Functional integration and dynamics of a Heisenberg ferromagnet at high temperatures

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(Submitted 3 July 1986)
Zh. Eksp. Teor. Fiz. **91**, 2313–2318 (December 1986)

We obtain a functional representation for the different-time spin correlators of a Heisenberg ferromagnet at high temperatures. Using this we calculate the asymptotic behavior of the spin correlation functions at small times.

1. INTRODUCTION

1. Attempts to describe the high-temperature dynamics of a Heisenberg ferromagnet from first principles, starting from the exchange Hamiltonian H, have been made by a large number of authors. A detailed survey of the corresponding theoretical results is contained in the experimental Ref. 1. In the limit of an infinite temperature T the different-time spin correlator $C^{\alpha\beta}(\mathbf{r},t)$ is define as

$$C^{\alpha\beta}(\mathbf{r},t)=\mathrm{Sp}(e^{itH}S_{\mathbf{R}}^{\alpha}e^{-itH}S_{\mathbf{R}+\mathbf{r}}^{\beta}). \tag{1.1}$$

Here $\mathbf{r}$ is the coordinate of the lattice site, α and β are the indexes of the components, and H is the Heisenberg Hamiltonian

$$H=-{}^1/_2 J_{ij}\mathbf{S}_i\mathbf{S}_j,\quad \mathbf{S}_i\equiv\mathbf{S}_{\mathbf{r}i} \tag{1.2}$$

(summation over repeated indexes is implied). The boundedness of the spin operators guarantees the existence of the trace (1.1). Thanks to rotational symmetry,

$$C^{\alpha\beta}(\mathbf{r},t)=\delta_{\alpha\beta}C(\mathbf{r},t).$$

2. As the basic method for evaluating the average (1.1) in the majority of the papers all possible schemes for decoupling the correlators have been used, amongst them very refined ones.[2] The exception is the paper by Lazuta and Maleev,[3] where a model considerably different from Ref. 2 was considered, using a diagram technique. Uncontrollable approximations contained in such an approach led to statements either about the exponential damping of single-site correlations[2] or about the existence of quasi-particles.[4] The usual regular methods (diagram techniques) are of little use in this case since the basic building blocks are propagators of weakly damped elementary excitations. On the other hand, Kubo's formula used by Blume and Hubbard[2] is inapplicable to non-commuting operators.

3. The object of the present paper is the calculation of the asymptotic behavior of the function $C(\mathbf{r},t)$ for $Jt\ll 1$ (and arbitrary r) using a functional integral for spin systems.[6] The direct expansion of $\exp(itH)$ in (1.1) in powers of t leads to an ultra-local series in r for $C(\mathbf{r},t)$, which indicates an (*a priori* obvious) non-analyticity of the function $C(\mathbf{r},t)$ at $t=0$. The functional representation of Ref. 6 is convenient only in the low–temperature phase, owing to the explicit asymmetry of the field variables. Following the prescription proposed in Ref. 6 we get in what follows a rotationally invariant functional representation for $C(\mathbf{r},t)$ and we find the main asymptotic behavior as $t\to 0$. Unfortunately we were not able to calculate the most interesting asymptotic behavior as $t=\infty$ (spin diffusion). This difficulty is not particular to spin systems.

2. FUNCTIONAL REPRESENTATION

Writing e^{itH} in the form $(e^{it\varepsilon H})^{1/\varepsilon}$, $\varepsilon\to 0$ and using the formula (see, e.g., Ref. 7) [1)]

$$\exp\left(\frac{i}{2}\varepsilon tJ_{ij}\mathbf{S}_i\mathbf{S}_j\right)$$

$$=N'\int\prod_i d\varphi_i\exp\left(\frac{i}{2}\varepsilon tJ_{ij}^{-1}\varphi_i\varphi_j+i\varepsilon t\varphi_j\mathbf{S}_j\right), \tag{2.1}$$

where J_{ij}^{-1} is the matrix which is the inverse of j_{ij}, N′ is a normalization factor, we can express $C^{\alpha\beta}(\mathbf{r}_i-\mathbf{r}_j t)$ in terms of the functional $Q(h)$:

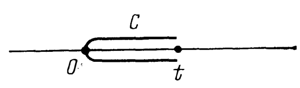
$$Q(\mathbf{h})=N\int D\varphi^{(1)}D\varphi^{(2)}\exp\left(\frac{i}{2}\int_C\varphi_i(t')J_{ij}^{-1}\varphi_j(t')\,dt'\right)$$

$$\times\prod_i\mathrm{Sp}\left\{T_C\exp\left[i\int_C(\varphi_i(t')+\mathbf{h}_i(t'))\mathbf{S}_i\,dt'\right]\right\}, \tag{2.2}$$

$$D\varphi\equiv\prod_i\prod_{t'}d\varphi(t',\mathbf{r}_i),$$

$$C^{\alpha\beta}(\mathbf{r}_i-\mathbf{r}_j,t)=\left.\frac{\partial^2Q(\mathbf{h})}{\partial h_{\alpha}^{(1)}(r_i)\,\partial h_{\beta}^{(2)}(r_j)}\right|_{h=0}, \tag{2.3}$$

where the contour C is



(2.4)

[the indexes (1) and (2) refer, respectively, to the lower and the upper branches] and

$$\mathbf{h}_n(t')=\mathbf{h}^{(1)}(r_n)\delta(t'-t)+\mathbf{h}^{(2)}(r_n)\delta(t'). \tag{2.5}$$

The T_C sign indicates the ordering of the operator exponent along the contour C.

Making the substitution $\varphi\to\varphi-\mathbf{h}$ and neglecting terms which do not contribute to (2.3) we get the expression

$$Q(\mathbf{h})=\int D\varphi^{(1)}D\varphi^{(2)}\exp\left\{i\int_0^t dt'(\varphi_i^{(1)}J_{ij}^{-1}\varphi_j^{(1)}-\varphi_i^{(2)}J_{ij}^{-1}\varphi_j^{(2)})\right.$$

0038-5646/86/121373-03$04.00

$$+\frac{1}{2}\mathbf{h}_i^{(1)}J_{ij}^{-1}[\boldsymbol{\varphi}_j^{(1)}(t)+\boldsymbol{\varphi}_j^{(2)}(t)]$$

$$+\frac{1}{2}\mathbf{h}_i^{(2)}J_{ij}^{-1}(\boldsymbol{\varphi}_j^{(1)}(0)+\boldsymbol{\varphi}_j^{(2)}(0))\Big\}$$

$$\times\prod_i \mathrm{Sp}\left\{T_C\exp\left(i\int_C \boldsymbol{\varphi}_i\mathbf{S}_i\,dt'\right)\right\}. \quad (2.6)$$

The calculation of T_C operating on the exponent as a functional of the field $\boldsymbol{\varphi}(t')$ reduces already in the particular case of spin $\frac{1}{2}$ to solving a Schrödinger equation in an arbitrary potential and is impossible in its general form. However, (see also Ref. 6) in the framework of the functional formalism one can avoid this difficulty. We introduce the operator $A(t)$:

$$A(t)=T_C\exp\left[i\int_C\boldsymbol{\varphi}(t')S\,dt'\right]$$

$$=T\exp\left[i\int_0^t\boldsymbol{\varphi}^{(1)}(t')S\,dt'\right]\tilde{T}\exp\left[-i\int_0^t\boldsymbol{\varphi}^{(2)}(t')S\,dt'\right], \quad (2.7)$$

where T and $\widetilde{T}$ indicate, respectively, the usual chronological and anti-chronological ordering. The operator $A(t)$ is determined by the differential equation

$$-i\dot{A}(t)=\boldsymbol{\varphi}^{(1)}(t)\mathbf{S}A(t)-A(t)\boldsymbol{\varphi}^{(2)}(t)\mathbf{S} \quad (2.8)$$

and the initial condition $A(0)=1$. We introduce explicitly the given operator $G(t)$:

$$G(t)=\exp\left\{i\int_0^t[\boldsymbol{\rho}^{(1)}(t')-\boldsymbol{\rho}^{(2)}(t')]\mathbf{S}\,dt'\right\} \quad (2.9)$$

and differentiate it with respect to time

$$i\dot{G}(t)=\int_0^1 d\tau\exp(i\tau\boldsymbol{\zeta}\mathbf{S})(\boldsymbol{\rho}^{(1)}-\boldsymbol{\rho}^{(2)})\mathbf{S}\exp[i(1-\tau)\boldsymbol{\zeta}\mathbf{S}]$$

$$=U_1(t)G(t)-G(t)U_2(t). \quad (2.10)$$

Here

$$\boldsymbol{\zeta}(t)=\int_0^t dt'[\boldsymbol{\rho}^{(1)}(t')-\boldsymbol{\rho}^{(2)}(t')],$$

$$U_1(t)=\int_0^1 d\tau\exp(i\tau\boldsymbol{\zeta}\mathbf{S})\boldsymbol{\rho}^{(1)}\mathbf{S}\exp(-i\tau\boldsymbol{\zeta}\mathbf{S}), \quad (2.11)$$

$$U_2(t)=\int_0^1 d\tau\exp(-i\tau\boldsymbol{\zeta}\mathbf{S})\boldsymbol{\rho}^{(2)}\mathbf{S}\exp(i\tau\boldsymbol{\zeta}\mathbf{S}).$$

Noting that under the integral sign in (2.11) there appeared spin rotation operators we get immediately

$$U_1(t)=\boldsymbol{\eta}_1(t)\mathbf{S},\quad U_2(t)=\boldsymbol{\eta}_2(t)\mathbf{S},$$

$$\boldsymbol{\eta}_1(t)=\boldsymbol{\rho}^{(1)}\frac{\sin|\boldsymbol{\zeta}|}{|\boldsymbol{\zeta}|}+\boldsymbol{\zeta}\frac{(\boldsymbol{\zeta}\boldsymbol{\rho}^{(1)})}{\boldsymbol{\zeta}^2}\left(1-\frac{\sin|\boldsymbol{\zeta}|}{|\boldsymbol{\zeta}|}\right)$$
$$+\frac{1}{\boldsymbol{\zeta}^2}[\boldsymbol{\zeta}\boldsymbol{\rho}^{(1)}](1-\cos|\boldsymbol{\zeta}|), \quad (2.12)$$

$$\boldsymbol{\eta}_2(t)=\boldsymbol{\rho}^{(2)}\frac{\sin|\boldsymbol{\zeta}|}{|\boldsymbol{\zeta}|}+\boldsymbol{\zeta}\frac{(\boldsymbol{\zeta}\boldsymbol{\rho}^{(2)})}{\boldsymbol{\zeta}^2}\left(1-\frac{\sin|\boldsymbol{\zeta}|}{|\boldsymbol{\zeta}|}\right)$$
$$-\frac{1}{\boldsymbol{\zeta}^2}[\boldsymbol{\zeta}\boldsymbol{\rho}^{(2)}](1-\cos|\boldsymbol{\zeta}|).$$

The transition in the functional integral (2.6) to the integration variables $\boldsymbol{\rho}(t')$ through the formulae

$$\boldsymbol{\varphi}^{(1)}(t')=\boldsymbol{\eta}_1(t'),\quad \boldsymbol{\varphi}^{(2)}(t')=\boldsymbol{\eta}_2(t') \quad (2.13)$$

puts T_c—the ordering constant in (2.7)—in the form (2.9). On can easily calculate the Jacobian of the change (2.13) and it is equal to

$$J=4\left[\prod_{t'=0}^{t'=t}\frac{1}{\boldsymbol{\zeta}^2(t')}(1-\cos|\boldsymbol{\zeta}(t')|)\right]^2. \quad (2.14)$$

The explicit expression for the functional integral in the ρ-variables is cumbersome and we shall not write it down. We merely note that the substitution (2.13) is strongly nonlocal in time.

3. ASYMPTOTIC BEHAVIOR AS $t\to 0$

1. To calculate the main asymptotic behavior as $t\to 0$ we can put (the index of the site number is temporarily dropped)

$$\boldsymbol{\rho}^{(1)}(t')=\boldsymbol{\rho}^{(1)}=\mathrm{const},$$
$$\boldsymbol{\rho}^{(2)}(t')=\boldsymbol{\rho}^{(2)}=\mathrm{const} \quad (3.1)$$

and we can consider $\boldsymbol{\rho}^{(1)}$ and $\boldsymbol{\rho}^{(2)}$ as independent integration variables. We have here made the rather natural assumption that our integral is concentrated on trajectories of a nonzero Hölder class, i.e., as $t_1\to t_2$

$$|\boldsymbol{\rho}(t_1)-\boldsymbol{\rho}(t_2)|\leqslant\mathrm{const}|t_1-t_2|^\alpha,\ \alpha>0.$$

For instance, for the simple case of a Brownian particle one can prove that $\alpha=\geqslant\frac{1}{2}$.[8] The first non-vanishing term in $\boldsymbol{\zeta}(t')$ is:

$$\boldsymbol{\zeta}(t')=t'(\boldsymbol{\rho}^{(1)}-\boldsymbol{\rho}^{(2)}), \quad (3.2)$$

the Jacobian is

$$J=1+O(t^2),$$

and the change of variables takes the form

$$\boldsymbol{\varphi}^{(1)}(t')=\boldsymbol{\rho}^{(1)}+\frac{t'}{2}[\boldsymbol{\rho}^{(1)}\boldsymbol{\rho}^{(2)}]+O(t^2),$$
$$\boldsymbol{\varphi}^{(2)}(t')=\boldsymbol{\rho}^{(2)}-\frac{t'}{2}[\boldsymbol{\rho}^{(1)}\boldsymbol{\rho}^{(2)}]+O(t^2). \quad (3.3)$$

We introduce new variables $\boldsymbol{\pi}$ and $\boldsymbol{\Phi}$:

$$\boldsymbol{\pi}=\boldsymbol{\rho}^{(1)}-\boldsymbol{\rho}^{(2)},\quad \boldsymbol{\Phi}=\boldsymbol{\rho}^{(1)}+\boldsymbol{\rho}^{(2)}. \quad (3.4)$$

Writing the trace of the operator (2.9) in the form

$$\mathrm{Sp}\exp\left\{i\int_0^t dt'(\boldsymbol{\rho}^{(1)}-\boldsymbol{\rho}^{(2)})\mathbf{S}\right\}=\exp\{g_S(t|\boldsymbol{\pi}|)\}$$
$$=\mathrm{const}\exp(-Dt^2\boldsymbol{\pi}^2/2), \quad (3.5)$$

where

$$g_S(x)=\sin[(S+{}^1/_2)x]/\sin(x/2),\quad D=g''_S(0), \tag{3.6}$$

we get asymptotic form of the functional integral $Q(\mathbf{h})$ in the form

$$Q(\mathbf{h})=N\int D\boldsymbol{\pi}\, D\boldsymbol{\Phi}\exp\Big\{it\boldsymbol{\pi}_iJ_{ij}^{-1}\boldsymbol{\Phi}_j+\frac{it^2}{4}\cdot\boldsymbol{\Phi}_iJ_{ij}^{-1}[\boldsymbol{\Phi}_j\boldsymbol{\pi}_j]$$
$$-\frac{1}{2}Dt^2\boldsymbol{\pi}_i\boldsymbol{\pi}_i+\mathbf{h}_iJ_{ij}^{-1}\boldsymbol{\Phi}_j\Big\}, \tag{3.7}$$
$$\mathbf{h}_i={}^1/_2(\mathbf{h}_i^{(1)}+\mathbf{h}_i^{(2)}).$$

Performing the linear substitution

$$\boldsymbol{\Phi}_i=J_{ij}\boldsymbol{\sigma}_j \tag{3.8}$$

and carrying out the Gaussian integration over the variable $\boldsymbol{\pi}$ we are led to the final expression for $Q(h)$:

$$Q(\mathbf{h})=\tilde{N}\int D\boldsymbol{\sigma}\exp\Big(-\frac{1}{2D}\sum_i\boldsymbol{\sigma}_i^2-\frac{t^2}{8}[\boldsymbol{\sigma}_iJ_{ij}\boldsymbol{\sigma}_j]^2+\mathbf{h}_i\boldsymbol{\sigma}_i\Big) \tag{3.9}$$

($\tilde{N}$ is the new normalization factor). We note some features of Eq. (3.9). Firstly, the integral (3.9) is Euclidean although it generates [in the sense of (2.3)] correlation functions in real time. This corresponds to the essence of the fact as there should be no propagating excitation as $T=\infty$. Secondly, the undesirable terms in the action containing odd powers in T cancelled in the integration over $\boldsymbol{\pi}$. Finally, the x expansion of (3.9) in t^2 reproduces the ultra-local expansion for (1.1).

2. Being interested in the coarse-scale structure of the correlations we go in (3.9) over to the continuum limit

$$Q(\mathbf{h})=\tilde{N}\int D\boldsymbol{\sigma}\exp\Big\{-\int d^3\mathbf{r}\Big(\frac{1}{2D}\boldsymbol{\sigma}^2+\alpha^2\frac{t^2}{8}[\boldsymbol{\sigma},\Delta\boldsymbol{\sigma}]^2+\mathbf{h}\boldsymbol{\sigma}\Big)\Big\}, \tag{3.10}$$

where α is connected with the exchange frequency $\omega_{\rm ex}$:

$$J(k)=J(0)-\omega_{ex}(\mathbf{k}a)^2 \tag{3.11}$$

as follows:

$$\alpha=\omega_{ex}a^{7/2}. \tag{3.12}$$

Here a is the size of the elementary cell in the lattice. The mass operator is on the single-loop level equal to (cutoff mementum $\Lambda=\pi/a$):

$$\Sigma^{(1)}(\mathbf{k})=D^2\omega_{ex}^2t^2\Big[\frac{16\pi^5}{7}-\frac{8\pi^3}{5}(\mathbf{k}a)^2+\pi(\mathbf{k}a)^4\Big]. \tag{3.13}$$

For the correlation function $C^{\alpha\beta}(r,t)$ we get the expression

$$C^{\alpha\beta}(\mathbf{r},t)=Da^3\delta_{\alpha\beta}\int\frac{d^3\mathbf{k}}{(2\pi)^3}e^{i\mathbf{kr}}\frac{1}{1+\Sigma^{(1)}(\mathbf{k})}\xrightarrow{t\to 0}$$
$$\to\delta_{\alpha\beta}\Big(\frac{2}{\pi}\Big)^{1/2}\frac{a}{\pi r\omega_{ex}t}\exp\Big(-\tilde{D}\frac{r}{a(\omega_{ex}t)^{1/2}}\Big)\sin\Big[\tilde{D}\frac{r}{a(\omega_{ex}t)^{1/2}}\Big].$$
$$\tilde{D}=(2/D^2\pi)^{1/4}. \tag{3.14}$$

The Dyson summation for the propagator $C(\mathbf{r},t)$ is in this case justified as it takes into account to each order in t^2 terms of the highest order in the derivative of $\delta(\mathbf{r})$ (in the continuum limit).

I am grateful to V. B. Cherepanov for many discussions and useful hints and to V. I. Belicher, V. S. L'vov, and E. V. Podivilov for useful advice. I am pleased to thank D. E. Khmel'nitskiĭ for his interest in this work.

[1)]One can in the limit as $\varepsilon\to 0$ neglect the fact that the spin operators in Eq. (2.1) do not commute.

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Translated by D. ter Haar