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К термодинамике спиновых систем в методе функций Грина

Методом двухвременных функций рассмотрена термодинамика модели Изинга с поперечным полем в приближении хаотических фаз. В отличие от обычного подхода параметр порядка определяется из минимума свободной энергии, а кинематические правила сумм используются для оценки точности приближения.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Aksionov V.L., Schreiber J. E17 - 11419

On the Thermodynamics of Spin Systems in the Green Function Method

The thermodynamics of the Ising model with transverse field is considered within RPA. Contrary to the conventional RPA, the order parameter is determined by the free energy while sum rules are used to check the accuracy.

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

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Applying the method of double-time Green functions (GF) [1,2] to spin systems, the equations for $\langle S^{\alpha}\rangle$ $(\alpha = x,y,z)$ are usually obtained from the kinematic sum rules. However, in such an approach the thermodynamic equilibrium cannot be ensured in general since the sum rules follow from operator identities rather than from equilibrium conditions. Besides, the accuracy of the used approximation is hard to estimate.

In the present letter a thermodynamically consistent procedure is proposed. With the help of GF the free energy F is calculated, from its minimum one gets $\langle S^{\alpha}\rangle$, and sum rules are employed for checking the accuracy of the approximation. We consider the Ising model with transverse field: $\mathcal{H} = -\Gamma\sum_n S_n^x - \frac{1}{2}\sum_{n,m} J_{nm} S_n^z S_m^z$, where the conventional RPA for GF yields an ambiguous result: the value of $\langle S^z\rangle$ exceeds that one in MFA for all temperatures contrary to the results obtained by the diagram technique [3,4].

To calculate F let us introduce $\mathcal{H}(\lambda) = \mathcal{H}_0 + \lambda(\mathcal{H} - \mathcal{H}_0)$, where $\mathcal{H}_0 = -\Gamma\sum_n S_n^x - \sum_n h_z S_n^z + \frac{1}{2}\sum_n h_z \langle S_n^z\rangle$, $h = \sum_m J_{nm}\langle S_m^z\rangle$. The order parameter $\sigma = \langle S_n^z\rangle$ is fixed and considered as a thermodynamical variable. Using the exact relation $\sum_n \langle S_n^y(t)\, i\frac{d}{dt} S_n^y(t)\rangle_\lambda = \langle \mathcal{H}\rangle_\lambda + \frac{1}{2}\Gamma N\langle S^x\rangle_\lambda$, F may be calculated by

$$F = F(\lambda = 0) + \int_0^1 d\lambda \Big[\sum_n \langle S_n^y(t)\, i \frac{d}{dt} S_n^y(t)\rangle_\lambda + N(\Gamma\langle S^x\rangle_\lambda + J_0\sigma^2)/2\Big], \qquad (1)$$

where $\langle ...\rangle_\lambda$ is the statistical average taken with $\mathcal{H}(\lambda)$.

With the help of the RPA results for GF /4/ and employing the spectral representation /1,2/ it can be shown that the integral in (1) vanishes, i.e., $F^{RPA} = F(\lambda = 0)$. Thus in this case F could be easily obtained and is given by that one of MFA. Possibly, this fact can be explained by the specific feature of the model where the interactions between transverse components of spin are absent, consequently, there is no contribution of collective dynamics to thermodynamic quantities. Hence $\delta F^{RPA}/\delta\sigma = 0$ leads to the equation for σ which is the same as in MFA /5/. Furthermore one can show that as well in the presence of an inhomogeneous field $H_m^\beta = \exp(i\vec{q}\vec{R}_m)H^\beta$ the integral in (1) does not contribute to F^{RPA}. That means that in RPA the isothermal susceptibility $\chi_{nm}^{T\alpha\beta} = \partial\langle S_n^\alpha\rangle/\partial H_m^\beta$ is given by the same expression as in MFA /5/.

Using these results, we are able to determine all the correlation functions $\langle S_n^\alpha S_m^\beta\rangle = \langle S_n^\alpha\rangle\langle S_m^\beta\rangle + f_{nm}^{\alpha\beta} + C_{nm}^{\alpha\beta}$, where $f_{nm}^{\alpha\beta}$ are obtained from the commutator GF /4/. $C_{nm}^{\alpha\beta}$ are some constants /6/ and as they cannot be completly derived from GF the thermodynamical relation $C_{nm}^{\alpha\beta} = k_B T(\chi_{nm}^{T\alpha\beta} - \chi_{nm}^{(-)\alpha\beta})$ must be applied, where $\chi_{nm}^{(-)\alpha\beta}$ is the isolated (Kubo-) susceptibility. It results in the equations:

$$C_{\vec{q}}^{zz} = h_z^2 b/\epsilon_{\vec{q}}^2 \left(1 - (\Gamma\langle S^x\rangle + h_z^2 b/k_B T)J_{\vec{q}}/h^2\right),$$
$$(\Gamma - \langle S^x\rangle J_{\vec{q}})C_{\vec{q}}^{zz} = h_z C_{\vec{q}}^{xz}, \quad (\Gamma - \langle S^x\rangle J_{\vec{q}})C_{\vec{q}}^{xz} = h_z C_{\vec{q}}^{xx}, \qquad (2)$$

where $4b = (1 - \mathrm{th}(h/2k_B T))$, $h^2 = \Gamma^2 + h_z^2$, $\langle S^x\rangle = \Gamma\sigma/h_z$, and $\epsilon_{\vec{q}}^2 = h_z^2 + \Gamma(\Gamma - \langle S^x\rangle J_{\vec{q}})$. It is of interest to note that the results agree with the ones of the diagrammatic approach handled also in RPA /3/.

The accuracy of the given RPA can now be checked by the relative deviation from the kinematic sum rules: $\Delta_{\alpha\alpha} = (4\langle(S_n^\alpha)^2\rangle - 1)$, $\Delta_{xz} = 4\langle S_n^z S_n^x\rangle$ ($\langle S_n^y\rangle = 0$) and from the dynamic one: $\Delta_p = 4i\frac{d}{dt}\langle S_n^y(t)\rangle$ (Fig.1). Numerical calculations were done for the model case, where $1/N\sum_{\vec{q}} f(J_{\vec{q}}) = \int_{-1}^{1} dx\,\rho(x) f(J_0 x)$, $\rho(x) = 2/\pi\sqrt{(1 - x^2)}$.

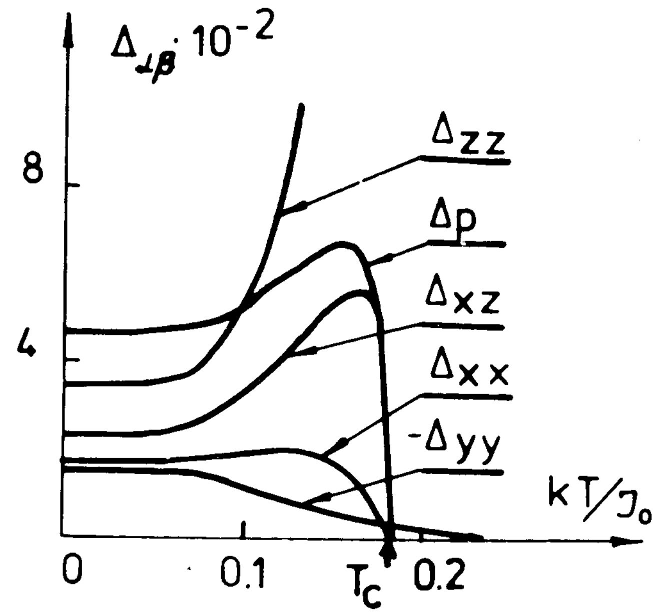

Fig.1. Temperature dependent deviations from sum rules for $\Gamma/J_0 = 0.4$.

As it is generally known, RPA poorly accounts for the longitudinal correlations, particular at T_c (Fig.2). Nevertheless, one can regard the proposed RPA as a good interpolation scheme to describe both the collective dynamics and the thermodynamics of the considered model.

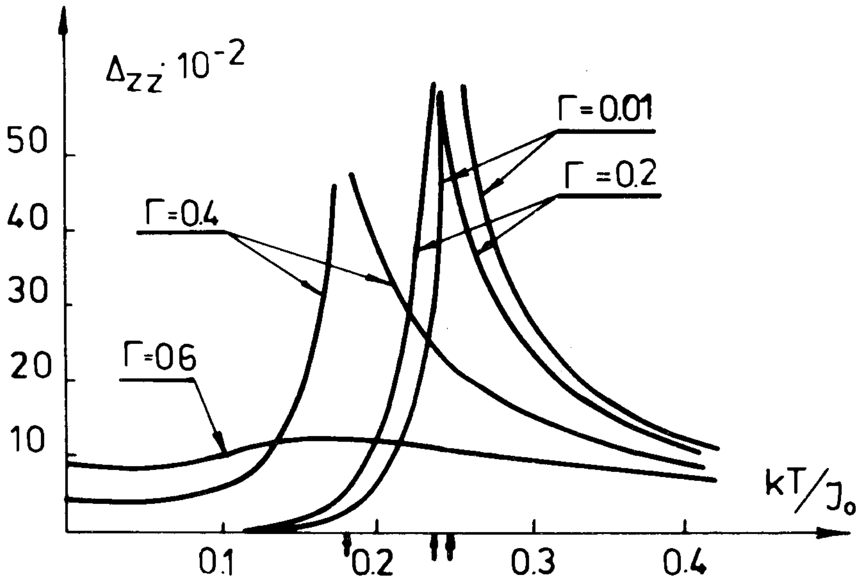

Fig.2. The deviation $\Delta_{zz} = 4\langle (S^z)^2 \rangle - 1$ versus temperature.

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