

Green's-function theory of the transverse Ising model

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Recent attempts to develop double-time Green's-function theories for the transverse Ising model (TIM) have been subject to certain difficulties; the appearance of zero-frequency poles in the commutator Green's function (CGF) led to the avoidance of CGF and an incomplete treatment based only upon anticommutator Green's functions (AGF), and ambiguities in the determination of some thermal averages. Upon decoupling the equations-of-motion hierarchy, we develop a consistent Green's-function theory of the TIM. The AGF and CGF are shown to provide consistent results, the problem of zero-frequency poles in CGF being treated appropriately. We resolve the ambiguity problem and obtain reasonable values for the Weiss critical field and the ground-state magnetization.

I. INTRODUCTION

The transverse Ising model (TIM) has been widely used to describe a variety of physical systems, e.g., in treatments of order-disorder ferroelectrics,^{1,2} van Vleck paramagnets,^{3,4} and systems exhibiting a cooperative Jahn-Teller phase transition.^{5,6} Attempts to develop double-time Green's-function (DTGF) theories of TIM have met with limited success. Wang and Cooper studied the spin- $\frac{1}{2}$ ($S = \frac{1}{2}$) case with DTGF in the $T = 0$ limit.⁷ While their approximate excitation spectrum correctly predicted a softening of the collective mode as $T \rightarrow T_c$, their procedure failed to satisfy certain $S = \frac{1}{2}$ operator identities. Ramakrishnan and Tanaka¹ also correctly predicted collective-mode softening as $T \rightarrow T_c$ but they were unable to provide analytic (or numerical) solutions for their complicated correlation expressions. More importantly, they treated only anticommutator DTGF, avoiding commutator DTGF because of the appearance of zero frequency poles in the latter. This precluded calculating the response of the system to external fields, e.g., the determination of dynamic susceptibilities.^{8,9}

In order to develop a fully self-consistent approximation scheme and describe the dynamic response of the system, we consider *both* the commutator and anticommutator DTGF managing any appearance of zero frequency poles in the former in an appropriate manner.^{10,11} Unlike other DTGF studies, ours is

based on equations of motion of a set of self-adjoint operator *observables*. Our use of this set and of commutator DTGF provide a very useful *direct* connection between the approximations and their impact on the predictions of the dynamical response following from our treatment of the TIM system. We demonstrate that the "symmetric" decoupling scheme of Ramakrishnan and Tanaka is inherently restricted to $T > T_c$. Then we develop an unambiguous scheme for all T based upon the concepts of cumulant averages.¹²⁻¹⁴

In this paper we consider the TIM for all T and $S = \frac{1}{2}$. Our excitation spectrum exhibits mode softening as $T \rightarrow T_c$, all $S = \frac{1}{2}$ identities are preserved, and we obtain expressions for the dynamical susceptibilities of interest. We also obtain an expression for the critical curve and obtain reasonable numerical values (when compared to series results¹⁵) for both the Weiss critical field (the transverse-field strength for which $T_c \rightarrow 0$) and T_c in the zero-transverse-field limit. We also obtain results for the magnetization versus transverse field in the ground state (at zero temperature).

II. DOUBLE-TIME GREEN'S FUNCTIONS

The retarded ($\rho = +1$) or advanced ($\rho = -1$) commutator ($\eta = -1$) or anticommutator ($\eta = +1$) double-time Green's function (DTGF) is defined by¹⁶

$$\langle\langle A(t); B(t') \rangle\rangle_{\rho}^{\eta} = -\frac{1}{2} i [(\rho + 1)\theta(t - t') + (\rho - 1)\theta(t' - t)] \langle [A(t), B(t')]_{\eta} \rangle, \quad (2.1)$$

where

$$A(t) = e^{iHt} A e^{-iHt}, \quad [A, B]_{\eta} = AB + \eta BA \quad (2.2)$$

and $\theta(t)$ is unity for $t > 0$ and zero for $t < 0$. The single angular brackets in Eq. (2.1) denote thermal average. It follows from Eq. (2.1) that $\langle\langle A(t); B(t') \rangle\rangle$ is a function of $t - t'$ only.

The Fourier transform of $\langle\langle A(t); B \rangle\rangle$ is defined by

$$\langle\langle A; B \rangle\rangle_{E+i\rho\epsilon}^{(\eta)} = \int_{-\infty}^{\infty} dt e^{i(E+i\rho\epsilon)t} \langle\langle A(t); B \rangle\rangle_{\rho}^{(\eta)}, \quad \epsilon \rightarrow 0^+ \quad (2.3)$$

and satisfies the equation of motion

$$E \langle\langle A; B \rangle\rangle_E^{(\eta)} = \langle[A, B]_{\eta}\rangle + \langle\langle [A, H]_-; B \rangle\rangle_E^{(\eta)}. \quad (2.4)$$

The GF on the right-hand side of Eq. (2.4) is generally of "higher order" and must be decoupled so

that a closed system of equations is obtained. Note that the Fourier-transformed GF as defined in Eq. (2.3) is sectionally holomorphic, the retarded (or advanced) GF being analytic in the upper (respectively, lower) half of the complex E plane.^{10,13}

It has been shown^{10,11} that the commutator DTGF cannot have a pole at $E=0$, i.e.,

$$C^{(-)} = 0, \quad (2.5)$$

where

$$C^{(\eta)} = \lim_{E \rightarrow 0} E \langle\langle A; B \rangle\rangle_E^{(\eta)} \quad (2.6)$$

and that the correlations $\langle BA(t) \rangle$ may be calculated from

$$\langle BA(t) \rangle = \frac{1}{4} (1 - \eta) C^{(+)} + \frac{i}{2\pi} \int_{-\infty}^{\infty} dE (e^{\beta E} + \eta)^{-1} e^{-iEt} \lim_{\epsilon \rightarrow 0^+} (\langle\langle A; B \rangle\rangle_{E+i\epsilon}^{(\eta)} - \langle\langle A; B \rangle\rangle_{E-i\epsilon}^{(\eta)}). \quad (2.7)$$

Also, the response of the system to an external field is described by the generalized susceptibility^{8,9}

$$\chi_{AB}(E) = - \lim_{\epsilon \rightarrow 0^+} \langle\langle A; B \rangle\rangle_{E+i\epsilon}^{(-)}, \quad (2.8)$$

where A and B are observables.

A self-consistent approximate scheme should provide the same result for $\langle BA(t) \rangle$ whether the approximate versions of the anticommutator DTGF ($\eta = +1$) or the approximate version of the commutator DTGF ($\eta = -1$) is used in Eq. (2.6). The approximate commutator DTGF *must* satisfy the analyticity condition (2.5). For observables A, B the approximate DTGF is directly related to measurement predictions by Eq. (2.8).

III. THE TRANSVERSE ISING MODEL ($S = \frac{1}{2}$)

The TIM Hamiltonian is given by

$$H_0 = -2\Omega_1 \sum_i S_i^x - 2\Omega_2 \sum_i S_i^y - \frac{1}{2} \sum_{ij} J_{ij} S_i^z S_j^z, \quad (3.1)$$

where S_i^x , S_i^y , and S_i^z are components of the spin- $\frac{1}{2}$ operator. Most treatments set $\Omega_2 = 0$ in Eq. (3.1) but we choose to retain the most general form of the TIM. Defining

$$P_i \equiv \frac{2\Omega_1 S_i^x + 2\Omega_2 S_i^y}{(\Omega_1^2 + \Omega_2^2)^{1/2}} \quad (3.2)$$

and

$$P = \prod_i P_i \quad (3.3)$$

we have

$$[P, H_0] = 0, \quad P^2 = 1 \quad (3.4)$$

and

$$PS_i^z P = -S_i^z. \quad (3.5)$$

From Eqs. (3.4) and (3.5) we then have

$$\langle S_i^z \rangle_0 = \frac{\text{Tr} e^{-\beta H_0} S_i^z}{\text{Tr} e^{-\beta H_0}} = \langle PS_i^z P \rangle_0 = -\langle S_i^z \rangle_0 = 0, \quad (3.6)$$

an *exact* result which demonstrates that a consequence of the inherent symmetry of Eq. (3.1) is the absence of a net z magnetization.

We consider the question of the stability of Eq. (3.1) in a vanishingly small, external symmetry-breaking z field. That is, we consider the Hamiltonian

$$H = H_0 - 2\Omega_3 \sum_i S_i^z \quad (3.7)$$

in the limit $\Omega_3 \rightarrow 0$. For Eq. (3.7) we have

$$[P, H] \neq 0, \quad (3.8)$$

i.e., broken symmetry. Equation (3.1) provides a mechanism for the presence of a phase such that

$$\lim_{\Omega_3 \rightarrow 0} \langle S_i^z \rangle = 0, \quad T > T_c \\ \neq 0, \quad T < T_c, \quad (3.9)$$

where T_c is a critical temperature and

$$\langle S_i^z \rangle = \text{Tr} e^{-\beta H} S_i^z / \text{Tr} e^{-\beta H}. \quad (3.10)$$

The mechanism is the final term in Eq. (3.1) by which the interactions between the z components of spin provide an internal z field, producing long-range z - z correlations. Thus, the TIM itself imposes the dominance of z - z correlations.

We define

$$A_{ij}^{\mu\nu(\eta)} = \langle \langle S_i^\mu; Q_j^\nu \rangle \rangle_E^{(\eta)}, \quad (3.11)$$

$$a_{ij}^{\mu\nu} = \langle Q_j^\nu S_i^\mu \rangle, \quad (3.12)$$

$$K_{ij}^{\mu\nu(\eta)} = \langle [S_i^\mu, Q_j^\nu]_\eta \rangle, \quad (3.13)$$

$$x = \langle S_i^x \rangle, \quad y = \langle S_i^y \rangle, \quad z = \langle S_i^z \rangle, \quad Q^\nu = \langle Q_j^\nu \rangle. \quad (3.14)$$

Here Q_j^ν is a member of our observable operator set $\{S_j^x, S_j^y, S_j^z\}$. As we shall see, the choice of Q_j^ν is *not* arbitrary (as it *appears* to be in most other Green's-functions procedures) but is determined by the physical situation to be described.

The equation of motion of our observable basis set are

$$i[S_i^x, H] = 2\Omega_3 S_i^y - 2\Omega_2 S_i^z + \sum_m J_{im} S_m^z S_i^y, \quad (3.15)$$

$$-i[S_i^y, H] = -2\Omega_3 S_i^x + 2\Omega_1 S_i^z - \sum_m J_{im} S_m^z S_i^x, \quad (3.16)$$

$$-i[S_i^z, H] = 2\Omega_2 S_i^x - 2\Omega_1 S_i^y. \quad (3.17)$$

Then the equations of motion of the Green's functions [Eq. (3.11)] are

$$EA_{ij}^{x\nu(\eta)} = K_{ij}^{x\nu(\eta)} - 2i\Omega_2 A_{ij}^{z\nu(\eta)} + 2i\Omega_3 A_{ij}^{y\nu(\eta)} + i \sum_m J_{im} \langle \langle S_m^z S_i^y; Q_j^\nu \rangle \rangle_E^{(\eta)}, \quad (3.18)$$

$$EA_{ij}^{y\nu(\eta)} = K_{ij}^{y\nu(\eta)} - 2i\Omega_3 A_{ij}^{x\nu(\eta)} + 2i\Omega_1 A_{ij}^{z\nu(\eta)} - i \sum_m J_{im} \langle \langle S_m^z S_i^x; Q_j^\nu \rangle \rangle_E^{(\eta)}, \quad (3.19)$$

$$EA_{ij}^{z\nu(\eta)} = K_{ij}^{z\nu(\eta)} - 2i\Omega_1 A_{ij}^{y\nu(\eta)} + 2i\Omega_2 A_{ij}^{x\nu(\eta)}. \quad (3.20)$$

Taking the thermal averages of both sides of Eqs. (3.15)–(3.17) gives the identities

$$\sum_m J_{im} \langle S_m^z S_i^y \rangle = 2\Omega_2 z - 2\Omega_3 y, \quad (3.21)$$

$$\sum_m J_{im} \langle S_m^z S_i^x \rangle = 2\Omega_1 z - 2\Omega_3 x, \quad (3.22)$$

$$0 = 2\Omega_2 x - 2\Omega_1 y. \quad (3.23)$$

We also note from Eq. (3.23) that

$$y = \left[\frac{x}{2\Omega_1} \right] 2\Omega_2 \quad (3.24)$$

and we can write

$$x = 2\Omega_1 \Gamma, \quad y = 2\Omega_2 \Gamma, \quad (3.25)$$

where Γ will be determined below.

IV. DECOUPLING SCHEMES

As expected, the GF's on the right-hand side of Eqs. (3.18) and (3.19) are of higher order than our basic GF's in Eq. (3.11) and must be approximately decoupled to provide a closed, soluble set of equations to replace Eqs. (3.18)–(3.20). In the symmetric decoupling approximation,^{1,17}

$$\langle \langle S_m^z S_i^y; Q_j^\nu \rangle \rangle_E^{(\eta)} = z A_{ij}^{y\nu(\eta)} + y A_{mj}^{z\nu(\eta)} \quad (4.1)$$

and

$$\langle \langle S_m^z S_i^x; Q_j^\nu \rangle \rangle_E^{(\eta)} = z A_{ij}^{x\nu(\eta)} + x A_{mj}^{z\nu(\eta)}. \quad (4.2)$$

In order to demonstrate the difficulties inherent in such a decoupling, we use the $\eta = +1$ form of Eqs. (4.1) and (4.2) and obtain the correlation approximations.

$$\langle Q_j^\nu S_m^z S_i^y \rangle = z a_{ij}^{y\nu} + y a_{mj}^{z\nu}, \quad (4.3)$$

$$\langle Q_j^\nu S_m^z S_i^x \rangle = z a_{ij}^{x\nu} + x a_{mj}^{z\nu}. \quad (4.4)$$

Since a description of the response of the system to a vanishingly small field in the z direction ($\Omega_3 \rightarrow 0$) requires determination of the GF $\langle \langle A; \sum_j S_j^z \rangle \rangle_E^{(-)}$, we consider the choice $Q_j^\nu = S_j^z$ in Eqs. (4.3) and (4.4) and obtain (for $m \neq i$)

$$\langle S_j^z S_m^z S_i^y \rangle = z \langle S_j^z S_i^y \rangle + y \langle S_j^z S_m^z \rangle = z a_{ij}^{yz} + y a_{mj}^{zz}, \quad (4.5)$$

$$\langle S_j^z S_m^z S_i^x \rangle = z \langle S_j^z S_i^x \rangle + x \langle S_j^z S_m^z \rangle = z a_{ij}^{zx} + x a_{mj}^{zz}. \quad (4.6)$$

For $j = m \neq i$ Eqs. (4.5) and (4.6) yield

$$z \langle S_m^z S_i^y \rangle = 0, \quad z \langle S_m^z S_i^x \rangle = 0, \quad (4.7)$$

while for $j = i \neq m$ Eqs. (4.5) and (4.6) yield

$$\langle S_m^z S_i^y \rangle = zx + iy \langle S_i^z S_m^z \rangle, \quad (4.8)$$

$$\langle S_m^z S_i^x \rangle = zy - ix \langle S_i^z S_m^z \rangle. \quad (4.9)$$

Since the correlations are real for $i \neq m$ and for TIM x and y do not vanish, Eqs. (4.7)–(4.9) imply therefore that

$$\langle S_i^z S_m^z \rangle = \langle S_m^z S_i^x \rangle = \langle S_m^z S_i^y \rangle = z = 0. \quad (4.10)$$

Thus, a symmetric decoupling treatment of the response of TIM to a vanishingly small z field is inherently limited to the linear-response region ($T > T_c$) where z vanishes if Ω_3 vanishes.

We propose a decoupling scheme, based upon the concept of the cumulant average, which is not inherently limited to any temperature range. The cumulant average of $\langle S_m^z(t) S_i^y(t) Q_j^\nu \rangle$, a typical correlation appearing in $\langle \langle S_m^z S_i^y; Q_j^\nu \rangle \rangle_E^{(\eta)}$, is defined by¹²

$$\begin{aligned} \langle S_m^z(t) S_i^y(t) Q_j^\nu \rangle &= z \langle S_i^y(t) Q_j^\nu \rangle + y \langle S_m^z(t) Q_j^\nu \rangle \\ &\quad + Q^\nu (\langle S_m^z S_i^y \rangle - 2zy) \\ &\quad + \langle S_m^z(t) S_i^y(t) Q_j^\nu \rangle_c, \end{aligned} \quad (4.11)$$

where the subscript c denotes cumulant average. Also,

$$\begin{aligned} \langle Q_j^y S_m^z(t) S_i^y(t) \rangle &= z \langle Q_j^y S_i^y(t) \rangle \\ &+ y \langle Q_j^y S_m^z(t) \rangle \\ &+ Q^y (\langle S_m^z S_i^y \rangle - 2zy) \\ &+ \langle Q_j^y S_m^z(t) S_i^y(t) \rangle_c. \end{aligned} \quad (4.12)$$

A decoupling is accomplished if we can assume

$$\langle S_m^z(t) S_i^y(t) Q_j^y \rangle_c = \langle Q_j^y S_m^z(t) S_i^y(t) \rangle_c = 0. \quad (4.13)$$

The question is, when is Eq. (4.13) a reasonable approximation? As shown by Kubo,¹² Eq. (4.13) is true if the set $\{S_m^z(t), S_i^y(t), Q_j^y\}$ can be divided into two or more groups which are statistically independent of each other. We now *assume* the existence of a region where

$$\lim_{\Omega_3 \rightarrow 0} z \neq 0. \quad (4.14)$$

This assumption (to be verified self-consistently by demonstrating the existence of such a phase under our approximations) is essentially an assumption that the dominant coupling in the system is the coupling of the z components of spin. This coupling produces an effective internal z field which is responsible for Eq. (4.14). If we choose

$$Q_j^y = S_j^z \quad (4.15)$$

in Eq. (4.13), the set in question is $\{S_m^z(t), S_i^y(t), S_j^z\}$, two members of which are coupled by the dominant z - z coupling and one member $[S_i^y(t)]$ of which is relatively independent of the others. Such a division of $\{S_m^z(t), S_i^y(t), Q_j^y\}$ is not possible for the other choices $(Q_j^y = S_j^x, S_j^y)$. Thus, only the choice (4.15) makes Eq. (4.13) consistent with the internal field interpretation of Eq. (4.14). We thus restrict ourselves to the choice (4.15). It is interesting to note that question of the choice of Q_j^y never arises in most decoupling approximations while here the choice is crucial and determined by physical considerations. If the remainder of our development is followed for different choices for Q_j^y (i.e., $Q_j^y = S_j^x$ or S_j^y), different results are obtained for the parameters of interest in the TIM. If one attempts to use the results from various Q_j^y choices simultaneously, "ambiguities" appear. Such ambiguities are a common feature of DTGF treatments of many-body systems,^{7,17} and depending upon the choice of basis operators, can also appear as a failure of the scheme to satisfy the $S = \frac{1}{2}$ "kinematic condition," $\langle (S^-)^2 \rangle = 0$. Recent decoupling schemes for the TIM^{7,18,19} do not satisfy this kinematic condition and therefore must be restricted to regions where $\langle (S^-)^2 \rangle$ is self-consistently "small" ($\Omega_1 \rightarrow \infty$ and $T_c \rightarrow 0$). Even in these regions, however, $\langle (S^-)^2 \rangle$ does *not* vanish, and the ambiguities

are *not* removed. These schemes are also restricted to $T > T_c$; thus the problems of zero frequency poles in the CGF did not appear. By distinguishing *a priori* between the different Q_j^y choices [here requiring Eq. (4.15)], cumulant decoupling *removes* these ambiguities

Using Eqs. (4.11)–(4.13), and (4.15), we obtain the approximation

$$\begin{aligned} \langle \langle S_m^z S_i^y, S_j^z \rangle \rangle_E^{(\eta)} &= z A_{ij}^{yz(\eta)} + y A_{mj}^{zz(\eta)} \\ &+ [(1 + \eta)/E] z (\langle S_m^z S_i^y \rangle - 2zy) \end{aligned} \quad (4.16)$$

and, similarly,

$$\begin{aligned} \langle \langle S_m^z S_i^x, S_j^z \rangle \rangle_E^{(\eta)} &= z A_{ij}^{xz(\eta)} + x A_{mj}^{zz(\eta)} \\ &+ [(1 + \eta)/E] z (\langle S_m^z S_i^x \rangle - 2zx). \end{aligned} \quad (4.17)$$

Using Eqs. (4.16) and (4.17) in Eqs. (3.18) and (3.19) and defining spatial Fourier transforms by, e.g.,

$$A_k^{xz(\eta)} = \sum_j e^{i\vec{k} \cdot \vec{r}_{ij}} A_{ij}^{xz(\eta)} \quad (4.18)$$

we obtain

$$A_k^{\mu z(\eta)} = \frac{1}{\Delta_k} (K_k^{\mu z(\eta)} E^2 + i L_k^{\mu z(\eta)} E - M_k^{\mu z(\eta)}) \quad \mu = x, y, z \quad (4.19)$$

where

$$L_k^{xz(\eta)} = (2\Omega_3 + zJ_0) K_k^{xz(\eta)} - 2\Omega_2(1 - \Gamma J_k) K_k^{zz(\eta)} - \Gamma_0^{yz(\eta)}, \quad (4.20)$$

$$L_k^{yz(\eta)} = -(2\Omega_3 + zJ_0) K_k^{yz(\eta)} + 2\Omega_1(1 - \Gamma J_k) K_k^{zz(\eta)} + \Gamma_0^{xz(\eta)}, \quad (4.21)$$

$$L_k^{zz(\eta)} = 2(\Omega_2 K_k^{xz(\eta)} - \Omega_1 K_k^{yz(\eta)}), \quad (4.22)$$

$$M_k^{xz(\eta)} = 2\Omega_1(1 - \Gamma J_k) D_k^{(\eta)} + (2\Omega_3 + zJ_0) \Gamma_0^{xz(\eta)}, \quad (4.23)$$

$$M_k^{yz(\eta)} = 2\Omega_2(1 - \Gamma J_k) D_k^{(\eta)} + (2\Omega_3 + zJ_0) \Gamma_0^{yz(\eta)}, \quad (4.24)$$

$$M_k^{zz(\eta)} = (2\Omega_3 + zJ_0) D_k^{(\eta)} - (2\Omega_1 \Gamma_0^{xz(\eta)} + 2\Omega_2 \Gamma_0^{yz(\eta)}), \quad (4.25)$$

$$\Gamma_0^{\mu z(\eta)} = (1 + \eta) z \Phi^{\mu z} N \delta_{k0}, \quad (4.26)$$

$$D_k^{(\eta)} = 2\Omega_1 K_k^{xz(\eta)} + 2\Omega_2 K_k^{yz(\eta)} + (2\Omega_3 + zJ_0) K_k^{zz(\eta)}, \quad (4.27)$$

and

$$\Delta_k = E(E^2 - \omega_k^2) \quad (4.28)$$

with

$$\omega_k^2 = (1 - \Gamma J_k)(2\Lambda)^2 + (2\Omega_3 + zJ_0)^2, \quad (4.29)$$

$$(2\Lambda)^2 = (2\Omega_1)^2 + (2\Omega_2)^2, \quad (4.30)$$

and

$$\begin{aligned} \Phi^{\mu z} &= \sum_m J_{im} (2zQ^\mu - \langle S_i^z S_m^z \rangle) \\ &= Q^\mu [(2J_0 - \Gamma^{-1})z + 2\Omega_3], \end{aligned} \quad (4.31)$$

where the last equality follows for $\mu = x$ and y from Eqs. (3.21), (3.22), and (3.25).

From Eq. (4.19) we find that the analyticity condition (2.5) requires

$$\lim_{E \rightarrow 0} EA_k^{\mu z(-)} = (1/\omega_k^2) M_k^{\mu z(-)} = 0 \quad (4.32)$$

for $\mu = x, y, z$. Using Eqs. (4.24)–(4.26) the condition (4.32) becomes

$$D_k^{(-)} = 0. \quad (4.33)$$

Now from Eqs. (3.13) and (4.19) we find

$$K_k^{xz(-)} = -iy, \quad K_k^{yz(-)} = ix, \quad K_k^{zz(-)} = 0 \quad (4.34)$$

and thus Eqs. (4.33) and (4.27) yield

$$2\Omega_1 y - 2\Omega_2 x = 0, \quad (4.35)$$

which is identity (3.23). Our CGF's thus satisfy the analyticity condition (2.5).

From Eqs. (4.12), (4.13), and (4.15) we obtain the correlation approximations

$$\langle S_j^z S_m^z S_i^y \rangle = z \langle S_j^z S_i^y \rangle + y \langle S_j^z S_m^z \rangle + z (\langle S_m^z S_i^y \rangle - 2zy), \quad (4.36)$$

$$\langle S_j^z S_m^z S_i^x \rangle = z \langle S_j^z S_i^x \rangle + x \langle S_j^z S_m^z \rangle + z (\langle S_m^z S_i^x \rangle - 2zx). \quad (4.37)$$

Note that the $\eta = +1$ forms of Eqs. (4.16) and (4.17) lead by means of Eqs. (2.7) to (4.36) and (4.37).

For $j = m \neq i$ Eqs. (4.36) and (4.37) give

$$z (\langle S_m^z S_i^y \rangle - zy) = 0, \quad (4.38)$$

$$z (\langle S_m^z S_i^x \rangle - zx) = 0, \quad (4.39)$$

while for $j = i \neq m$ Eqs. (4.36) and (4.37) give, using Eqs. (4.38) and (4.39)

$$y (\langle S_j^z S_m^z \rangle - z^2) + \frac{1}{2} i (\langle S_m^z S_i^y \rangle - zy) = 0, \quad (4.40)$$

$$x (\langle S_j^z S_m^z \rangle - z^2) - \frac{1}{2} i (\langle S_m^z S_i^x \rangle - zx) = 0. \quad (4.41)$$

Then Eqs. (4.38)–(4.41) have the solutions

$$a_{im}^{xz} = \langle S_m^z S_i^x \rangle = zx(1 - \delta_{mi}) + \frac{1}{2} iy \delta_{mi}, \quad (4.42)$$

$$a_{im}^{yz} = \langle S_m^z S_i^y \rangle = zy(1 - \delta_{mi}) - \frac{1}{2} ix \delta_{mi}, \quad (4.43)$$

$$a_{im}^{zz} = \langle S_m^z S_i^z \rangle = z^2(1 - \delta_{mi}) + \frac{1}{4} \delta_{mi}. \quad (4.44)$$

and we *do not* have to restrict ourselves to the $z = 0$ case.

Using Eqs. (4.42) and (4.43) in Eqs. (3.22) and (3.21) gives

$$z(2\Omega_2 - yJ_0) - 2\Omega_3 y = 0, \quad (4.45)$$

$$z(2\Omega_1 - xJ_0) - 2\Omega_3 x = 0, \quad (4.46)$$

so that

$$\lim_{\Omega_3 \rightarrow 0} z(2\Omega_2 - yJ_0) = 0, \quad (4.47)$$

$$\lim_{\Omega_3 \rightarrow 0} z(2\Omega_1 - xJ_0) = 0, \quad (4.48)$$

and, in the phase described by Eq. (4.14) we must have

$$\lim_{\Omega_3 \rightarrow 0} y = 2\Omega_2/J_0, \quad (4.49)$$

$$\lim_{\Omega_3 \rightarrow 0} x = 2\Omega_1/J_0. \quad (4.50)$$

From Eqs. (4.45), (4.46), and (3.25) we have

$$\Gamma = (2\Omega_3 + zJ_0)^{-1} z, \quad z \neq 0. \quad (4.51)$$

If $\Omega_3 = 0$ and $z = 0$, then Γ is not determined by Eq. (4.51); but must instead be determined from the solution to a transcendental equation [see Eq. (5.39) below].

V. RESPONSE OF THE TRANSVERSE ISING SYSTEM TO A UNIFORM z FIELD

We now consider the basic question for TIM: Does the system provide a nonvanishing z in the limit of $\Omega_3 \rightarrow 0$? First we assume a negative answer; i.e., we consider the linear-response region where^{8,9}

$$\begin{aligned} x &= x_0 + \chi_{xz}(2\Omega_3) + \dots, \\ y &= y_0 + \chi_{yz}(2\Omega_3) + \dots, \\ z &= \chi_{zz}(2\Omega_3) + \dots \end{aligned} \quad (5.1)$$

The static susceptibilities are given by

$$\chi_{\mu z} = -A_{0,0}^{\mu z(-)}(E=0), \quad (5.2)$$

where the extra zero subscript indicates that all thermal averages are calculated for $\Omega_3 = 0$ which means, from Eq. (3.6), that $z_0 = 0$.

For finite k , E , and Ω_3 we have from Eq. (4.19)

$$A_k^{xz(-)} = -(E^2 - \omega_k^2)^{-1} [iyE + (2\Omega_3 + zJ_0)x], \quad (5.3)$$

$$A_k^{yz(-)} = (E^2 - \omega_k^2)^{-1} [ixE - (2\Omega_3 + zJ_0)y], \quad (5.4)$$

$$A_k^{zz(-)} = (E^2 - \omega_k^2)^{-1} [(2\Lambda)^2 \Gamma]. \quad (5.5)$$

In the $k = 0$, $\Omega_3 = 0$, $z_0 = 0$ limit we find from Eq. (5.2)

that

$$\chi_{xz} = \chi_{yz} = 0, \quad \chi_{zz} = \Gamma_0(1 - \Gamma_0 J_0)^{-1}, \quad (5.6)$$

where we used

$$\omega_{00}^2 = (2\Lambda)^2(1 - \Gamma_0 J_0). \quad (5.7)$$

From Eq. (5.6) we thus have that the series (5.1) diverge; i.e.,

$$\lim_{\Omega_3 \rightarrow 0} z \neq 0 \quad (5.8)$$

if

$$\Gamma_0 \rightarrow 1/J_0, \quad (T \rightarrow T_c), \quad (5.9)$$

for then $\chi_{zz} \rightarrow \infty$ and the expansion in powers of Ω_3 does not converge for any Ω_3 . Thus, Eq. (5.9) defines a critical temperature T_c and since then $\omega_{k,0} \rightarrow 0$ at $\bar{k} = 0$, it predicts a softening of the collective mode at T_c . The $\bar{k} = 0$ mode corresponds to the lowest energy (in-phase) motion of the protons.²⁰ For $\bar{k} \neq 0$ the motions are out of phase. Moreover, mode softening corresponds to large displacements so that x_0 approaches $2\Omega_1/J_0$ and y_0 approaches $2\Omega_2/J_0$ from below (becoming larger) as $T \rightarrow T_c$. Then, since $J_k < J_0$, $\omega_{k,0} = 0$ has no solution except for $\bar{k} = 0$ and $T = T_c$.

Below T_c Eq. (4.14) holds, and from Eq. (4.51)

$$\Gamma = 1/J_0, \quad T < T_c, \quad \Omega_3 = 0. \quad (5.10)$$

In order to proceed we need the correlations x , y , and z in the $\Omega_3 \rightarrow 0$ limit. The *exact* values of these

$$\lim_{i, \epsilon \rightarrow 0} \frac{i}{2\pi} \int_{-\infty}^{\infty} dE (e^{\beta E} - 1)^{-1} e^{-iEt} (G_{E+i\epsilon} - G_{E-i\epsilon}) = -\frac{1}{2}\alpha_1 + \frac{1}{2}\alpha_0 \omega_k^{-1} \coth \frac{1}{2}\beta\omega_k, \quad (5.17)$$

where

$$G_E = \frac{\alpha_1 E + \alpha_0}{E^2 - \omega_k^2}. \quad (5.18)$$

Then we find from Eqs. (4.19) and (2.7), using Eq. (3.25)

$$a_k^{xz} = \frac{1}{2} C^{xz(+)} + i \Omega_2 \Gamma - \Omega_1 (2\Omega_3 + zJ_0) \omega_k^{-1} \Gamma \coth \frac{1}{2}\beta\omega_k, \quad (5.19)$$

$$a_k^{yz} = \frac{1}{2} C^{yz(+)} - i \Omega_1 \Gamma - \Omega_2 (2\Omega_3 + zJ_0) \omega_k^{-1} \Gamma \coth \frac{1}{2}\beta\omega_k, \quad (5.20)$$

$$a_k^{zz} = \frac{1}{2} C^{zz(+)} + \frac{1}{2} (2\Lambda)^2 \omega_k^{-1} \Gamma \coth \frac{1}{2}\beta\omega_k. \quad (5.21)$$

Utilizing Eqs. (5.12)–(5.14), and (5.16), $(2\Omega_2)$ times Eq. (5.19) minus $(2\Omega_1)$ times Eq. (5.20) yields the relation

$$2\Omega_2 a_k^{xz} - 2\Omega_1 a_k^{yz} - \frac{1}{2} i \Gamma (2\Lambda)^2 = \frac{1}{2} (2\Omega_3 + zJ_0) \omega_0^{-2} (2\Omega_2 \Gamma_0^{x(+)} - 2\Omega_1 \Gamma_0^{y(+)}) = 0, \quad (5.22)$$

where the last equality follows from Eqs. (4.26), (4.28), and (3.21)–(3.23). Also we find that $(2\Omega_1)$ times Eq. (5.19) plus $(2\Omega_2)$ times Eq. (5.20) yields $(2\Omega_3 + zJ_0)$ times the identity following from Eq. (5.21), viz.,

$$0 = (2\Omega_3 + zJ_0) \omega_k^{-2} (2\Omega_1 a_k^{xz} + 2\Omega_2 a_k^{yz}) - [1 - (2\Omega_3 + zJ_0)^2 \omega_k^{-2}] a_k^{zz} + \frac{1}{2} (2\Lambda)^2 \Gamma \omega_k^{-1} \coth \frac{1}{2}\beta\omega_k - \frac{1}{2} \omega_0^{-2} (2\Omega_1 \Gamma_0^{x(+)} + 2\Omega_2 \Gamma_0^{y(+)}). \quad (5.23)$$

correlations are not available since we do not know the exact GF's. We now make the additional self-consistent approximation of obtaining these correlations from our approximate GF's.

To evaluate the $a_k^{\mu z}$ correlations from the $A_k^{\mu z(-)}$ GF's, we need the values of the limiting functions $C^{\mu z(+)}$:

$$C^{\mu z(+)} = \lim_{E \rightarrow 0} E A_k^{\mu z(+)} = \omega_k^{-2} M_k^{\mu z(+)} \quad (5.11)$$

We have from Eqs. (4.23)–(4.25)

$$C^{xz(+)} = 2\Omega_1 (1 - \Gamma J_k) \omega_k^{-2} D_k^{(+)} + (2\Omega_3 + zJ_0) \omega_0^{-2} \Gamma_0^{x(+)}, \quad (5.12)$$

$$C^{yz(+)} = 2\Omega_2 (1 - \Gamma J_k) \omega_k^{-2} D_k^{(+)} + (2\Omega_3 + zJ_0) \omega_0^{-2} \Gamma_0^{y(+)}, \quad (5.13)$$

$$C^{zz(+)} = (2\Omega_3 + zJ_0) \omega_k^{-2} D_k^{(+)} - \omega_0^{-2} (2\Omega_1 \Gamma_0^{x(+)} + 2\Omega_2 \Gamma_0^{y(+)}). \quad (5.14)$$

Therefore, since

$$K_k^{\mu z(+)} = K_k^{\mu z(-)} + 2a_k^{\mu z} \quad (5.15)$$

and $K_k^{\mu z(-)}$ is given in Eq. (4.34), we find using Eq. (3.25)

$$D_k^{(+)} = (2\Omega_1) 2a_k^{xz} + (2\Omega_2) 2a_k^{yz} + (2\Omega_3 + zJ_0) 2a_k^{zz}. \quad (5.16)$$

For $\eta = -1$ we see from Eqs. (5.3)–(5.5), and (2.7) that we must evaluate integrals of the form²¹:

Alternatively for $\eta = +1$ we see from Eqs. (4.19) and (2.7) that we must evaluate integrals of the form²¹:

$$\lim_{\epsilon, t \rightarrow 0} \frac{i}{2\pi} \int_{-\infty}^{\infty} dt (e^{\beta E} + 1)^{-1} e^{-iEt} (G_{E+i\epsilon} - G_{E-i\epsilon}) = \frac{1}{2} \alpha_2 - \frac{1}{2} \alpha_1 \omega_k^{-1} \tanh \frac{1}{2} \beta \omega_k, \quad (5.24)$$

where

$$G_E = \frac{\alpha_2 E^2 + \alpha_1 E + \alpha_0}{E(E^2 - \omega_k^2)}. \quad (5.25)$$

Then we find from Eqs. (4.19) and (2.7)

$$a_k^{\mu z} = \frac{1}{2} K_k^{\mu z(+)} - (iL_k^{\mu z(+)} / 2\omega_k) \tanh \frac{1}{2} \beta \omega_k, \quad \mu = x, y, z, \quad (5.26)$$

i.e.,

$$a_k^{xz} = -\frac{1}{2} iy + a_k^{yz} - i\omega_k^{-1} [(2\Omega_3 + zJ_0) (\frac{1}{2} ix + a_k^{yz}) - 2\Omega_2 (1 - \Gamma J_k) a_k^{xz} - \frac{1}{2} \Gamma_0^{y(+)}] \tanh \frac{1}{2} \beta \omega_k, \quad (5.27)$$

$$a_k^{yz} = \frac{1}{2} ix + a_k^{xz} - i\omega_k^{-1} [(2\Omega_3 + zJ_0) (\frac{1}{2} iy - a_k^{xz}) + 2\Omega_1 (1 - \Gamma J_k) a_k^{yz} + \frac{1}{2} \Gamma_0^{x(+)}] \tanh \frac{1}{2} \beta \omega_k, \quad (5.28)$$

$$a_k^{zz} = a_k^{zz} - i\omega_k^{-1} [2\Omega_2 (-\frac{1}{2} iy + a_k^{xz}) - 2\Omega_1 (\frac{1}{2} ix + a_k^{yz})] \tanh \frac{1}{2} \beta \omega_k. \quad (5.29)$$

Now $(2\Omega_2)$ times Eq. (5.29) minus $(2\Omega_1)$ times Eq. (5.30) yields $(i\omega_k)$ times Eq. (5.23); also $(2\Omega_1)$ times Eq. (5.29) plus $(2\Omega_2)$ times Eq. (5.30) yields $(2\Omega_3 + zJ_0)$ times Eq. (5.22); finally Eq. (5.31) yields Eq. (5.22) directly. Thus, when properly treated, both CGF and AGF yield the same result. Bloomfield and Nafari¹⁰ showed that CGF and AGF lead to the same correlation identities only if the correct Fourier inversion formula (2.7) is used and if Eq. (2.5) is imposed as a condition on the CGF's.

Summing Eq. (5.23) over k we find [summing Eq. (5.22) yields an identity]:

$$(2\Omega_3 + zJ_0) \left(\frac{2\Omega_1}{N} \sum_k \frac{a_k^{xz}}{\omega_k^2} + \frac{2\Omega_2}{N} \sum_k \frac{a_k^{yz}}{\omega_k^2} + (2\Omega_3 + zJ_0) \frac{1}{N} \sum_k \frac{a_k^{zz}}{\omega_k^2} \right) - z \frac{(2\Omega_1 \Phi^{xz} + 2\Omega_2 \Phi^{yz})}{\omega_0^2} + \Gamma(2\Lambda)^2 \frac{1}{2N} \sum_k \frac{1}{\omega_k} \coth \frac{1}{2} \beta \omega_k - \frac{1}{4} = 0. \quad (5.30)$$

This equation relates z , Λ , Ω_3 , and β to each other and is valid for finite z and Ω_3 both above, below, and on the critical curve. This contrasts with the symmetric decoupling approximation which is valid only for $T > T_c$, $\Omega_3 = z = 0$. For the region $T > T_c$ we set z and Ω_3 to zero and obtain from Eq. (5.30)

$$\frac{1}{2} = \Gamma_0 (2\Lambda)^2 N^{-1} \sum_k \omega_k^{-1} \coth \frac{1}{2} \beta \omega_{k0}, \quad (5.31)$$

where

$$\omega_{k0}^2 = (1 - \Gamma_0 J_k) (2\Lambda)^2. \quad (5.32)$$

One can determine Γ_0 from Eq. (5.31) and then from Eq. (5.6) the static susceptibility for $T > T_c$. The *critical curve* is defined by Eq. (5.9) and is determined by inserting Eq. (5.9) into Eqs. (5.31) and (5.32)

$$\frac{1}{2} = 2\Lambda (J_0 N)^{-1} \sum_k (1 - J_k/J_0)^{-1/2} \coth[\beta_c \Lambda (1 - J_k/J_0)^{1/2}], \quad (5.33)$$

where $\beta_c = (kT_c)^{-1}$. The *Weiss condition*²² is obtained by solving Eq. (5.33) for that value of $2\Lambda/J_0$ for which $T_c = 0$. This gives

$$\left(\frac{2\Lambda}{J_0} \right)_w = \left[2N^{-1} \sum_k (1 - J_k/J_0)^{-1/2} \right]^{-1}. \quad (5.34)$$

Values of the sum in Eq. (5.34) are available for simple cubic (sc), bcc, and fcc lattices.^{7,19} Thus, Eq. (5.34) gives, for sc, bcc, and fcc, respectively,

$$\left(\frac{2\Lambda}{J_0} \right)_w = 0.449, \quad 0.460, \quad 0.466. \quad (5.35)$$

The series results¹⁵ are 0.423 (sc), 0.435 (bcc), and 0.444 (fcc).

TABLE I. Ground-state magnetization vs transverse field for bcc lattice [from Eq. (5.38) at $T=0$].

z	$2\Lambda/J_0$	z	$2\Lambda/J_0$	z	$2\Lambda/J_0$
0	0.461	0.2789	0.380	0.4049	0.265
0.1036	0.450	0.2992	0.366	0.4214	0.243
0.1470	0.441	0.3182	0.352	0.4374	0.219
0.1805	0.430	0.3368	0.337	0.4527	0.190
0.2090	0.418	0.3546	0.321	0.4686	0.156
0.2343	0.406	0.3716	0.303	0.4845	0.111
0.2574	0.393	0.3888	0.285	0.5	0

If we let $\Lambda \rightarrow 0$ in Eq. (5.33), the *pure Ising* limit (the "other end" of the critical curve) is obtained. In this limit Eq. (5.33) gives

$$\left(\frac{kT_c}{J_0}\right)_I = \frac{1}{4} \left[N^{-1} \sum_k (1 - J_k/J_0)^{-1} \right]^{-1}. \quad (5.36)$$

The Watson sums in Eq. (5.36) being readily available,²³ we obtain for sc, bcc, and fcc

$$\left(\frac{kT_c}{J_0}\right)_I = 0.1649, \quad 0.179, \quad 0.1859. \quad (5.37)$$

The series results¹⁵ are 0.188 (sc), 0.200 (bcc), and 0.205 (fcc).

For $T < T_c$ and $\Omega_3 = 0$ Eq. (5.30) becomes, using

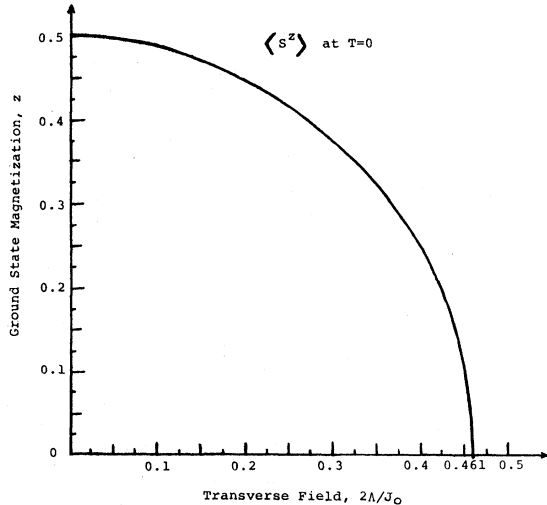


FIG. 1. Magnetization z vs transverse field $2\Lambda/J_0$ at $T=0$ for bcc lattice from Eq. (5.38) and Table I. Note $z=0$ corresponds to the Weiss field of Eq. (5.35) where $T_c = T=0$, while $\Lambda=0$ corresponds to the Ising limit where (kT_c/J_0) is given in Eq. (5.37). The curve meets the two axes perpendicularly.

Eq. (5.10)

$$\begin{aligned} \frac{1}{4} - \zeta^2 \lambda^2 + \zeta^2 \lambda^2 [1 - (\frac{1}{4} - \zeta^2 \lambda^2) \lambda^{-2}] \frac{1}{N} \sum_k \nu_k^{-2} \\ = \frac{\lambda}{2N} \sum_k \nu_k^{-1} \coth \beta \Lambda \nu_k, \end{aligned} \quad (5.38)$$

where

$$\lambda = 2\Lambda/J_0, \quad \zeta = z/\lambda, \quad (5.39)$$

$$\nu_k^2 = \omega_k^2 / (2\Lambda)^2 = 1 - J_k/J_0 + \zeta^2, \quad (5.40)$$

and where we have used, from Eqs. (4.42)–(4.44), and (4.28), and (5.10)

$$a_k^{xz} = \frac{1}{2} iy + zx (N \delta_{k0} - 1), \quad (5.41)$$

$$a_k^{yz} = -\frac{1}{2} ix + zy (N \delta_{k0} - 1), \quad (5.42)$$

$$a_k^{zz} = \frac{1}{4} + z^2 (N \delta_{k0} - 1), \quad (5.43)$$

$$\Phi^{\mu z} = z J_0 Q^\mu. \quad (5.44)$$

We can readily solve Eq. (5.38) by iteration for the ground-state ($T=0$) value of z using series expansion.⁷ The result for the bcc lattice is presented in Table I and Fig. 1.

VI. SUMMARY AND CONCLUSIONS

The transverse Ising model (Ising model with additional internal fields, Ω_1 coupled to S^x and Ω_2 coupled to S^y) is studied in the presence of a finite external field Ω_3 coupled to S^z . An exact identity shows that $\langle S^x \rangle$ or $\langle S^y \rangle$ is directly proportional to Ω_1 or Ω_2 , respectively, both above and below the critical temperature T_c . On the other hand above T_c $\langle S^z \rangle$ is directly proportional to Ω_3 ; while below T_c $z \neq 0$ even when $\Omega_3 \rightarrow 0$.

The response of a system to an external field is given by the generalized dynamical susceptibility. To

calculate the generalized susceptibility the commutator Green's functions are needed. Then account must be taken of the fact that a CGF cannot have a pole at $E=0$. Our treatment fits the zero frequency condition and utilizes the proper inversion formula for calculating the correlations from the CGF's. The CGF's and AGF's, calculated in the complex energy plane, should lead to the same temporal or static correlation functions. This will be the case only if: (1) the correct Fourier inversion formula is used to calculate the correlation functions and (2) the analyticity condition at $E=0$ is imposed on the CGF's. In fact the CGF analyticity condition may lead to correlation function identities. If this is the case, these same identities will express themselves as self-consistency conditions among the correlation functions calculated from the AGF's. An example of this relationship is seen in the calculation herein of the zero frequency $M_k^{\mu\nu(-)}=0$ equations [see Eq. (4.32)]. Identity (3.23) automatically satisfies the zero frequency condition for $\nu=z$ [see Eqs. (4.33) and (4.35)]. For $\nu=x$ (4.45) and for $\nu=y$ (4.46) satisfies the respective zero frequency condition. Also as noted after Eq. (4.37) these relationships follow from the AGF inversion formula.

The symmetric decoupling approximation is shown to be valid only for $T > T_c$ and for $\Omega_3 = z = 0$. We have developed an unambiguous scheme for all T utilizing the concept of cumulant averages. Our cumulant decoupling approximation, based upon the statistical independence of different groups of opera-

tors, is determined by the fact that the dominant coupling in the system is between z components of spin. In particular this leads us to select S^z as the trailing operator in our double time Green's-function formalism.

In common with the current decoupling schemes, ours produces GF's with poles on the real axis; i.e., undamped excitations. An improved version of cumulant decoupling would recognize that the approximation (4.13) with Eq. (4.15) is weakest when $j=i$ because $S_j^y(i)$ and S_j^z would be correlated by virtue of their being on a common site while $S_m^z(i)$ would still be correlated to S_j^z through the internal field. An improved treatment would have formal properties in common with single-site-impurity problems where GF techniques have lead to damped excitations.¹³

We have examined the equations of motion of the set of operators which are directly coupled to the internal and external fields for both the disordered ($T > T_c$) and ordered ($T < T_c$) regions. All $S = \frac{1}{2}$ operator identities are satisfied. Collective-mode softening is found as $T \rightarrow T_c$. Expressions for the dynamical susceptibility have been found; the critical curve formula was obtained and numerical values for the Weiss critical field and T_c in the Ising limit have been calculated. Furthermore we have derived expressions relating the magnetization and finite internal and external fields for all temperatures. Thus for the first time there has been carried out a self-consistent determination of the dynamical solution of a DTGF theory of the TIM.

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²¹We used $\lim_{\epsilon \rightarrow 0^+} [1/(\omega - i\epsilon) - 1/(\omega + i\epsilon)] = 2\pi i \delta(\omega)$.

We note that Eq. (11) in Ref. 10 contains a sign misprint and should read: $1/(\omega \pm i\epsilon) = P/\omega \mp \pi i \delta(\omega)$, where P/ω means that a Cauchy principal-value integral is to be taken and $\delta(\omega)$ is the Dirac δ function. Also we need

$\eta[e^{-\beta\omega} + \eta]^{-1} \pm (e^{\beta\omega} + \eta)^{-1} \eta = (1, \tanh \frac{1}{2}\beta\omega)$, which corrects Eq. (43) of Ref. 10.

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