ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ
ДУБНА

E17 - 11359

V.L.Aksionov, H.Konvent, J.Schreiber

COMMUTATOR AND ANTICOMMUTATOR GREEN FUNCTIONS IN THE ISING MODEL WITH TRANSVERSE FIELD

1978

E17 - 11359

V.L.Aksionov, H.Konvent,[1] J.Schreiber[2]

COMMUTATOR AND ANTICOMMUTATOR GREEN FUNCTIONS IN THE ISING MODEL WITH TRANSVERSE FIELD

Submitted to "physica status solidi"

[1] Technical University Wroclaw, Institute of Physics, Poland.
[2] On leave from Technical University Dresden, Section of Physics, GDR.

Аксенов В.Л., Конвент Г., Шрайбер Ю. E17 - 11359

Коммутаторные и антикоммутаторные функции Грина в модели Изинга с поперечным полем

Обсуждается применение техники спектральных представлений в методе двухвременных функций Грина для модели Изинга с поперечным полем в приближении хаотических фаз. Вычислены коммутаторные и антикоммутаторные функции Грина. Корреляционные функции вычисляются с учетом особенности спектральной интенсивности при нулевой частоте. В данном подходе не удается полностью определить корреляционные функции, однако удается получить уравнение для параметра порядка на основе кинематических правил сумм. В отличие от предыдущих работ это уравнение лишено неоднозначностей. Численный расчет показывает, что корректное применение спектральных представлений в ПХФ приводит к нефизическим результатам.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1978

Aksionov V.L., Konvent H., Schreiber J. E17 - 11359

Commutator and Anticommutator Green Functions in the Ising Model with Transverse Field

The zero-frequency anomaly of spectral functions is analyzed in the framework of RPA, and a unique equation for the order parameter is derived using kinematic sum rules.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1978

The Ising model with transverse field $\mathcal{H} = -\Gamma\sum_n S_n^x - 1/2\sum_{n,m} J_{nm} S_n^z S_m^z$ is widely used in solid state physics[1]. Frequently, the considerations are based on the method of double-time Green functions [2,3] (GF), mainly working in RPA[4]. However, so far there are some troubles to obtain a unique equation for $\langle S_n^z\rangle$; by exploiting kinematic sum rules, as it is usually done for spin systems, various sum rules yield different equations for $\langle S_n^z\rangle$, ref. [4,5]. In the present letter it is shown that this ambiguity can be removed by a correct treatment of the zero-frequency anomaly of spectral functions [6-8], however, the resulting $\langle S_n^z\rangle$ exhibits unphysical behaviour. By using the spectral representation [2,3], correlation functions must be given as ($\alpha,\beta = x,y,z$)

$$\langle S_n^\alpha S_m^\beta\rangle = f_{nm}^{\alpha\beta} + C_{nm}^{\alpha\beta} + \langle S_n^\alpha\rangle\langle S_m^\beta\rangle$$

$$f_{nm}^{\alpha\beta} = i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\{G_{mn}^{(-)\beta\alpha}(\omega+i\epsilon) - G_{mn}^{(-)\beta\alpha}(\omega-i\epsilon)\}/(e^{\omega/kT}-1), \qquad (1)$$

$$\epsilon \to 0^+ ,$$

where $G_{nm}^{(-)\alpha\beta}(\omega)$ is the commutator GF (CGF). The physical reason for the existence of $C_{nm}^{\alpha\beta}$ is the presence of constants of motion for $\mathcal{H}$, ref. [7]. We note that this circumstance is well known [6-8], although the existence of $C_{nm}^{\alpha\beta}$ often escaped notice. Formally, $C_{nm}^{\alpha\beta}/\pi$ appears as the residue of a pole at $\omega = 0$ in the anticommutator GF (AGF)[8]. Solving the equation of motion for CGF and AGF in RPA[4] one obtains the following matrix for $f_g^{\alpha\beta} = \sum_{n-m} \exp(ig(R_n - R_m)) f_{nm}^{\alpha\beta}$

$$f_g = \begin{vmatrix} h_z\langle S^z\rangle A_g & i\langle S^z\rangle/2 & -h_z\langle S^x\rangle A_g \\ -i\langle S^z\rangle/2 & \epsilon_g^2\langle S^x\rangle A_g/\Gamma & i\langle S^x\rangle/2 \\ -h_z\langle S^x\rangle A_g & -i\langle S^x\rangle/2 & \Gamma\langle S^x\rangle A_g \end{vmatrix}, \qquad (2)$$

where $A_g = \mathrm{cth}(\epsilon_g/2kT)/2\epsilon_g$, $h_z = \sum_m J_{nm}\langle S_m^z\rangle$, and $\epsilon_g = (h_z^2+\Gamma^2-\Gamma\langle S^x\rangle J_g)^{1/2}$ is the energy of spin waves. The AGF yield

$$C_g^{\alpha y} = 0,\quad B_g C_g^{xz} = h_z C_g^{xx}, \quad B_g C_g^{zz} = h_z C_g^{xz}, \qquad (3)$$

where $B_g = \Gamma - \langle S^x\rangle J_g$, $C_g^{xz} = C_g^{zx}$. In the calculations we have used the relation $\Gamma\langle S^z\rangle = h_z\langle S^x\rangle$, which one can obtain from the condition $i\frac{d}{dt}\langle S_n^\alpha(t) S_m^\beta(t)\rangle = 0$ handled also in RPA. As can be seen the relations between $C_g^{\alpha\beta}$'s in eq. (3) also follow from the equilibrium conditions. To close the procedure, kinematic sum rules – $\langle (S_n^\alpha)^2\rangle = 1/4$ and $\langle S_n^z S_n^x\rangle = i\langle S_n^y\rangle/2 = 0$ – will be applied as usual. Taking yet into account $i\frac{d}{dt}\langle S_n^y(t)\rangle = 0$ and $2\langle S_n^y(t) i\frac{d}{dt} S_n^y(t)\rangle = \Gamma\langle S_n^x\rangle - \sum_m J_{nm}\langle S_n^z S_m^z\rangle$, where the right-hand side of this equation is determined by $G_{nn}^{(-)yy}(\omega)$, contrary to previous calculations (cf. [4,5]), we obtain $\langle (S_n^x)^2\rangle = \langle (S_n^y)^2\rangle = \langle (S_n^z)^2\rangle = 1/N\sum_g \epsilon_g^2 A_g/J_0$ $(T \le T_c)$. Consequently, $\langle S^z\rangle$ is given by the unique self-consistent equation

$$1/2 = 1/N\sum_g (\epsilon_g/J_0)\,\mathrm{cth}(\epsilon_g/2kT). \qquad (4)$$

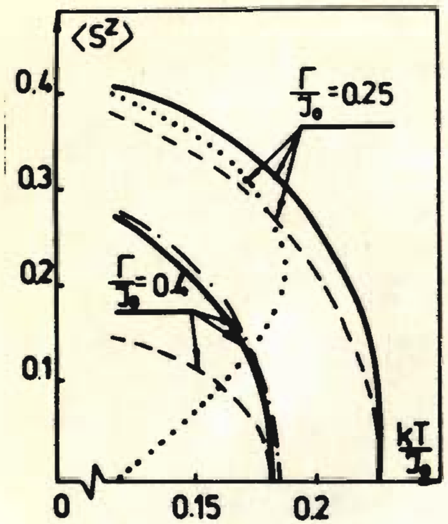

Fig. 1. $\langle S^z\rangle$ as a function of T according to Eq. (4) (–·–) to MFA (——), to (5) (– –), and to (4) (...).

Numerical calculations were done for the case, where $1/N\sum_g F(J_g)$ is approximated by $\int_{-1}^{1} d\bar{\omega}\,\rho_0(\bar{\omega}) F(J_0\bar{\omega})$, $\rho_0(\bar{\omega}) = (2/\pi)(1-\bar{\omega}^2)^{1/2}$. At $\Gamma/J_0 = 0.25$ the difference $\langle S^z\rangle^{RPA} - \langle S^z\rangle^{MFA}$ cannot be seen in our Fig. 1, but with increasing Γ/J_0 the deviations become larger and are positive at all T. Because RPA includes some kinds of fluctuations, $\langle S^z\rangle^{RPA}$ should be smaller than (or at least equal to) $\langle S^z\rangle^{MFA}$ but not opposite. Just such a behaviour is obtained within the diagrammatic approach for RPA[5] (dashed line in Fig. 1) and is also indicated by high- and low-temperature expansions (cf. [1]). Hence, in our opinion, the failure of our approach is not connected with the RPA decoupling procedure, but with the fact that we have applied sum rules for determination of the order parameter. Within a certain approximation they can be used as identities for the estimation of accuracy. The order parameter $\langle S^z\rangle$, however, must be found from thermodynamical conditions, i.e., from the minimum of the free energy.

The authors are indepted to Dr. N.M.Plakida for useful discussions.

REFERENCES

1. Stinchombe R.B. J.Phys., 1973, C6, p.2459-524.
2. Bogolubov N.N., Tjablikov S.V. Dokl Akad. Nauk SSSR, 1959, 126, p.126.
3. Zubarev D.N. Sov.Phys.Usp., 1960, 3, p.320.
4. Konvent H., Weller W. Acta Phys.Pol., 1972, A41, p.717.
5. Levitsky R.R., Stasjuk I.V. Ukrayin Fiz.Zh., 1974, 19, p.1331.
6. Kwok P.C., Schultz T.D. J.Phys., 1969, C2, p.1196.
7. Suzuki M. Physica, 1971, 51, p.271.
8. Ramos J.G., Gomes A.A. Nuovo Cim., 1971, 3A, p.441.

Received by Publishing Department
on March 1, 1978.