

Spectral-density method for classical systems: Heisenberg ferromagnet

L. S. Campana, A. Caramico D'Auria, M. D'Ambrosio, and U. Esposito
Istituto di Fisica della Facoltà di Ingegneria, Università di Napoli, Napoli, Italy
and Gruppo Nazionale di Struttura della Materia, Napoli, Italy

L. De Cesare

Istituto di Fisica dell'Università di Salerno, Salerno, Italy
and Gruppo Nazionale di Struttura della Materia, Salerno, Italy

G. Kamieniarz

Institute of Physics, A. Mickiewicz University, Poznan, Poland
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We formulate the spectral-density method in classical statistical mechanics in strict analogy with the known quantum version, and we apply it to the classical Heisenberg ferromagnetic model in an external field. A new formula for the magnetization in the classical formulation of spin-vector Green functions is derived for arbitrary spatial dimensionality. Furthermore, the static properties of the one- and three-dimensional cases are considered in detail. We obtain accurate results over a wide range of temperatures with the external field for the one-dimensional model and without field for the three-dimensional model. In the first case very good agreement with the exact numerical transfer-matrix data is also found in the region of higher temperature where the interacting-boson approach fails. In particular the zero-field susceptibility results are found to be consistent with the exact results obtained by Fisher.

I. INTRODUCTION

The spectral-density method^{1,2} (SDM) gives a systematic unperturbative procedure for obtaining successive approximations in order to investigate the thermal properties of many-body systems. The method has been widely used for quantum systems¹⁻⁷ that also involve phase transitions,^{2-4,6} and its effectiveness has been also checked extensively.

Since classical systems have assumed an important role in the modern theory of critical phenomena,⁸ it is of particular interest to develop in classical statistical mechanics an unperturbative scheme that makes it possible to obtain systematic and untrivial approximations. Only recently⁹ has the SDM been formulated for classical systems and applied to a classical Heisenberg ferromagnetic chain. However, only preliminary results have been presented.

The purpose of this paper is twofold. Firstly we reformulate, in a more detailed way, the classical spectral-density method (CSDM) on the basis of the classical analog¹⁰ of the quantum two-time temperature Green functions, in strict analogy with the well-known quantum version. Then, in order to check its effectiveness, we apply it to classical Heisenberg ferromagnets of arbitrary spatial dimensionality. Furthermore, as examples for numerical and analytic results, we consider in detail the one-dimensional case and also give some data for the three-dimensional case where long-range order exists at finite temperature. This will be accomplished to the lowest order in the CSDM; the theoretical results for some static quantities are discussed and compared with the data obtained by the transfer-matrix method and by the

interacting-boson approach.¹¹

Our choice of investigating a magnetic chain in order to test the method is connected with the widespread interest recently shown in classical one-dimensional systems from both the theoretical and experimental points of view.¹² A strong impetus for such studies has been given by the discovery that true one-dimensional systems do exist in reality. This is particularly true for magnetic properties, and in this respect $(\text{CD}_3)_4\text{NMnCl}_3$ (TMMC), CsNiF_3 , and $\text{CuCl}_2 \cdot 2\text{NC}_5\text{H}_5$ seem to be nearly ideal one-dimensional magnetic systems.^{13,14} Furthermore, the existence of computer simulations^{15,16} for Heisenberg ferromagnetic chains with and without applied fields offers a complementary and valid tool for suggesting and guiding various theoretical approaches.

In this paper some new elements appear. Firstly, we derive, in general, a Lehman spectral decomposition for classical systems that is very similar to the quantum counterpart. Furthermore, we obtain a new formula for the magnetization in the classical formulation of spin-vector Green functions. Finally, on the basis of simple calculations, we have results for any temperature with an external field for the one-dimensional model and without an applied field for the three-dimensional model, which are consistent with exact numerical and analytical data.

The organization of the paper is as follows. In Sec. II we introduce the classical spectral density for two arbitrary dynamic variables and formulate the CSDM. Within this formulation, some known results of the classical statistical mechanics are also presented in a new form that is more appropriate for the application of the method. In Sec. III the general formalism developed in

Sec. II is applied to the classical isotropic Heisenberg ferromagnet with arbitrary dimensionality. Here a detailed investigation of the main thermodynamic properties of one- and three-dimensional models is also presented. Finally, some conclusions are drawn in Sec. IV.

II. THE SPECTRAL-DENSITY METHOD FOR CLASSICAL SYSTEMS

Following Ref. 10, we consider the classical two-time temperature-dependent retarded and advanced Green functions for two arbitrary dynamical variables A and B :

$$\begin{aligned} G_{AB}^{(r)}(t-t') &= \Theta(t-t') \langle \{A(t), B(t')\} \rangle, \\ G_{AB}^{(a)}(t-t') &= -\Theta(t'-t) \langle \{A(t), B(t')\} \rangle, \end{aligned} \quad (1)$$

where $\Theta(x)$ is the step function, $\langle \rangle$ stands for the usual statistical average, and $\{A, B\}$ is the Poisson bracket of A and B . In Eq. (1) the dynamic variables A and B depend on the time via the coordinates $q(t) \equiv \{q_i(t)\}$ and the momenta $p(t) \equiv \{p_i(t)\}$. They satisfy the equation of motion

$$\frac{dA(t)}{dt} = \{A(t), H\}, \quad (2)$$

where $H = H(p, q)$ is the Hamiltonian of the system. As is known, the formal solution of Eq. (2) can be written in the form

$$A(t) = e^{iL t} A, \quad (3)$$

where $A = A(0)$ and L is the Liouville operator defined by

$$iLA = \{A, H\}. \quad (4)$$

In analogy with the quantum case,^{1,2} we now introduce the classical spectral density for A and B :

$$\Lambda_{BA}(\tau) = -i \langle \{B, A(\tau)\} \rangle. \quad (5)$$

Then, it is easy to show that the Green function $G_{AB}(\omega)$, related to the Fourier transforms of (1) and defined in the whole complex ω plane with a cut along the real axis, has the spectral representation

$$G_{AB}(\omega) = \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \frac{\Lambda_{BA}(\omega')}{\omega - \omega'}, \quad (6)$$

where $\Lambda_{BA}(\omega)$ is the Fourier transform of $\Lambda_{BA}(\tau)$,

$$\begin{aligned} \Lambda_{BA}(\omega) &= -i \langle \{B, A(\tau)\} \rangle_{\omega} \\ &= \int_{-\infty}^{+\infty} d\tau e^{i\omega\tau} \Lambda_{BA}(\tau). \end{aligned} \quad (7)$$

Also, the dynamic correlation function $\langle A(\tau)B \rangle$ can be easily expressed in terms of $\Lambda_{BA}(\omega)$. This possibility lies on the known result¹⁰

$$\begin{aligned} -\langle \{B, A(\tau)\} \rangle &= T^{-1} \frac{d}{d\tau} \langle A(\tau)B \rangle \\ &= T^{-1} \langle \{A(\tau), H\}B \rangle, \end{aligned} \quad (8)$$

which connects the Poisson bracket of two dynamical variables and the corresponding dynamical correlations function, T being the temperature. From relation (8) one

obtains in fact

$$\langle A(\tau)B \rangle = T \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{\Lambda_{BA}(\omega)}{\omega} e^{-i\omega\tau}. \quad (9)$$

Thus if one determines independently the spectral densities it is possible to obtain the correlation and the Green functions and therefore the physical properties of a classical system. Our purpose is just to show that for classical systems also one can construct a formalism (in strict analogy with the well-known quantum version) that makes it possible to formulate a CSDM for a systematic calculation of the spectral density.

As a first step we show that, also for the present $\Lambda_{BA}(\omega)$, a spectral decomposition can be derived in the form of an infinite sum of δ functions. Following Ref. 17, we introduce a Hilbert space \mathcal{S} of the classical dynamical variables with a scalar product defined by

$$\begin{aligned} \langle \psi | \phi \rangle &= \frac{1}{N! \mathcal{L}^{dN}} \int \psi^*(p, q) \phi(p, q) e^{-H(p, q)/T} dp dq \\ &= \mathcal{Z} \langle \psi^*(p, q) \phi(p, q) \rangle, \end{aligned} \quad (10)$$

where d is the spatial dimensionality and \mathcal{Z} the partition function of a system with dN degrees of freedom. In this space we consider the eigenvalue equation for the Hermitian operator L

$$L\psi_k = \omega_k \psi_k. \quad (11)$$

An important property of the Liouville operator is that all its eigenfunctions are complex¹⁰ and it is immediately proven that if ψ_k is an eigenfunction of L with eigenvalue ω_k , then ψ_k^* is also an eigenfunction of L with eigenvalue $-\omega_k$. If we assume that $\{\psi_k\}$ is a complete set of orthonormal eigenfunctions, for two arbitrary dynamical variables A and B we can consider the series expansions

$$\begin{aligned} A(p, q) &= \sum_k \langle \psi_k^* | A \rangle \psi_k^*(p, q), \\ B(p, q) &= \sum_k \langle \psi_k | B \rangle \psi_k(p, q). \end{aligned} \quad (12)$$

We now observe that from Eqs. (7) and (8) it follows that

$$\begin{aligned} \Lambda_{BA}(\omega) &= \frac{\omega}{T} \int_{-\infty}^{+\infty} d\tau e^{i\omega\tau} \langle A(\tau)B \rangle \\ &= \frac{\omega}{T} (N! \mathcal{L}^{dN} \mathcal{Z})^{-1} \\ &\quad \times \int e^{-H(p, q)/T} B(p, q) \\ &\quad \times \int_{-\infty}^{+\infty} d\tau e^{i(\omega+L)\tau} A(p, q) dp dq. \end{aligned} \quad (13)$$

Then, taking into account Eqs. (11) and (12) and the orthonormality and completeness conditions in \mathcal{S} , from (13) we obtain

$$\Lambda_{BA}(\omega) = 2\pi \frac{\omega}{T} \mathcal{Z}^{-1} \sum_k \langle \psi_k | B \rangle \langle \psi_k^* | A \rangle \delta(\omega - \omega_k), \quad (14)$$

which is the desired spectral decomposition to be compared with the quantum analog²

$$\Lambda_{BA}(\omega) = 2\pi(e^{\omega/T} + \eta)\mathcal{Z}^{-1} \times \sum_{k,k'} \langle k | B | k' \rangle \langle k' | A | k \rangle \times e^{-E_k/T} \delta(\omega - E_k + E_{k'}) \quad (\eta = \pm 1).$$

Of course, if $A = B^*$, we have $\langle \psi_k^* | A \rangle = \langle \psi_k | B \rangle^*$ and therefore

$$\Lambda_{BB^*}(\omega) = 2\pi \frac{\omega}{T} \mathcal{Z}^{-1} \sum_k |\langle \psi_k | B \rangle|^2 \delta(\omega - \omega_k) \quad (15)$$

is a real quantity.

Note that, from (8) and (13), if we put formally

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} d\tau e^{i(\omega+L)\tau} = \delta(\omega+L), \quad (16)$$

it is possible to write $\Lambda_{BA}(\omega)$ in the compact form

$$\Lambda_{BA}(\omega) = 2\pi \frac{\omega}{T} \langle B \delta(\omega+L) A \rangle = -2\pi i \langle \{B, \delta(\omega+L) A\} \rangle, \quad (17)$$

which must be considered the operational version of the spectral decomposition (14).

The successive step is to show that, also for the classical case, it is possible to write an infinite system of moments for $\Lambda_{BA}(\omega)$. If we use the definition (5) for $\Lambda_{BA}(\tau)$ and the equation of motion (2), one has

$$\frac{d^m \Lambda_{BA}(\tau)}{d\tau^m} = -i \langle \{B, (iL)^m A(\tau)\} \rangle \quad (m=0,1,2,\dots). \quad (18)$$

Then, taking the Fourier transform of Eq. (18) and using the relations (16) and (17), we have

$$(-i\omega)^m \Lambda_{BA}(\omega) = -2\pi i \langle \{B, (iL)^m \delta(\omega+L) A\} \rangle. \quad (19)$$

Finally, integration over ω yields

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \omega^m \Lambda_{BA}(\omega) = i^{m-1} \langle \{B, (iL)^m A\} \rangle \quad (m=0,1,2,\dots). \quad (20)$$

The Poisson brackets involved in the relations (20) can be evaluated, at least in principle, and the result gives the m th moment of the spectral density. Therefore, the sequence of Eqs. (20) represents a "moment problem," the solution of which would yield the spectral density. Unfortunately, as in the quantum case, this problem cannot be solved exactly, and one must look for an approximate solution of the spectral density. Suggested by the form of Eq. (14), we seek an approximation for $\Lambda_{BA}(\omega)$ in the form

$$\Lambda_{BA}(\omega) = 2\pi \sum_{k=1}^n \lambda_k^{(B,A)} \delta(\omega - \omega_k^{(B,A)}), \quad (21)$$

where n is a finite integer. The parameters $\lambda_k^{(B,A)}$ and $\omega_k^{(B,A)}$ are to be determined as a solution of the set of $2n$ integral equations obtained by inserting the expression (21) into the first $2n$ moment equations (20). This is the

purpose of CSDM.

Physically, the parameters $\omega_k^{(B,A)}$ that appear in (21) take the role of effective eigenvalues of the Liouville operator. From (6) and (9) it follows that they are still, as in the quantum case, the poles of the Green function $G_{AB}(\omega)$, and each of them represents a possible mode of undamped oscillation for the correlation function $\langle A(\tau)B \rangle$.

It must be stressed that the evaluation of the right-hand sides of Eqs. (20) require the introduction of the higher-order spectral densities. Therefore higher-order moment problems should be considered, but the difficulty of calculations increases considerably. Therefore, in order to solve self-consistently the system of Eqs. (20), it is usually necessary to use some extra decoupling procedures and thus introduce additional approximations in the CSDM.

III. CLASSICAL HEISENBERG FERROMAGNET

We apply the formalism developed in the preceding section to the classical Heisenberg ferromagnet described by the Hamiltonian

$$H = -\frac{1}{2} \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j - h \sum_j S_j^z, \quad (22)$$

where \vec{S}_i ($i=1, \dots, N$) are the classical spins, $J_{ij} > 0$ is the ferromagnetic exchange constant restricted to the nearest neighbors, and h is the external magnetic field.

We define the Fourier transforms of the spin vectors and the exchange integral as

$$\vec{S}_{\vec{k}} = \sum_j e^{-i\vec{k} \cdot \vec{r}_j} \vec{S}_j, \quad (23)$$

$$J(\vec{K}) = \sum_j J_{ij} e^{-i\vec{K} \cdot (\vec{r}_i - \vec{r}_j)} = J(0) \gamma_{\vec{K}}, \quad (24)$$

where

$$J(0) = zJ, \quad \gamma_{\vec{K}} = \frac{1}{z} \sum_{\vec{\delta}} e^{i\vec{K} \cdot \vec{\delta}}, \quad (25)$$

and z is the coordination number. It is also convenient to introduce the new dynamical variables

$$S_i^{\pm} = S_i^x \pm S_i^y, \quad (26)$$

so that

$$S^2 = (S^z)^2 + S^+ S^-. \quad (27)$$

The model can be appropriately described by the $2N$ canonical variables φ_i, S_i^z ($i=1,2,\dots,N$), where φ_i is the angle between the projection of \vec{S}_i in the x - y plane and the x axis. The Poisson brackets of the spin components are

$$\{S_{\vec{k}}^{\pm}, S_{\vec{q}}^z\} = \pm i S_{\vec{k}+\vec{q}}^{\pm}, \quad (28)$$

$$\{S_{\vec{k}}^{\pm}, S_{\vec{q}}^{\mp}\} = -2i S_{\vec{k}+\vec{q}}^z. \quad (29)$$

It can easily be seen that, in terms of the Fourier components, one has

$$H = -hS_0^z - \frac{1}{2N} \sum_{\vec{q}} J(\vec{q})(S_{\vec{q}}^+ S_{-\vec{q}}^- + S_{\vec{q}}^z S_{-\vec{q}}^z). \quad (30)$$

According to the CSDM we introduce the spectral density

$$\Lambda_{\vec{k}}(\omega) = -i \langle \{S_{-\vec{k}}^-, S_{\vec{k}}^+(\tau)\} \rangle_{\omega} \quad (31)$$

and assume that it can be represented approximately by one δ function

$$\Lambda_{\vec{k}}(\omega) = 2\pi A_{\vec{k}} \delta(\omega - \omega_{\vec{k}}), \quad (32)$$

where $A_{\vec{k}}$ and $\omega_{\vec{k}}$ are parameters that will be determined from the moment equations (20).

From the zero-moment equation we have

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \Lambda_{\vec{k}}(\omega) = 2Nm,$$

where $m = \langle S^z \rangle$. Thus it immediately follows that $A_{\vec{k}} = 2Nm$. From the first-moment equation we have

$$\begin{aligned} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \omega \Lambda_{\vec{k}}(\omega) &= 2h \langle S_0^z \rangle + J(0)(1 - \gamma_{\vec{k}}) \\ &\times \frac{1}{N} \sum_{\vec{q}} \gamma_{\vec{q}} (\langle S_{\vec{q}}^+ S_{-\vec{q}}^- \rangle \\ &\quad + 2 \langle S_{\vec{q}}^z S_{-\vec{q}}^z \rangle). \end{aligned} \quad (33)$$

The transverse correlation function appearing on the right-hand side of Eq. (33) can be readily calculated. The expression (9) leads to

$$\langle S_{\vec{k}}^+ S_{-\vec{k}}^- \rangle = 2TNm / \omega_{\vec{k}}. \quad (34)$$

The longitudinal correlation function in (33) cannot be easily calculated within our scheme, and we resort to the decoupling $\langle S_{\vec{k}}^z S_{-\vec{k}}^z \rangle \rightarrow \langle S_{\vec{k}}^z \rangle \langle S_{-\vec{k}}^z \rangle$, neglecting the correlations between Fourier transforms of the S^z components of the spin. The mean value $m = \langle S^z \rangle$ of the angular momentum provides us with another difficulty because the classical counterpart of the quantum kinematic rule for the z components of the spin does not exist. We suggest the calculation of the magnetization according to the following procedure. Let us introduce the higher-order spectral density defined as

$$\Omega(\omega) = \frac{1}{N^2} \sum_{\vec{q}} \sum_{\vec{k}} (-i \langle \{S_{-\vec{q}}^z S_{-\vec{k}}^-, S_{\vec{q}+\vec{k}}^+(\tau)\} \rangle_{\omega}), \quad (35)$$

Performing the decoupling, we have

$$\begin{aligned} \langle \{S_{-\vec{q}}^z S_{-\vec{k}}^-, S_{\vec{q}+\vec{k}}^+(\tau)\} \rangle_{\omega} \\ = \langle S_{-\vec{q}}^z \rangle (1 + \alpha) \langle \{S_{-\vec{k}}^-, S_{\vec{q}+\vec{k}}^+(\tau)\} \rangle_{\omega}, \end{aligned} \quad (36)$$

and we can reduce the higher-order spectral density to the more simple form

$$\Omega(\omega) = m(1 + \alpha) \frac{1}{N} \sum_{\vec{k}} \Lambda_{\vec{k}}(\omega), \quad (37)$$

where α is an unknown parameter. Requiring the original

spectral density (35) and the reduced spectral density to preserve the zero-moment equation, we obtain

$$m^2(1 + \alpha) = S^2 - \frac{3}{2} \langle S^+ S^- \rangle. \quad (38)$$

From Eq. (38) it follows that for high temperatures, when $m \rightarrow 0$, the isotropy condition $\langle S^+ S^- \rangle = \frac{2}{3} S^2$ is fulfilled regardless of the value of α . At low temperatures, when the angular momentum S^z is nearly saturated and, for Eq. (27), $S^+ S^-$ is small, α goes to 0 according to Eq. (38) and

$$S^z \simeq S - \frac{1}{2} \frac{S^+ S^-}{S}. \quad (39)$$

Now the expansion for m in terms of $\langle S^+ S^- \rangle$ and α can be compared with that following from Eq. (39). These two expansions will coincide if the parameter α is given by the expression

$$\alpha = - \frac{\langle S^+ S^- \rangle}{2S^2}. \quad (40)$$

This leads to the following formula for the magnetization:

$$m^2 = \frac{S^2 - \frac{3}{2} \langle S^+ S^- \rangle}{1 - \frac{1}{2} (\langle S^+ S^- \rangle / S^2)}, \quad (41)$$

where

$$\langle S^+ S^- \rangle = 2Tm \frac{1}{N} \sum_{\vec{q}} \frac{1}{\omega_{\vec{q}}} \quad (42)$$

and

$$\omega_{\vec{k}} = h + mJ(0)(1 - \gamma_{\vec{k}}) \left[1 + \frac{T}{m} \frac{1}{N} \sum_{\vec{q}} \frac{\gamma_{\vec{q}}}{\omega_{\vec{q}}} \right]. \quad (43)$$

Equations (41)–(43) represent the closed system that will be solved explicitly for the one- and three-dimensional models in the remaining part of the section. For the first time such a system has been obtained in terms of the classical spins, enabling us to explore the temperature region where standard bosonlike formulation¹¹ fails.

A. One-dimensional model

The general results (41)–(43) now resolve themselves into

$$\omega_k^* = h^* + \sigma Q(1 - \gamma_k), \quad (44)$$

$$Q = 1 + T^* [(h^* + \sigma Q) / K_{T^*} - 1] / \sigma^2 Q, \quad (45)$$

$$\sigma^2 = (1 - 3\sigma T^* / K_{T^*}) / (1 - \sigma T^* / K_{T^*}), \quad (46)$$

where we introduced the dimensionless quantities

$$\frac{\omega_k}{J(0)S} = \omega_k^*, \quad \frac{h}{J(0)S} = h^*, \quad \frac{T}{J(0)S^2} = T^*,$$

and

$$\sigma = m/S, \quad K_{T^*}^2 = h^*(h^* + 2\sigma Q).$$

The magnetization, evaluated in a numerical way for a wider range of parameters, is reported in Fig. 1, and a comparison between our results and the corresponding

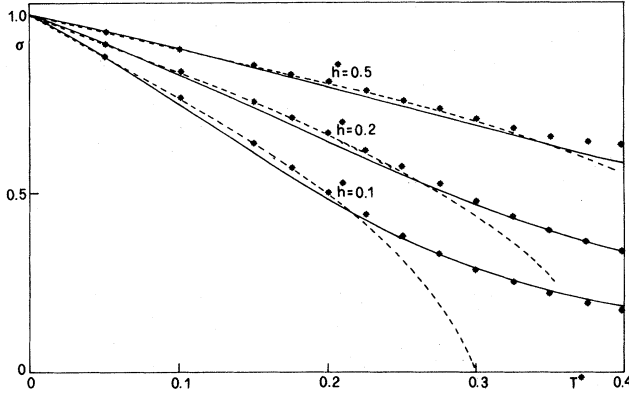


FIG. 1. The magnetization σ vs temperature T^* for different values of the magnetic field h^* . The dashed and the solid lines report the interacting-boson and the present results, respectively. The asterisks represent the exact transfer-matrix results.

transfer-matrix and interacting-boson¹¹ data is shown. A very good agreement with the exact transfer-matrix results is found also in the region of higher temperatures where the interacting-boson theory fails.

It is possible to obtain an expression for the transverse correlation length ξ_1 . By using the result (34) for the static correlation function and the definition

$$\xi_1^2 = -\frac{1}{2} \lim_{k \rightarrow 0} \frac{d^2}{dk^2} \langle S_k^+ S_{-k}^- \rangle / \langle S_k^+ S_{-k}^- \rangle, \quad (47)$$

we obtain

$$\xi_1 = (\sigma Q / 2h^*)^{1/2}. \quad (48)$$

The corresponding numerical results are plotted in Fig. 2 and compared with other calculations.¹¹ The behavior of

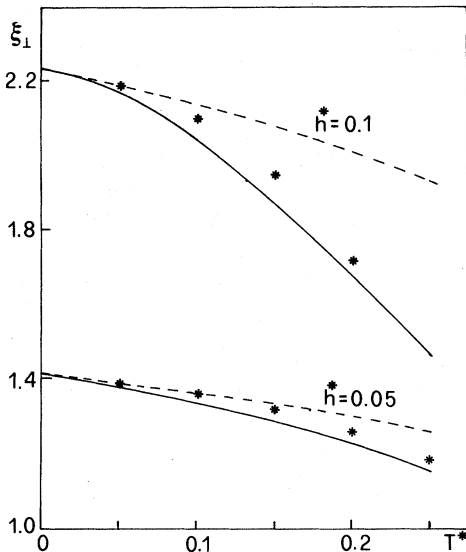


FIG. 2. Temperature (T^*) dependence of the transverse correlation length ξ_1 for different values of the magnetic field h^* . The dashed and the solid lines report the interacting-boson and the present predictions, respectively. The asterisks represent the exact transfer-matrix results.

ξ_1 , given by exact numerical transfer-matrix results, is well reproduced by our calculations throughout the temperature region reported here.

Analytical results can be obtained in special asymptotic regions. Expanding Eqs. (44)–(46) in terms of $T^* \ll (h^*)^{1/2}$ we obtain

$$\sigma = 1 - \frac{T^*}{K} \left[1 + \frac{T^*}{h^* + 2} \left(1 - \frac{h^*}{K} \right) + \frac{T^*}{2K} \right], \quad (49)$$

$$\begin{aligned} \omega_k^* &= h^* + (1 - \cos k) \\ &\times \left\{ 1 - T^* \left[1 - \frac{h^*}{K} \right] \right. \\ &\quad \left. + (T^*)^2 \left[\left(\frac{h^*}{K} - 1 \right) \left[1 - \frac{h^*}{K} - \frac{h^{*2}}{K^3} \right] \right. \right. \\ &\quad \left. \left. - \frac{1}{2K^2} \right] \right\}, \quad (50) \end{aligned}$$

where $K^2 = h^*(h^* + 2)$. For small magnetic fields [$(h^*)^{1/2} \ll 1$], the result (49) resolves into that found by Balucani *et al.*¹¹ Different numerical factors correspond to the different units. The only difference is that the term $(T^*/K)^2$ in expression (49) is not present in Eq. (42) of Ref. 11.

Let us consider the opposite limit $h^* \ll T^*$. When the magnetic field becomes very small the magnetization approaches zero, causing the divergence of the parameter Q and the frequency ω_k^* . In analogy with the quantum case³ we remove this divergence by modifying the divergent term in expression (43). The modification

$$\frac{1}{m} \frac{1}{N} \sum_q \frac{\gamma_q}{\omega_q} \rightarrow \frac{m}{S^2} \frac{1}{N} \sum_q \frac{\gamma_q}{\omega_q} \quad (51)$$

is found not to alter the results for $m \neq 0$. The data reported in Figs. 1 and 2 remain practically unchanged under this modification. In regard to Eqs. (49) and (50) for the magnetization and the frequency in the low-temperature region [$T^* \ll (h^*)^{1/2}$], the new expression for σ coincides with the previous one whereas the $(T^*)^2$ term of the expression for ω_k^* is only slightly affected. The modification (51) is related to a slightly different decoupling of corresponding Green functions which reproduces the previous results and does not fail in the range $m \rightarrow 0$.

In the limit $h^* \ll T^*$ for the magnetization one has $\sigma = \chi h^*$, where χ is the paramagnetic susceptibility. To first order with respect to h^* , the left-hand side of Eq. (46) vanishes, so that the set of equations (45) and (46) is reduced to

$$\chi(3Q^2 - 4Q + 3T^*) - 1 = 0, \quad (52)$$

$$Q = \frac{1}{2} [(3\chi T^*)^2 - 1] / \chi, \quad (53)$$

where, of course, the modification (51) is taken into account. The susceptibility for high ($T^* \gg 1$) and low ($T^* \ll 1$) temperatures is found to be

$$\chi = \frac{1}{3T^*} \left[1 + \frac{1}{3T^*} + \frac{2}{3} \left(\frac{1}{3T^*} \right)^2 + \dots \right] \quad (54)$$

and

$$\chi = \frac{8}{3} \left[\frac{1}{3T^*} \right]^2, \quad (55)$$

respectively. The only difference between these results and the corresponding exact counterparts¹⁸ is that the coefficient $\frac{2}{3}$ appears instead of $\frac{1}{2}$ in the formula (54) and $\frac{8}{3}$ instead of 3 in the formula (55). For the first time the results obtained are consistent with those of Fisher.¹⁸ Very recently Balucani *et al.*¹⁹ have shown the vanishing of the magnetization in the limit $h^* \rightarrow 0$ by having recourse to a new approach which goes beyond the framework of the Green-function theory, however.

B. Three-dimensional model

Let the magnetic field $h^* \rightarrow 0$. Then the expressions (41)–(43) can be reduced to

$$\omega_{\vec{k}}^* = \sigma Q (1 - \gamma_{\vec{k}}), \quad (56)$$

$$\sigma = [1 - 3T^*F(-1)/Q] / [1 - T^*F(-1)/Q], \quad (57)$$

where the lattice sum $F(-1)$ is defined as

$$F(-1) = \frac{1}{N} \sum_{\vec{q}} \frac{1}{1 - \gamma_{\vec{q}}} \quad (58)$$

and

$$Q = \frac{1}{2} \left[1 + \left(1 + \frac{4T^*}{N} \sum_{\vec{q}} \frac{\gamma_{\vec{q}}}{1 - \gamma_{\vec{q}}} \right)^{1/2} \right]. \quad (59)$$

The zero-field magnetization σ versus T^* is presented in Fig. 3 for the cubic lattices [the values of $F(-1)$ are tak-

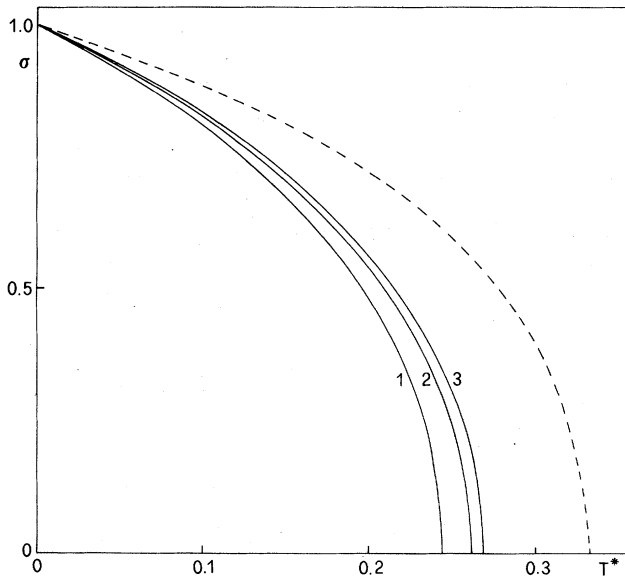


FIG. 3. Temperature (T^*) dependence of the magnetization σ in zero field for 3D classical Heisenberg ferromagnet. The curves 1,2,3 represent the present data for the sc, bcc, fcc lattices, respectively. The dashed curve represents the MFA result.

TABLE I. The dimensionless critical temperature for 3D classical Heisenberg ferromagnet.

T_c^*	MFA	RPA	CSDM	HTS
sc	0.333	0.220	0.245	0.241
bcc	0.333	0.239	0.262	0.257
fcc	0.333	0.248	0.269	0.265

en from Callen²⁰] and compared with the molecular-field approximation (MFA) result. At very low temperatures the magnetization depends linearly on temperature and is explicitly given by the formula

$$\sigma = 1 - T^*F(-1) \left\{ 1 + T^* \left[1 + \frac{1}{2}F(-1) \right] \right\}. \quad (60)$$

The magnetization falls off to 0 at the critical temperature

$$T_c^* = \left[1 + \frac{1}{3F(-1)} \frac{1}{N} \sum_{\vec{q}} \frac{\gamma_{\vec{q}}}{1 - \gamma_{\vec{q}}} \right] / 3F(-1). \quad (61)$$

The numerical values are reported in the Table I as CSDM results. We present also classical random-phase-approximation (RPA) results which can be obtained by dropping the second term in large parentheses of Eq. (61). Our CSDM results are very close to the exact high-temperature-series (HTS) results of Rushbrooke *et al.*²¹ whereas our RPA data coincide with those obtained by Tahir-Kheli⁴ for the quantum model in the limit $S \rightarrow \infty$.

IV. CONCLUSIONS

In this paper we have presented the classical analog of the SDM already developed for quantum systems. The formulation, which has general validity in classical statistical mechanics, has been applied to a d -dimensional classical Heisenberg ferromagnet. General moment equations, to be solved self-consistently, have been obtained to the lowest order in the CSDM and a new formula for the magnetization has been introduced. Apart from some numerical results concerning the three-dimensional case in zero field in good agreement with the exact HTS ones, we have explored more extensively the one-dimensional case, due to its widespread interest. For this, the magnetization is evaluated in a numerical way for a wide range of parameters T and h and compared with the corresponding transfer-matrix and interacting-boson¹¹ data. Very good agreement with the exact transfer-matrix results is also found in the region of higher temperature where the interacting-boson theory fails. Analytic expressions for the magnetization and susceptibility are also obtained in some regions. For the first time, the zero field results appear to be consistent with the exact results obtained by Fisher.¹⁸ In our opinion, all the previous results for magnetic systems constitute a good test of the effectiveness of the CSDM. Finally, we wish to emphasize that, due to its general character, this method also offers a possibility for investigating the macroscopic properties of other classical models and to include in the theory damping effects in a very simple and systematic way.^{7,22}

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