(1-\delta_{\mathbf{n}\mathbf{0}})\Delta(\mathbf{n}) \tag{61}$$

for the generating pseudopotential. The parameter α is chosen such that the energy expectation value (10) attains a minimum. We note that the optimized *Ansatz* (61) reproduces the exact results on the ground-state energy and other physical quantities in the strong-coupling limit ($\lambda\to 0$) and in the weak-coupling regime ($\lambda\to\infty$).

The HNC equations (37),(39) associated with the disordered state and the HNC equations (43) and (47)–(49) corresponding to the ordered phase are solved in HNC/0 approximation, i.e., by neglecting the elementary contributions. We emphasize that these equations are derived for an infinitely extended spin lattice in the limit $N\to\infty$ at fixed lattice constant. Of course, the actual numerical calculations for solving the HNC equations are carried out on a finite lattice with periodic boundary conditions.

We have performed numerical calculations at all ranges of the coupling parameter λ for square and simple cubic lattices. Here, we report on some results on the optimal order parameter M and, particularly, on the critical coupling parameter λ_c where the magnetization vanishes. In a series of figures, we display the optimal results for the ground-state energy, the spin-exchange strength, the static structure factor at zero wave number, the spatial distribution function $G(\mathbf{n})$, and the magnon energies at vanishing momentum $\hbar\mathbf{k}$, as functions of the external field. The results are compared with results derived from series expansions in powers of λ or λ^{-1} reported in Refs. 38 and 39.

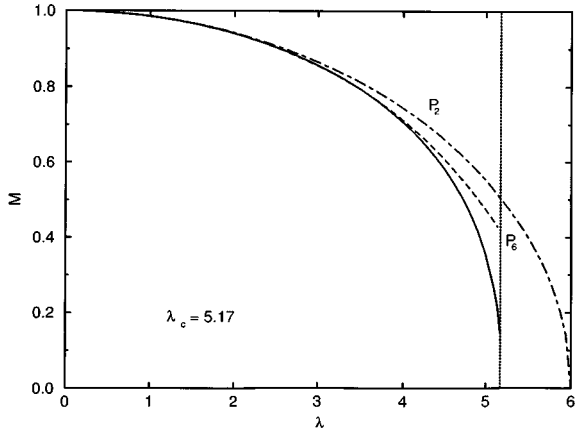

FIG. 1. Optimized CBF results (in HNC/0 approximation) for the order parameter M (magnetization in the x direction) as a function of the coupling parameter λ (solid curve). The long-range order vanishes at the critical point $\lambda_c=5.17$. For comparison we also show the results of perturbation theory, in second order (molecular-field approximation, denoted P_2) and in sixth order (P_6).

Figure 1 shows the numerical results for the optimal order parameter M. The calculation is done for a $32\times32\times32$ lattice with periodic boundary conditions in the range $0\leqslant\lambda\leqslant5.14$ of the coupling strength and checked against the results for a $8\times8\times8$ lattice. We find that finite-size effects are very small and may be ignored as long as we do not probe the fine structure of the magnetization and the other physical quantities of interest in the region $|\lambda-\lambda_c|\leqslant0.05$ very close to the critical point λ_c. The value of the critical parameter calculated within the present realization of the CBF theory is $\lambda_c\approx5.17$. This result is in very good agreement with the result of Ref. 38, $\lambda_c\approx5.21$, derived from perturbation theory in conjunction with Padé approximation techniques. The order parameter M expanded in powers of the parameter λ in the ordered state is represented, up to sixth order by[38]

$$M = 1 - \frac{1}{2}\left(\frac{\lambda}{6}\right)^2 - 0.255\left(\frac{\lambda}{6}\right)^4 - 0.1672\left(\frac{\lambda}{6}\right)^6 + \cdots . \tag{62}$$

For a convenient comparison we plot the results in second order—representing the molecular-field approximation—and in sixth order in Fig. 1.

A similar CBF calculation of the optimal order parameter and the critical transverse field of the two-dimensional Ising model on a square lattice yields $\lambda_c\approx3.12$ for the critical coupling parameter. The result agrees very well with the value $\lambda_c\approx3.14$ reported in Ref. 38 that is believed to be the most

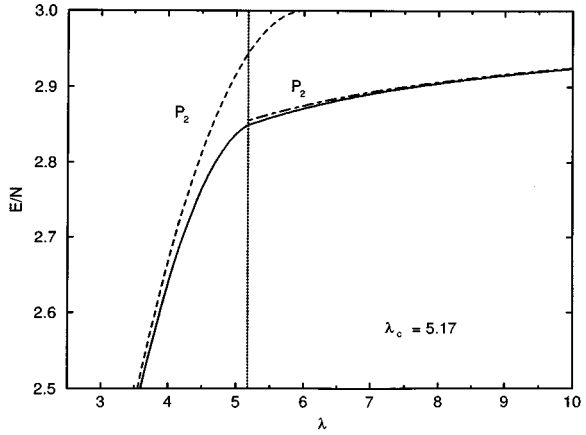

FIG. 2. Numerical results for the optimal ground-state energy per lattice site based on the *Ansätze* (12)–(14) and (61), in HNC/0 approximation. The results are compared with those of second-order perturbation theory for the disordered phase, Eq. (64), $\lambda>\lambda_c$, and for the ordered phase, Eq. (63), which represent the results of the molecular-field approximation at $0\leqslant\lambda\leqslant 4$.

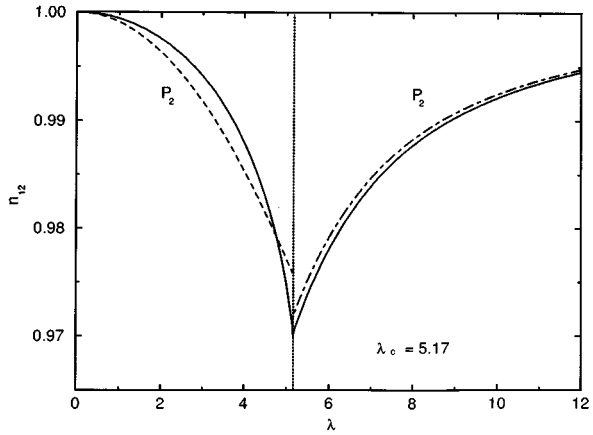

FIG. 3. CBF results (in HNC/0 approximation) for the spin-exchange strength n_{12} of Eq. (28) [related by Eq. (9) to the transverse magnetization], compared with the results (65) and (66) of second-order perturbation expansions in powers of λ and λ^{-1}, respectively.

reliable result within a *first-principles* approach.[44] Our result may be also compared with results of other microscopic approaches.[45,51–55]

The numerical results on the optimal ground-state energy (10) of a simple cubic spin-lattice as a function of the coupling parameter λ are presented in Fig. 2 together with the results of second-order perturbation theory,[38,39]

$$\frac{E}{N}=\lambda\left\{1-\frac{\lambda}{12}+\cdots\right\},\quad \lambda<\lambda_c, \tag{63}$$

$$\frac{E}{N}=3\left\{1-\frac{1}{4}\lambda^{-1}+\cdots\right\},\quad \lambda>\lambda_c. \tag{64}$$

The CBF results merge with the results (63) and (64) for $0\leqslant\lambda<2.5$ and $\lambda>10$, respectively. They depend smoothly on the coupling parameter in the transition range.

Figure 3 displays the numerical results on the spin-exchange strength versus the external field. Since the spins are not correlated in the limits of strong ($\lambda\to 0$) and weak ($\lambda\to\infty$) coupling, the function n_{12} must approach unity in these limits. Our data agree very well with the perturbative results[38,39] in second order, in the range $0\leqslant\lambda<0.5$ and $15<\lambda$,

$$n_{12}=1-0.0328\left(\frac{\lambda}{6}\right)^2+\cdots,\quad \lambda<\lambda_c, \tag{65}$$

$$n_{12}=A=1-0.0208\left(\frac{6}{\lambda}\right)^2+\cdots,\quad \lambda>\lambda_c. \tag{66}$$

Results on the behavior of the spatial correlations are displayed in Figs. 4–6. The static structure function (16) at vanishing wave vector $\mathbf{k}$ is shown in Fig. 4. This quantity is a measure of the correlation length of the interacting spin system. Since the spins are uncorrelated as $\lambda\to 0$ or $\lambda\to\infty$, the spatial distribution function $G(\mathbf{n})$ vanishes in these limits and, consequently, quantity $S(0)$ approaches unity. Perturbation theory[38] yields the expansion

$$S(0)=1+\frac{1}{2}\left(\frac{6}{\lambda}\right)+0.3125\left(\frac{6}{\lambda}\right)^2+0.2326\left(\frac{6}{\lambda}\right)^3+0.1742\left(\frac{6}{\lambda}\right)^4+\cdots \tag{67}$$

for the disordered phase. The fourth-order approximation is plotted in Fig. 4 (dot-dashed curve). For a coupling parameter $\lambda>15$ the CBF results are well represented by the perturbative results in fourth order. In the transition range $\lambda\simeq\lambda_c$ the CBF results exhibit a rather sharp but finite peak indicating a maximum for the correlation length. However, this result signals the limitations of the approximate *Ansatz* (61) presently adopted. If the structure function (16) corresponds to the exact ground state, quantity $S(0)$ diverges at the critical point. Consequently, *Ansatz* (61) is not flexible enough to describe correctly the asymptotic behavior of the spatial dis-

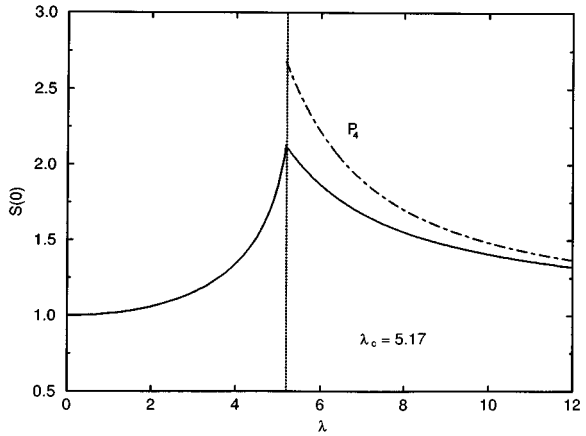

FIG. 4. The static structure function $S(0)$ at zero momentum corresponding to the *Ansätze* (12)–(14) and optimized choice (61), in HNC/0 approximation. The CBF results at coupling parameters in the range $\lambda>\lambda_c$ (disordered phase) are compared with the results of expansion (67), up to fourth order.

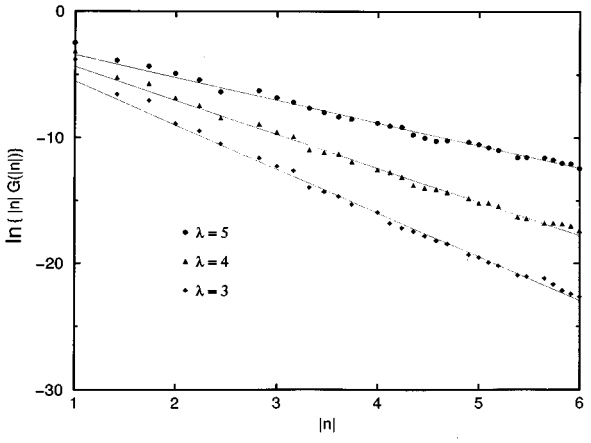

FIG. 5. Plot of the logarithm of the function $|\mathbf{n}|G(\mathbf{n})$ versus the lattice distance $|\mathbf{n}|$ at constant transverse field ($\lambda=3,4,5$). The spatial distribution function $G(\mathbf{n})$ corresponds to an ordered state described by the *Ansätze* (12)–(14) and (61) with the optimal parameter α. The numerical calculation is based on the CBF formalism in conjunction with the HNC/0 approximation. The data are well represented by straight lines, thus confirming the suggested exponential behavior (68).

tribution function $G(\mathbf{n})$ that leads to a divergent correlation length. To improve the present result we should (i) implement the strict functional optimization procedure described in Sec. VI and (ii) incorporate systematically the correlation effects generated by pseudopotentials of triplet, quadruplet,... n-tuplet type in addition to the pairpotentials $u(\mathbf{n})$ and $u_M(\mathbf{n})$ considered in *Ansätze* (13) and (14). We stress, however, that we aim primarily at a reliable quantitative study outside of the narrow region of the fine structure of the transition where theories of critical exponents are appropriate.

The CBF results on the U(1) lattice gauge model[31,32] suggest that the asymptotic behavior of the spatial distribution function $G(\mathbf{n})$ corresponding to *Ansätze* (12)–(14) should be well represented by the classical dependence

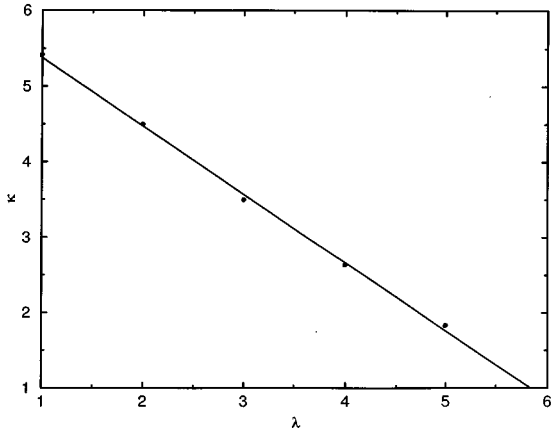

FIG. 6. CBF results (in HNC/0 approximation) for the inverse correlation length κ of the distribution function $G(\mathbf{n})$ that characterizes the structure of the ordered phase ($0\leqslant\lambda\leqslant\lambda_c$). The correlation length increases with increasing strength of the transverse magnetic field but remains finite (due to the approximations made) at the critical point λ_c.

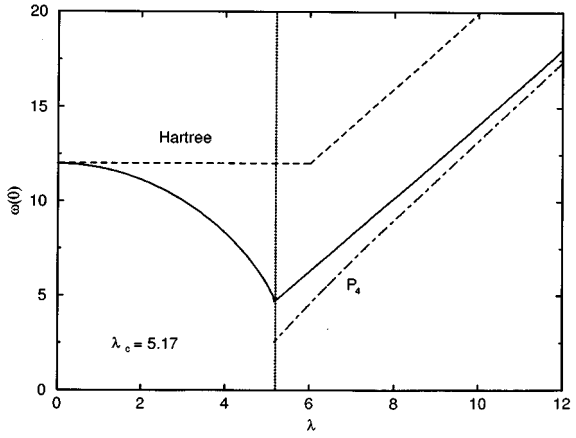

FIG. 7. Numerical results for the magnon energy gap $\omega(0)$ at zero wave number, in Feynman approximation (15). The CBF data correctly reproduce the exact dependence on the coupling parameter λ in the limits $\lambda\to0$ and $\lambda\to\infty$. The results for the paramagnon energy are compared with the perturbation results (69), in the fourth-order approximation. The Hartree energies are depicted by a broken line. In the transition region $\lambda\simeq\lambda_c=5.17$, the gap exhibits a minimum. Due to the approximations adopted, the minimum is not deep enough and, consequently, the magnon mode is not completely soft.

$$G(\mathbf{n})\simeq\frac{G_0}{|\mathbf{n}|}\,e^{-\kappa|\mathbf{n}|}, \tag{68}$$

where the inverse correlation length κ depends on the transverse magnetic field. We therefore plot the quantity $\ln\{|\mathbf{n}|G(\mathbf{n})\}$ in Fig. 5 versus the distance $|\mathbf{n}|$ at various coupling parameters, $\lambda<\lambda_c$. The linear dependence confirms very well the suggested behavior (68). The slope of each line gives the inverse correlation length κ as a function of the field strength λ. The result is shown in Fig. 6. The quantity κ decreases linearly with increasing strength of the transverse magnetic field $\lambda<\lambda_c$. An analogous behavior is found in the paramagnetic region.

As expected, the increase of the correlation length κ^{-1} is not rapid enough to reproduce correctly the singularity at the critical point associated with the true ground state. If we wish to improve the description of the fine structure in the transition region very close to the critical parameter λ_c, we must appropriately generalize the *Ansätze* (12)–(14) and (61) or we must proceed to the next level within the CBF theory where perturbative corrections are taken into account.[1–3]

In Fig. 7 we present our numerical results on the magnon energies at $\hbar\mathbf{k}=0$, calculated in Feynman approximation (15), as a function of the field strength λ. The calculated data may be compared with the results in the Hartree approximation and with the results[38] based on the series expansion ($\lambda>\lambda_c$),

$$\omega(0)=2\lambda\left\{1-\frac{1}{2}\left(\frac{6}{\lambda}\right)-0.0833\left(\frac{6}{\lambda}\right)^2-0.03747\left(\frac{6}{\lambda}\right)^3+\cdots\right\}. \tag{69}$$

The CBF results correctly reproduce the exact results corresponding to the true excited states at small transverse fields ($\lambda\to0$) and at very large coupling parameters ($\lambda\to\infty$). The

CBF results show a drastic reduction of the energy gap $\omega(0)$ as the critical region $\lambda \simeq \lambda_c$ is approached. Thus, the presently adopted *Ansätze* (12)–(14) and (61) take already account of a substantial portion of long-range effects but do not lead to a complete softening of the excitation mode at the critical point. Employment of the solutions of the Euler-Lagrange equations (54) and (58) and incorporation of "backflow" effects[56,3,14] into the *Ansatz* for the magnon states and triplet correlations[49] into the *Ansätze* (13),(14) may remedy this shortcoming of the presently adopted approximation close to the transition.

In summary, CBF theory at its variational level has been adapted to treat the ground and excited states of the Ising model in a transverse magnetic field. HNC equations have been derived for the spatial distribution functions associated with a suitable class of correlated many-body ground states of Hartree-Jastrow type. These distribution functions determine the energy functional, the transverse magnetization, the magnon energies, and other physical quantities of interest. An optimal version of the theory has been given in terms of Euler-Lagrange equations, consisting of a renormalized Hartree equation for the order parameter and a paired-magnon condition for the best pseudopotential.

A detailed numerical application of the theory has been performed in HNC/0 approximation, based on a one-parameter form for the pseudopotential. We have studied the dependence of various properties of the model on the transverse field. In particular, we have reported results on the spatial distribution function and its correlation length, on the static structure function, on the spin-exchange strength, and on the magnon energy gap. The results agree correctly with exact results of standard perturbation expansions in the strong- and weak-coupling regime. Since CBF theory is, in spirit, a nonperturbative approach its application is not limited to these particular regions of the phase space. The approach, therefore, permits one to bridge the gap between the regions where perturbative approaches are valid and the (narrow) transition region where scaling theories of phase transitions are appropriate. We have shown that the CBF analysis yields accurate numerical results on the critical points in two and three spatial dimensions.

We finally note that the CBF approach is formulated for infinitely extended systems, i.e., we are not limited to a numerical analysis of small finite lattices.

The present numerical application of the variational-CBF formalism should be complemented in future numerical work by a strict functional optimization of the pseudopotential $u(\mathbf{n})$. Solving the Euler-Lagrange equations (54) and (58) we can properly take account of the long-range effects of this function which are missing in the nearest-neighbor *Ansatz* (61). However, we believe that in the near term it would be more fruitful to extend the formalism to a quantitative description of the properties of lattice systems at finite temperatures. Such a generalization of the CBF approach has been already developed for quantum fluids such as liquid ^{4}He (Refs. 8, 11, 13, 14, and 57) at low temperatures and has led to the formulation of a correlated density matrix theory at more elevated temperatures.[58,59] The implementation of these approaches to spin lattices would permit systematic studies of real crystalline materials where the structural phase transitions are driven by a pseudospin mechanism.[39]

The formalism presented here can be directly applied for a numerical study of the $Z(2)$ lattice gauge model in two spatial dimensions,[42–45] for investigating the properties of Ising models with spin interactions $\Delta(\mathbf{n})$ that are not restricted to the form (2), or—with only minor modifications—to a CBF analysis of antiferromagnetic phases, etc.

Concluding this discussion of future properties we point out that the methods we have explored may be adapted to the treatment of more complex spin models, such as anisotropic Heisenberg models, mixtures of spin systems (alloys), and other models of interest in condensed-matter physics.[60–62,26,34]

ACKNOWLEDGMENTS

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APPENDIX: THE DISTRIBUTION FUNCTION $\hat{G}(\mathbf{n})$

The functional D_{12}, Eq. (30), is determined by the nodal and nonnodal components of the modified distribution functions[47]

$$g_\alpha(\mathbf{n}) = 1 + X_\alpha(\mathbf{n}) + N_\alpha(\mathbf{n}), \tag{A1}$$

with $\alpha = +$ or $-$. The associated HNC equations relating the functions $X_\alpha(\mathbf{n})$ and $N_\alpha(\mathbf{n})$ are

$$X_\alpha(\mathbf{n}) = (1-\delta_{\mathbf{n0}})\exp\{\tfrac{1}{2}u_{\alpha\alpha}(\mathbf{n}) + \tfrac{1}{2}u_{+-}(\mathbf{n}) + N_\alpha(\mathbf{n}) + E_\alpha(\mathbf{n})\} - N_\alpha(\mathbf{n}) - 1, \tag{A2}$$

$$N_\alpha(\mathbf{n}) = \sum_\beta \rho_\beta \sum_{\mathbf{m}} X_\beta(\mathbf{n}-\mathbf{m})\{X_{\beta\alpha}(\mathbf{m}) + N_{\beta\alpha}(\mathbf{m})\}. \tag{A3}$$

The generating pseudopotentials in Eq. (A2) may be written in the form

$$u_{++}(\mathbf{n}) + u_{+-}(\mathbf{n}) = M u_M(\mathbf{n}),$$
$$u_{--}(\mathbf{n}) + u_{+-}(\mathbf{n}) = -M u_M(\mathbf{n}), \tag{A4}$$

due to Eqs. (20). They vanish at $M=0$ and, consequently, Eqs. (A2) and (A3) have the solutions $X_\alpha(\mathbf{n}) = N_\alpha(\mathbf{n}) \equiv 0$, $\mathbf{n} \neq \mathbf{0}$. The distribution functions (A1) for the disordered state are therefore given by $g_\alpha(\mathbf{n}) = 1 - \delta_{\mathbf{n0}}$ and the quantity D_{12} vanishes identically. However, spatial correlations contribute to the distribution functions (A1) if the state is ordered.

To cast the HNC equations (A2) and (A3) into a more convenient form we decompose the functions (A1) and their X and N components according to[47]

$$2g_\alpha(\mathbf{n}) = g_{\alpha\alpha}(\mathbf{n}) + g_{+-}(\mathbf{n}) + 2\hat{G}_\alpha(\mathbf{n}),$$
$$2X_\alpha(\mathbf{n}) = X_{\alpha\alpha}(\mathbf{n}) + X_{+-}(\mathbf{n}) + 2\hat{X}_\alpha(\mathbf{n}), \tag{A5}$$
$$2N_\alpha(\mathbf{n}) = N_{\alpha\alpha}(\mathbf{n}) + N_{+-}(\mathbf{n}) + 2\hat{N}_\alpha(\mathbf{n}).$$

This enables us to eliminate the pseudopotentials (A4) in the hypernet equations (A2) and to reformulate the set of equations (A2),(A3) in terms of the functions $\hat{X}_\alpha(\mathbf{n})$ and $\hat{N}_\alpha(\mathbf{n})$,

$$\hat{X}_\alpha(\mathbf{n})=(1-\delta_{\mathbf{n0}})\{g_{\alpha\alpha}(\mathbf{n})g_{+-}(\mathbf{n})\}^{1/2}\exp\{\hat{N}_\alpha(\mathbf{n})+\hat{E}_\alpha(\mathbf{n})\} -\hat{N}_\alpha(\mathbf{n})-\tfrac{1}{2}\{g_{\alpha\alpha}(\mathbf{n})+g_{+-}(\mathbf{n})\}, \tag{A6}$$

$$\hat{N}_\alpha(\mathbf{n})=\sum_\beta \rho_\beta \sum_{\mathbf{m}} \hat{X}_\beta(\mathbf{m}-\mathbf{n})\{X_{\beta\alpha}(\mathbf{n})+N_{\beta\alpha}(\mathbf{n})\}. \tag{A7}$$

We may cast Eqs. (A6) and (A7) into a simple and more convenient form by employing the linear decompositions

$$\begin{aligned}\hat{X}_+(\mathbf{n})&=\hat{X}_0(\mathbf{n})+M(1-M)\hat{X}(\mathbf{n})+M(1+M)^{-1}G(\mathbf{n}),\\ \hat{X}_-(\mathbf{n})&=\hat{X}_0(\mathbf{n})-M(1+M)\hat{X}(\mathbf{n})-M(1-M)^{-1}G(\mathbf{n}),\end{aligned} \tag{A8}$$

and

$$\begin{aligned}\hat{N}_+(\mathbf{n})&=\hat{N}_0(\mathbf{n})+M(1-M)\hat{N}(\mathbf{n}),\\ \hat{N}_-(\mathbf{n})&=\hat{N}_0(\mathbf{n})-M(1+M)\hat{N}(\mathbf{n}).\end{aligned} \tag{A9}$$

Elementary algebraic manipulations involving Eqs. (A7) and the definitions (A8),(A9) lead to the chain equation (49) and the relation

$$\hat{X}_0(\mathbf{n})+\hat{N}_0(\mathbf{n})=0. \tag{A10}$$

This equation establishes a condition on the functions $g_+(\mathbf{n})$ and $g_-(\mathbf{n})$. From Eqs. (25)–(27) there follows

$$\rho_+ g_{++}(\mathbf{n})+g_{+-}(\mathbf{n})+\rho_- g_{--}(\mathbf{n})=2(1-\delta_{\mathbf{n0}}), \tag{A11}$$

and, with Eqs. (A5), (A8), (A9), and (A10), we arrive at the sum rule

$$\rho_+ g_+(\mathbf{n})+\rho_- g_-(\mathbf{n})=(1-\delta_{\mathbf{n0}}). \tag{A12}$$

Further, relations (25)–(27) and the decompositions (A8),(A9) allow us to express the function $\hat{N}_0(\mathbf{n})$ in terms of the distribution functions $G(\mathbf{n})$, $\hat{G}(\mathbf{n})=\hat{X}(\mathbf{n})+\hat{N}(\mathbf{n})$, and the nodal portion $\hat{N}(\mathbf{n})$. The result is

$$\begin{aligned}\hat{N}_0(\mathbf{n})=&-\tfrac{1}{2}\ln\{1-G(\mathbf{n})\}+M^2\hat{N}(\mathbf{n})\\ &-\tfrac{1}{4}\ln\{1+(1-M)(1+M)^{-1}G(\mathbf{n})\}\\ &-\tfrac{1}{4}\ln\{1+(1+M)(1-M)^{-1}G(\mathbf{n})\}\\ &+\tfrac{1}{2}\ln\{1-M(1+M)\hat{G}(\mathbf{n})\}\\ &+\tfrac{1}{2}\ln\{1+M(1-M)\hat{G}(\mathbf{n})\}.\end{aligned} \tag{A13}$$

Insertion of expressions (A8), (A9), and (A13) into the hypernet equations (A6) leads us, after a few elementary algebraic steps, to a single hypernet equation for the functions $\hat{X}(\mathbf{n})$ and $\hat{N}(\mathbf{n})$. The explicit form is given by Eq. (48).

Employing Eqs. (A8), (A9), and (A13), we may write the functional (30) in terms of functions $G(\mathbf{n})$, $\hat{G}(\mathbf{n})$, and $\hat{N}(\mathbf{n})$. The explicit result on quantity $D_{12}-\frac{1}{2}(D_1+D_2)$ is presented in Eq. (51).

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