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Spin-1/2 modified Callen decoupling procedures in the Green's-function theory of ferromagnetism*

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In this note modified Callen decoupling procedures in first-order Green's-function theory of ferromagnetism are analyzed for spin-1/2. While the low-temperature results present the same difficulties as the original approximation, the intermediate- and high-temperature ones are better than those obtained with the first-order decoupling schemes previously published. For a better understanding of these approximations we have also applied them to the two-spin system.

Recently the present authors[1] introduced a first-order decoupling procedure [from now on referred to as Coutinho-Fittipaldi decoupling (CFD)] in the Green's-function theory of ferromagnetism, devised to give a better treatment for the spin kinematics. In that paper various first-order decoupling schemes were reviewed and analyzed in view of their influence on the spin kinematics and the renormalization of quasiparticle energies.

In a recent paper Swendsen[2] presented a modification in Callen's decoupling[3] (MCD) whose motivation was based on the best possible result for the Curie temperature. This approximation was used to obtain polynomial expressions for the Curie temperature of Heisenberg ferromagnets with first- and second-nearest-neighbor exchange interaction and to investigate magnetic phase transitions. The decoupling method was illustrated by application to the europium chalcogenides. However, the ability of the MCD to treat the special case of spin $\frac{1}{2}$ was not explicitly analyzed in Ref. 2 and consequently only the results for the Curie temperature were discussed in Ref. 1.

The purpose of this note is to investigate the results of the modified Callen decoupling of Ref. 2 (MCD-I) for spin $\frac{1}{2}$ as well as those of a possible variant (MCD-II). We analyze their results for several low- and high-temperature thermodynamic properties of the Heisenberg model (nearest-neighbor only), with especial attention to the treatment of spin kinematics and renormalization of quasiparticle energies. We have also applied the two decouplings to the two-spin system, concluding that almost all the agreements, departures, and discrepancies which appear in the Heisenberg ferromagnet are also present in this simple model. This note should complete the analysis made in Ref. 1.

First, we note that the MCD-I scheme[2] presents a spurious T^3 term in the low-temperature spontaneous magnetization series, for spin $\frac{1}{2}$, which shows that it has the same difficulties[4] as the original Callen's decoupling[3] (CD). This difficulty can be overcome if we include an extra term in the termination function α defined in Ref. 2, to take the form,

$$\alpha = \frac{1}{2S^2}\frac{S-1}{S+1}\langle S^z\rangle + \frac{1}{S(S+1)}\left(\frac{\langle S^z\rangle}{S}\right)^3 - \frac{2}{3}\left(\frac{\langle S^z\rangle}{S}\right)^3 \delta_{S,1/2} \; . \tag{1}$$

It can be easily seen by inspection of the low-temperature results for the magnetization that the last term in Eq. (1) does eliminate the T^3 term, as was pointed out by Swendsen.[5] We call the decoupling with the termination function defined in Eq. (1) the MCD-II. We note that this new α does not affect the predicted value of the Curie temperature, nor the high-temperature zero-field susceptibility series, when compared with MCD-I. With this choice of α one obtains a low-temperature series expansion of the magnetization free from the spurious term T^3 and with a T^4 term (which is absent in CD and MCD-I) given by $-3\pi\nu\zeta(\frac{3}{2})\zeta(\frac{5}{2})Q\tau^4$, where $Q=\frac{2}{3}$. Note that the Q factor predicted by MCD-II is lattice-structure independent and its value is worse than that given by Dembinski's[6] decoupling (DD), when compared with those calculated by Dyson[7] (see Table II of Ref. 1). Another result from Eq. (1) is that the treatment for the spin kinematics at low temperature indicates an improvement as compared to that of Callen,[3] namely

$$\langle (S_g^-)^2 S_g^+ S_j^+ \rangle \approx \tfrac{4}{3}\zeta^2(\tfrac{3}{2})\tau^3 \; . \tag{2}$$

(For a discussion of this subject the reader is referred to Ref. 1 with special attention to Table I).

Unfortunately, however, the predicted renormalization of quasiparticle energies does not give a correct spin-wave behavior at low temperature. As in random-phase-approximation (RPA) decoupling,[8] it leads to an inaccurate renormalization factor for the spin-wave energies which is not proportional to the thermodynamic energy. As pointed out by Keffer and Loudon,[9] in the low-temperature region the renormalization factor is expected to be proportional to the thermodynamic energy, with a

TABLE I. Coefficients a_2 and a_3 of the susceptibility series $\chi = \frac{1}{4}\beta\mu^2 \sum_{n=0} a_n (T_m/T)^n$. The first coefficients a_0 and a_1 are equal to one in all approximations.

	Baker *et al.*[a]			MCD			CFD[b]		
	sc	bcc	fcc	sc	bcc	fcc	sc	bcc	fcc
a_2	0.66	0.75	0.83	0.78	0.83	0.89	0.83	0.88	0.91
a_3	0.40	0.54	0.63	0.58	0.68	0.75	0.61	0.72	0.79

[a] Reference 12.

[b] Reference 1.

leading temperature term arising in $T^{5/2}$. Recalling the definition of the renormalization factor R given by Callen,[3] one thus obtains as a consequence of the Eq. (1),

$$R = 1 - \tfrac{4}{3}\zeta(\tfrac{3}{2})\tau^{3/2} - \tfrac{5}{3}\pi\nu\zeta(\tfrac{5}{2})\tau^{5/2} + O(\tau^{7/2}) . \tag{3}$$

We can show that this discrepancy is connected with the fact that the inclusion of the extra term in Eq. (1) does not ensure that $\alpha \to 1$ as $\langle S^z \rangle \to \frac{1}{2}$, which is a basic feature in Callen's approach.[2,3] Furthermore, we can also show that in the framework of a Callen-type decoupling (spin-$\frac{1}{2}$ case) we cannot give simultaneously correct renormalization of quasiparticle energies and no appearance of the spurious T^3 term.[10]

While the low-temperature results of the MCD schemes are not very good, the intermediate- and high-temperature ($T = T_C$ and $T \gg T_C$) ones are better than those obtained with the first-order decoupling schemes previously published. The Curie temperature was imposed in an *ad hoc* procedure to agree with the Tahir-Kheli[11] expression which predicts T_C values in agreement with the Padé-approximant results[12] to within 5%, 3%, and 2% for the sc, bcc, and fcc lattices, respectively.

The results for the zero-field susceptibility series, however, were not reported in Ref. 2. Here, we shall present the results for the first few coefficients (spin $\frac{1}{2}$), which reads

$$\chi = \frac{\beta\mu^2}{4}\left[1 + \left(\frac{T_m}{T}\right) + \frac{\gamma_0 - \frac{4}{3}}{\gamma_0}\left(\frac{T_m}{T}\right)^2 + \frac{\gamma_0^2 - \frac{8}{3}\gamma_0 - \epsilon}{\gamma_0^2}\left(\frac{T_m}{T}\right)^3 + O\left(\frac{T_m}{T}\right)^4\right], \tag{4}$$

where $\epsilon = -\frac{7}{9}$ for sc and bcc, and $\frac{41}{9}$ for fcc, μ is the Bohr magneton times the gyromagnetic ratio, γ_0 is the number of nearest neighbors, T_m is the Curie temperature of the molecular field theory, and $\beta = (k_B T)^{-1}$. In Table I we list the coefficients given by MCD and CFD[1] approximations and compare them with the values evaluated by Baker *et al.*[12] It is worth mentioning that MCD is the first decoupling scheme in first-order Green's-function theory of ferromagnetism able to improve the a_2 coefficient (see Table IV of Ref. 1).

To understand better the MCD introduced here, as well as the MCD presented by Swendsen,[2] we have applied them to the two-spin system coupled by exchange. This simple system has been used by the present authors[1,13] and Ramos[13] to study the validity of the Tyablikov (RPA), Callen (CD), Dembinski (DD), and CF (CFD) decoupling procedures. The advantage of this method is that the comparison with the exact results can be analytically done over the whole range of temperature. Of course its limitation is that it is not a realistic model for an infinite ferromagnetic crystal. We refer to Refs. 1 and 13 for a better understanding of this problem. Here we shall present the results when using the MCD-I and MCD-II following the notation of the Ref. 1 (hereafter we use the indices I and II in the place of MCD-I and MCD-II for the sake of simplicity).

The correlation functions are

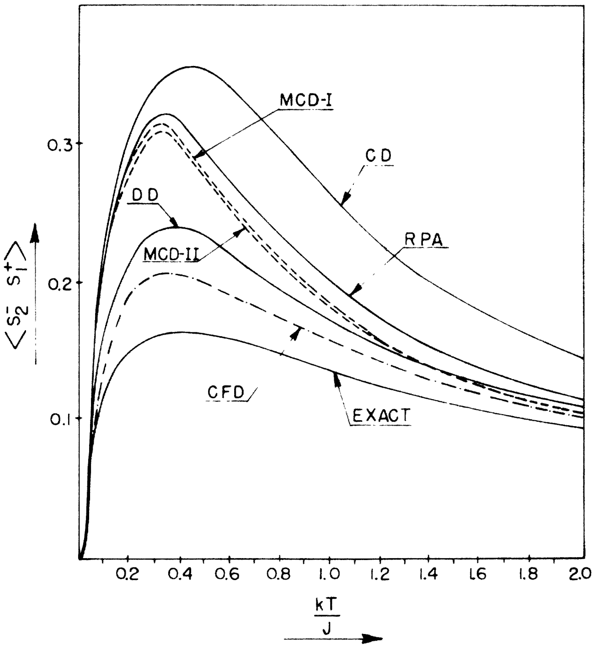

FIG. 1. Temperature dependence of the transverse correlation function for the two-spin system, calculated for $S = \frac{1}{2}$ and $\mu h/J = 0.1$. The dashed lines show the results obtained from both modified Callen decouplings. The solid and dash-dot curves were obtained in Ref. 1.

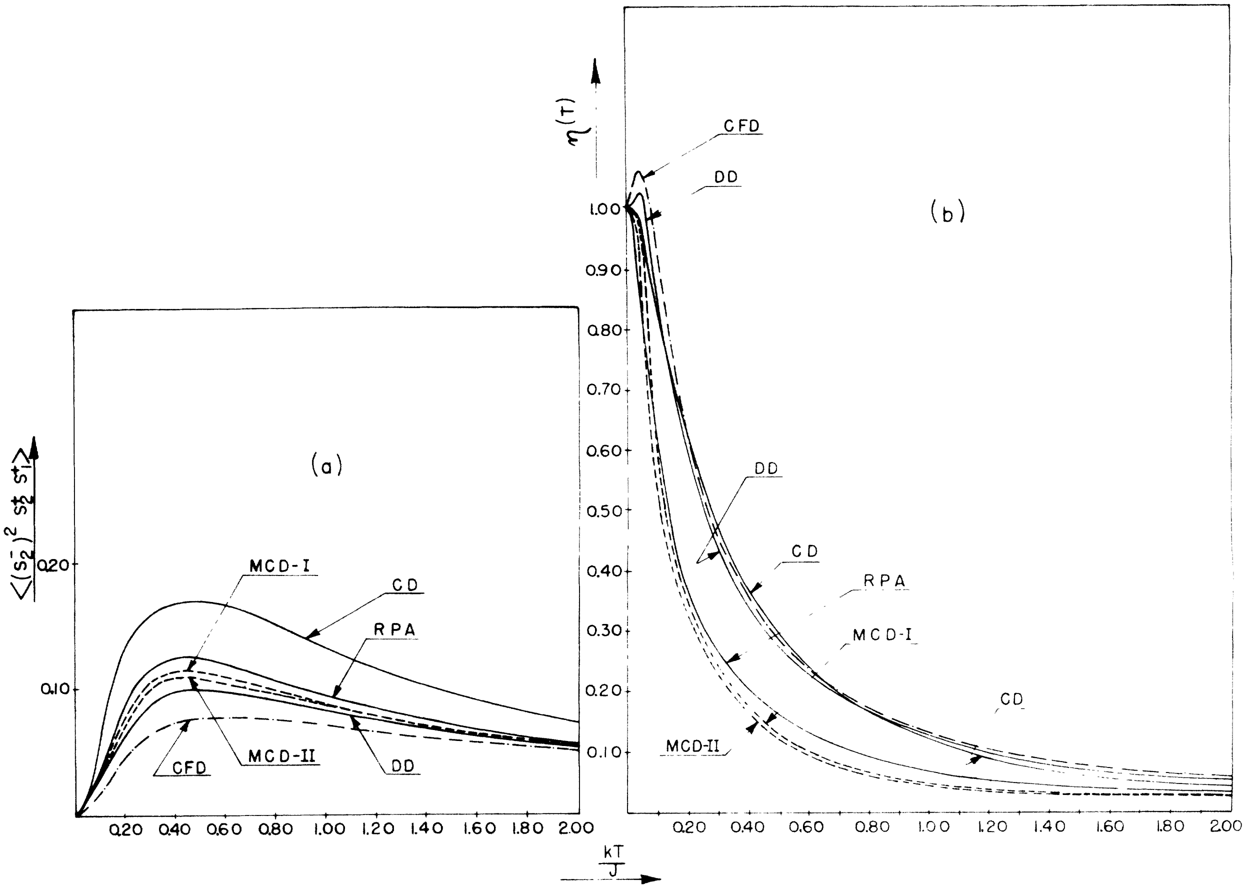

FIG. 2. Temperature dependence of the correlation function $\langle (S_2^-)^2 S_2^+ S_1^+ \rangle$ and the renormalization factor $\eta(T)$ (see the definition in the text) for the two-spin system ($S=\frac{1}{2}$): (a) treatment of spin kinematics: (b) behavior of the renormalized energies. The dashed lines show the results obtained from both modified Callen decouplings. The solid and dash-dot curves were obtained in Ref. 1. Note that the exact energies correspond to $\eta = 1$ and $\eta = 0$.

$$\langle S_2^- S_1^+ \rangle_{\mathrm{I,II}} = \langle S^z \rangle_{\mathrm{I,II}} \Delta^-_{\mathrm{I,II}} , \tag{5}$$

$$\langle S^- S^+ \rangle_{\mathrm{I,II}} = \langle S^z \rangle_{\mathrm{I,II}} \Delta^+_{\mathrm{I,II}} , \tag{6}$$

$$\langle (S_2^-)^2 S_2^+ S_1^+ \rangle_{\mathrm{I,II}} = (1+\alpha_{\mathrm{I,II}})(\tfrac{1}{2} - \langle S^z \rangle_{\mathrm{I,II}}) \langle S_2^- S_1^+ \rangle_{\mathrm{I,II}} , \tag{7}$$

where

$$\Delta^\pm_{\mathrm{I,II}} = [\exp(a/t) - 1]^{-1} \pm (\exp\{[a + 4(\langle S^z \rangle_{\mathrm{I,II}} + \alpha_{\mathrm{I,II}} \langle S_2^- S_1^+ \rangle_{\mathrm{I,II}})]/t\} - 1)^{-1} , \tag{8}$$

$$\alpha_{\mathrm{I}} = 2\langle S^z \rangle_{\mathrm{I}} [\tfrac{1}{3}(16 \langle S^z \rangle_{\mathrm{I}}^2 - 1)] , \tag{9}$$

$$\alpha_{\mathrm{II}} = 2\langle S^z \rangle_{\mathrm{II}} [\tfrac{1}{3}(8 \langle S^z \rangle_{\mathrm{II}}^2 - 1)] , \tag{10}$$

and

$$t = k_B T/J , \qquad a = \mu h/J . \tag{11}$$

The temperature-dependent Green's-function poles are given by

$$E_1 = \mu h , \tag{12}$$

$$E_2 = \mu h + 2J\eta_{\mathrm{I,II}}(T) , \tag{13}$$

where

$$\eta_{\mathrm{I,II}}(T) = 2(\langle S^z \rangle_{\mathrm{I,II}} + \alpha_{\mathrm{I,II}} \langle S_2^- S_1^+ \rangle_{\mathrm{I,II}}) . \tag{14}$$

The poles of the exact Green's function which correspond to the exact excitation energies of the system are obtained for $\eta = 1$ and $\eta = 0$.[14]

The results of Eqs. (5), (7), and (14) as well as the exact and the ones obtained with other decoupling schemes[1] are shown in Figs. 1 and 2. Figure 1 reveals that both modified Callen decouplings are better than CD and RPA and worse than DD and CFD over a large range of temperature with a slight improvement of MCD-II over MCD-I in this region of temperature. However, the results indicate that both MCD schemes at higher temperatures are practically indistinguishable and reach the exact results more rapidly than DD and CFD. It is worth mentioning that other thermodynamic quantities (such as magnetization and zero-field magnetic susceptibility), not explicitly given here, follow the same behavior. Figure 2(a) shows that the spin kinematics in both MCD schemes is also treated better than CD and RPA in the whole temperature range. We can see from Fig. 2(b) that near the exact pole corresponding to $\eta = 1$, the MCD-I follows the low-temperature renormalized energy of CD, whereas MCD-II follows that of RPA. On the other hand, at higher temperatures both MCD schemes reach the exact energies corresponding to $\eta = 0$, more rapidly than all other approximations, which reveals once more the reliable performance of these approximations in this region of temperature.

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