Short-duration limit of the correlation functions of two widely separated spins at high temperatures

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The first term of the power series in the time is found for the correlation function of two spins separated by a large distance for the case of an anisotropic Heisenberg paramagnet at high temperatures.

An important role is played in the dynamics of spin systems at high temperatures by the temporal correlation functions

$$\Gamma_\alpha(\mathbf{r},t)=\frac{\mathrm{Sp}\{S_i^\alpha(t)S_j^\alpha\}}{\mathrm{Sp}\,(S_i^\alpha)^2}, \tag{1}$$

where $S_i^\alpha(t)$ is the αth component (or the αth projection, where $\alpha=x,y,z$) of the spin at site i (with radius vector $\mathbf{r}_i$) in the Heisenberg representation, and $\mathbf{r}=\mathbf{r}_i-\mathbf{r}_j$. The correlation function has been calculated through the solution of an integral equation in Refs. 1–5 and many other places. After Laplace transforms are taken, and a switch is made to reciprocal-lattice vectors $\mathbf{k}$, the solution can be written in the form

$$\Gamma_\alpha(\mathbf{k},p)=[p-G_\alpha(\mathbf{k},p)]^{-1}, \tag{2}$$

where p is the transformation parameter and $G_\alpha(\mathbf{k},p)$ is the kernel of the equation (it is also called the "memory function" or "mass operator"). The numerous studies which have been carried out differ primarily in the approximate method used to find this kernel. In Refs. 1–5, the thrust of the effort was on calculating the spectra of correlation functions and their behavior after a fairly long time.

Kolokolov[6] has recently pointed out another interesting limit for functions (1): the short-duration limit, i.e., $t\to 0$, $r\to\infty$. The result which Kolokolov found for $\Gamma_\alpha(\mathbf{k},t)$ was derived by a functional-integration method for spin systems without the use of general expression (2). In the present paper we find correlation function (1) in this limit by working from (2). This method is considerably simpler than that proposed in Ref. 6 and is easy to check. In particular, it can be checked against the known exact result for a one-dimensional XY chain.[7] This ability to check the results is not a minor matter, in view of the discrepancies among the results.

We thus consider a system of spins at the sites of a cubic lattice with an anisotropic Heisenberg Hamiltonian

$$\mathcal{H}=\sum_{i\neq j}(\mathcal{J}_{ij}{}^x S_i{}^x S_j{}^x+\mathcal{J}_{ij}{}^y S_i{}^y S_j{}^y+\mathcal{J}_{ij}{}^z S_i{}^z S_j{}^z), \tag{3}$$

where $\mathcal{J}_{ij}^\alpha=\mathcal{J}^\alpha$ is an exchange integral. This integral is zero except in the case of nearest neighbors. We then calculate correlation functions (1) as $t\to 0$. (In the calculations below, we will write the specific equations for the z projection, since the equations for the two other projections can be found easily through a cyclic interchange of projection indices.) We know[8,9] that there exists a certain neighborhood of the point $t=0$ in which functions (1) have no singular points and can be expanded in converging series in positive powers of the time:

$$\Gamma_z(\mathbf{r},t)=\sum_{n=m}^{\infty}M_{2n}{}^z(\mathbf{r})\frac{t^{2n}}{(2n)!},$$
$$G_z(\mathbf{r},t)=\sum_{n=m}^{\infty}G_{2n}{}^z(\mathbf{r})\frac{t^{2n-2}}{(2n-2)!}. \tag{4}$$

If $\mathbf{r}$ is large, and for a nearest-neighbor interaction, the two series in (4) begin with terms with a high power that can be expressed in terms of the number of steps (links) in the shortest path which goes through nearest neighbors from site $\mathbf{r}_i$ to site $\mathbf{r}_j=\mathbf{r}_i+\mathbf{r}$:

$$m=r_x+r_y+r_z.$$

Here r_x, r_y, r_z are the projections of the vector $\mathbf{r}$ onto the principal axes of the cubic lattice and expressed in units of the lattice constant. On a cubic lattice, there are N_m such paths:

$$N_m=\frac{m!}{r_x!r_y!r_z!}. \tag{5}$$

Since we are interested in the limit $t\to 0$, we will retain in (4) only the first terms of the series, which have the lowest powers of the time for the given $\mathbf{r}$ and which correspond to the shortest paths. The relationship between the coefficients of the two series in (4) is easily established with the help of (2):

$$M_{2m}^z(\mathbf{r})=G_{2m}^z(\mathbf{r})+\sum G_{2m_1}^z(\mathbf{l}_1)G_{2(m-m_1)}^z(\mathbf{r}-\mathbf{l}_1)+\dots$$
$$+\sum G_2{}^z(\mathbf{l}_1)G_2{}^z(\mathbf{l}_2)\dots G_2{}^z(\mathbf{r}-\mathbf{l}_1-\mathbf{l}_2-\dots-\mathbf{l}_{m-1}). \tag{6}$$

The shortest path to the point $\mathbf{r}$ is broken up into two regions in the second term in (6). These two regions are $\mathbf{l}_1$ and $\mathbf{r}-\mathbf{l}_1$. In the third term, the shortest path is broken up into three regions: $\mathbf{l}_i$, $\mathbf{l}_2$, $\mathbf{r}-\mathbf{l}_1-\mathbf{l}_2$ (etc.). A summation is carried out over all possible positions of the vectors $\mathbf{l}_1$, $\mathbf{l}_2$,..., $\mathbf{l}_{m-1}$.

We turn now to the calculation of the coefficients in (6). The equation of motion of the spins is taken in tensor form:

$$\frac{d}{dt}\mathbf{S}_i(t)=\hat{h}_i(t)\mathbf{S}_i(t)=\sum_\alpha h_i{}^\alpha(t)\hat{\varepsilon}^\alpha\mathbf{S}_i(t), \tag{7}$$

where $\hat{\varepsilon}^\alpha$ is a unit axial tensor, and

$$h_i{}^\alpha(t)=2\sum_j\mathcal{J}_{ij}{}^\alpha S_j{}^\alpha(t) \tag{8}$$

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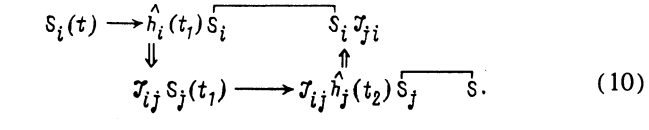
and is the α-th projection of the local magnetic field created by the surroundings at site i. An advantage of writing the equation of motion in this way is that this equation is the same in form for both ordinary vectors $\mathbf{S}_i$ and vector operators in the quantum-mechanical case. Solving Eq. (7) by an iterative method, we find the series

$$\mathbf{S}_i(t)=\mathbf{S}_i+\int_0^t \hat{h}_i(t_1)\mathbf{S}_i dt_1+\int_0^t dt_1\int_0^{t_1} dt_2\,\hat{h}_i(t_1)\hat{h}_i(t_2)\mathbf{S}_i+\dots\ . \tag{9}$$

In terms of local fields, the correlation function $\Gamma_\alpha(\mathbf{r},t)$ in (1) determines the contribution of the field from spin j to the resultant flip of spin i (and vice versa). The simplest correlation, with $m=1$, is formed between nearest neighbors. Series (4) for this correlation function begins with a quadratic term. To find it, we substitute the second term of (9) into (1). In expression (8) for the field, we again adopt as $S_j^\alpha(t)$ the second term of the corresponding iterative series, in which it is sufficient to retain only the field from spin i in the original orientation. For clarity, we diagram this procedure:

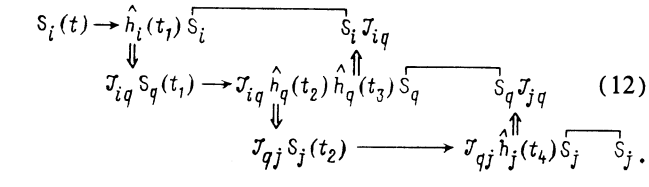


(10)

When the trace is taken, nonvanishing results come from the squared projections $(S_i^\alpha)^2$ and $(S_j^\alpha)^2$, the formation of which is indicated by the upper bracket in this diagram. We thus find

$$\Gamma_z(\mathbf{r},t)=\tfrac{4}{3}S(S+1)\mathcal{J}_{ij}^x\mathcal{J}_{ij}^y t^2+O(t^4). \tag{11}$$

For the correlation function of spin i with the next-nearest neighbor, the first term in series (4) has a fourth power of the time. The corresponding coefficient [$m=2$ in (6)] is the sum of two parts. The second of the two is the product of two of the nearest-neighbor coefficients found above, while the first is new. To single it out, we write the time dependence of the fields in diagram form:



(12)

Guided by (12), we find for paths $i\to q\to j$: the following expression for the first part:

$$2[\tfrac{4}{3}S(S+1)]^2\mathcal{J}_{iq}^x\mathcal{J}_{iq}^y\mathcal{J}_{qj}^x\mathcal{J}_{qj}^y\frac{t^4}{4!}. \tag{13}$$

If the arrows pointing up and down on the product $\hat{h}_q(t_2)\hat{h}_q(t_3)$ in (12) are interchanged, i.e., if the contribution of spin i is singled out from $\hat{h}_q(t_2)$, and that of spin j from $\hat{h}_q(t_3)$, we find two diagrams of the type in (10) connected in series. The contribution from that process is represented by the second part of (6). Taking the higher-order terms of iterative series (9), we can also construct other diagrams,[10] but for given values of i and j they lead to higher powers of the time, so we will ignore them.

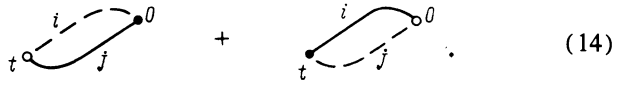
An expression for $G_4^z(\mathbf{r})$ can be found by dividing (13) by $t^4/4!$ This coefficient stands in front of different powers of the time in the two series in (4). This result is not surprising, since the correlation function in the integral equation is expressed in terms of a double integral of the memory function. When we find the latter from diagrams (10), (12), etc., we will thus not carry out an integration over the outermost time variables.

Replacing $\hat{h}_j(t_4)S_j$ on the last line of diagram (12) by the next term of the iterative series, $\hat{h}_j(t_4)\hat{h}_j(t_5)S_j$, we can tack on another stage; i.e., we can derive an expression for $G_6^z(\mathbf{r},t)$ for a correlation which is conveyed from i to j through two intermediate spins in succession. This procedure can be continued by adding on yet other new stages. At first glance this method looks complicated, but it actually is not. In the first place, the structure of the original coefficients in (6) is such that one can separate the spin and lattice variables. Specifically, we can choose one of the shortest paths which leads from i to j, evaluate the coefficient which is determined by the interaction [see (3)] of the spins at the sites of this path, move on to another path, and sum the results. Under these conditions the result for an individual path,

$$\overline{G}_{2m^z}(t)=\frac{\overline{G}_{2m^z}t^{2m-2}}{(2m-2)!},$$

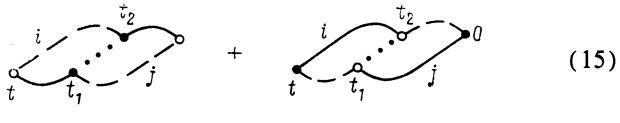
depends on only the number of steps (m), not on the position in the lattice.

The procedure outlined above for calculating $\overline{G}_{2m}^z(t)$ takes a particularly simple form when we represent it by a time diagram in accordance with the following rules.[10,11] We depict the spins participating in the interaction by lines, and the interaction itself (a flip of one of the spins in the field of its neighbor) by a vertex, i.e., by a point at which lines intersect. We depict a given projection of a spin at a site in the following way: x by a solid line, y by a dashed line, and z by a dotted line. We depict by ○ a vertex corresponding to $\mathcal{J}^x[\frac{4}{3}S(S+1)]^{1/2}$, and by ● a vertex corresponding to $\mathcal{J}^y[\frac{4}{3}S(S+1)]^{1/2}$. At the $2m$ vertices of each diagram we place the time variables t_0 ($=t$), t_1, t_2,..., t_{2m-2}, t_{2m-1} ($=0$) from left to right. Over these variables (except the outermost) we carry out an integration between limits set by the neighboring vertices on the same line. On the diagrams, the outermost lines correspond to the spins in the initial and final sites (i and j), while the sequence of interior lines corresponds to the sequence of spins at the intermediate sites on the selected path. For example, the two terms in (10) which contribute to (11) are represented in the same way by the diagram:



(14)

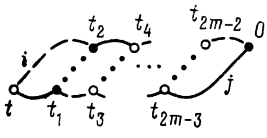
The two terms in (12) and (13), on the other hand, are represented by the two diagrams



(15)

which, although differing in the form of their projections,

are given by identical explicit expressions. In the general case of a correlation which is conveyed along a chain of m units, $\overline{G}^{z}_{2m}(t)$ is represented, as in (14) and (15), by the sum of two diagrams which convert into each other after the x lines and x vertices are interchanged with the y lines and the y vertices, respectively. Here is one of them for odd values of m:



(16)

For even values of m we should replace the x projections by y projections, and vice versa, in the second half of diagram (16) [beyond the ellipsis (...)]. Explicit expressions, identical for the two diagrams, can easily be found from (16) in accordance with the rules formulated above. Combining these expressions, we find

$$\overline{G}_{2m}{}^{z}(t)=g^{m}\int dt_1\int dt_2\ldots\int dt_{2m-2}, \tag{17}$$

where the integration limits are chosen in accordance with the rules, and $g=4/3S(S+1)\mathcal{J}^{x}\mathcal{J}^{y}$.

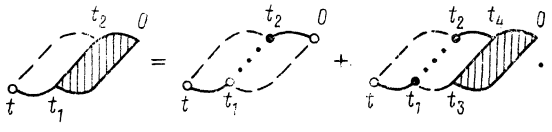
A direct integration in (17) becomes complicated at large values of m, so we will take a different approach. From these functions we form the series

$$G(t)={}^{1}/_{2}\sum_{m=1}^{\infty}\overline{G}_{2m}{}^{z}\frac{t^{2m-2}}{(2m-2)!}, \tag{18}$$

which is a series in the number of shortest-path steps. We denote by $G(t,t_2)$ the sum of the series without its first term before the integration over the third vertex [we have in mind the diagram representation of its terms in (14)–(16)]. We obviously have

$$G(t)=g+\int_{0}^{t}G(t,t_2)\,dt_2. \tag{19}$$

Using the diagram form of series (18), we see that the following equation holds for the function $G(t,t_2)$:



(20)

Alternatively, in explicit form, we have

$$G(t,t_2)=g^{2}\int_{t_2}^{t}dt_1\left[1+\int_{0}^{t_2}dt_4G(t_1,t_4)\right]. \tag{21}$$

Strictly speaking, we would have to introduce two functions $G(t,t_2)$, which differ in the positions of the x and y projections; we would have to sum the first diagrams and the second diagrams in (14)–(16) separately. However, since the series are equal in the limit under consideration here, we can treat them as if they were the same. Writing the function $G(t,t_2)$ as a series in powers of the time variables, and finding the coefficients of this series from Eq. (21), we obtain

$$G(t,t')=(t-t')\sum_{n=0}^{\infty}g^{n+2}\frac{(tt')^{n}}{n!(n+1)!}. \tag{22}$$

From (19) we then find

$$G(t)=\sum_{n=0}^{\infty}g^{n+1}\frac{t^{2n}}{n!(n+1)!}=\frac{gI_1(2tg^{1/2})}{t}, \tag{23}$$

where $I_1(t)$ is the Bessel function of imaginary argument of index one. Finally, comparing (18) with (23), we find

$$\overline{G}^{z}_{2m}=2[{}^{1}/_{3}S(S+1)\mathcal{J}^{x}\mathcal{J}^{y}]^{m}\frac{(2m-2)!}{m!(m-1)!}. \tag{24}$$

Once the coefficients $\overline{G}^{z}_{2m}(\mathbf{r})$ have been found on the same shortest path, we can find all the coefficients for the correlation functions $\overline{\Gamma}_{z}(\mathbf{r},t)$ from (6), by substituting (24) into the latter and carrying out the summation. The result is found most easily by substituting $2G(t)$ (after Laplace transforms are taken) into (2) and taking the coefficient of the appropriate power of the time in the expression which results. In this manner we obtain for $\overline{\Gamma}_{z}(\mathbf{r},t)$ as $t\to 0$

$$\overline{\Gamma}_{z}(\mathbf{r},t)=t^{2m}[{}^{1}/_{3}S(S+1)\mathcal{J}^{x}\mathcal{J}^{y}]^{m}(m!)^{-2}+O(t^{2m+2}). \tag{25}$$

The result in (25) does not depend on whether there is an interaction with spins which are not on the selected path or between z projections of the spins. Consequently, this result can be extended to one-dimensional chains with an XY interaction ($\mathcal{J}^{z}=0$), for which an exact solution is known.[7] With $\mathcal{J}^{x}=\mathcal{J}^{y}=\mathcal{J}$ and $S=\frac{1}{2}$, this solution can be expressed as the square of a Bessel function of index m:

$$\Gamma_{z}(m,t)=[\mathcal{J}_{m}(2\mathcal{J}t)]^{2}. \tag{26}$$

The first term of a power series of this function in the time is the same as (25).

Finally, we turn to the correlation function $\Gamma_{\alpha}(\mathbf{r},t)$ which we have been seeking. To find it we should sum the contributions in (25) from all the shortest paths which lead from i to j; i.e., we should multiply (25) by the combinational factor in (5). As a result we find the expression

$$\Gamma_{z}(\mathbf{r},t)=t^{2m}[{}^{1}/_{3}S(S+1)\mathcal{J}^{x}\mathcal{J}^{y}]^{m}(m!r_x!r_y!r_z!)^{-1}+O(t^{2m+2}). \tag{27}$$

Expression (27) is valid at any value of $\mathbf{r}$. For spins which are far apart, the dependence on the distance between them ($r=|\mathbf{r}|$) can be singled out explicitly in (27) by applying Stirling's formula and replacing x^{n} by $\exp(n\ln x)$. In particular, when sites i and j are on a [111] diagonal, i.e., at $r_x=r_y=r_z=r/3^{1/2}$, $m=r3^{1/2}$, we find

$$\Gamma_{z}(\mathbf{r},t)\approx\frac{3^{1/2}}{(2\pi r)^{2}}\left(\frac{\mathcal{J}^{x}\mathcal{J}^{y}}{|\mathcal{J}^{x}\mathcal{J}^{y}|}\right)^{m}\times\exp\left\{-r3^{1/2}\ln\frac{3^{1/2}r}{e^{2}S(S+1)|\mathcal{J}^{x}\mathcal{J}^{y}|t^{2}}\right\}, \tag{28}$$

When the sites are arranged along crystallographic axes ($m=r$) we find

$$\Gamma_{z}(\mathbf{r},t)\approx\frac{1}{2\pi r}\left(\frac{\mathcal{J}^{x}\mathcal{J}^{y}}{|\mathcal{J}^{x}\mathcal{J}^{y}|}\right)^{m}\times\exp\left\{-r\ln\frac{3r^{2}}{4e^{2}S(S+1)|\mathcal{J}^{x}\mathcal{J}^{y}|t^{2}}\right\}. \tag{29}$$

According to the expressions which have been derived, the correlation function has an exponential dependence on

the distance; the argument of the exponential function and the coefficient in front of it are both spatially anisotropic. Another property of the correlation function is that it is positive in the case $\mathcal{J}^x\mathcal{J}^y>0$, while in the case $\mathcal{J}^x\mathcal{J}^y<0$ it changes sign as we go from site to site.

We see a different picture when we look at the long-range interaction. In this case, any site can be reached in a single step, so the series in (4) begin with the quadratic term in (11); this is the term which determines the distance dependence of $\Gamma_z(\mathbf{r},t)$ in the limit $t\to 0$ under consideration here. For a dipole-dipole interaction, for example, we would have $\Gamma_z(\mathbf{r},t)\sim r^{-6}$.

We are left with the question of the role played, with increasing time, by the discarded terms of series (4). Here we must consider (first) a possible lengthening of the path along which the correlation propagates to the given point and (second) the interactions with the spins surrounding the trajectory. We know from the theory of a random walk on a lattice that the number of paths which contain $r_\alpha+p_\alpha$ steps to one side and p_α steps to the opposite side along each direction is

$$\frac{(r_x+r_y+r_z+2p_x+2p_y+2p_z)!}{(r_x+p_x)!p_x!(r_y+p_y)!p_y!(r_z+p_z)!p_z!}. \tag{30}$$

An increase in this factor makes random walks with maximally choppy trajectories preferable. In our case of the correlation functions $\Gamma_\alpha(\mathbf{r},t)$, the result of a lengthening of the path can be estimated from the expression given above for a shortest path of m steps, by setting

$$m=\sum_\alpha (r_\alpha+2p_\alpha)$$

and by multiplying (25) by (30). The large factor $(m!)^2$ in the denominator limits the growth of (30) with increasing path length and makes the shortest paths preferable even for finite times. Under the new conditions, however, we can no longer ignore the interactions between (on the one hand) the spins of the main chain, i.e., those at the sites of the shortest path, and (on the other) the surroundings. The random local fields from the spins of the surroundings are superimposed on the fields exerted by the spins of the main chain on each other, and they disrupt the correlation among the latter spins. On a qualitative level, an increase in the time can be dealt with by multiplying the initial terms of time series (27) by some decreasing functions of the time.

In conclusion we wish to stress that we have found an exact expression for the first nonvanishing coefficient of the power-series expansion of the correlation function $\Gamma_\alpha(\mathbf{r},t)$ in the time. The power can be arbitrarily high for spins which are far apart. It is important to know these coefficients for testing calculations of correlation functions and also for choosing values of the adjustable parameters when these coefficients are given approximately. In Ref. 12 the coefficients of these series were calculated only up to terms of the eighth power. The results were the same under identical conditions. Finally, Kolokolov[6] calculated the correlation functions for spins which are far apart, as we mentioned in the first part of this paper. The result which he found in the limit $t\to 0$ is entirely different. In the first place, it leads to the conclusion that the functions are not analytic at $t=0$, in contradiction of known theorems.[8,9] Second, it differs from (25)–(29) in that it has an oscillatory behavior as a function of the distance in the isotropic case. In addition to the final result, found in the continuum limit, we would question expression (3.9) of Ref. 6, for a basic functional in the site representation. We have not been able to derive a power series in the time from that expression, despite assurances from the author.

[1] P. Resibois and M. DeLeener, Phys. Rev. **152**, 305, 318 (1966).
[2] P. Borckmans and D. Walgraef, Phys. Rev. **167**, 282 (1968); Phys. Rev. B **7**, 563 (1973).
[3] F. C. Barreto and G. F. Reiter, Phys. Rev. B **6**, 2555 (1972); **9**, 46 (1974).
[4] T. Kawasaki, Prog. Theor. Phys. **41**, 322 (1969).
[5] V. P. Kalashnikov and S. V. Tret'yakov, Fiz. Met. Metalloved. **59**, 1075 (1985).
[6] I. V. Kolokolov, Zh. Eksp. Teor. Fiz. **91**, 2313 (1986) [Sov. Phys. JETP **64**, 1373 (1986)].
[7] S. Katsura, T. Horiguchi, and M. Suzuki, Physica **46**, 67 (1970).
[8] H. Araki, Commun. Math. Phys. **14**, 120 (1969).
[9] D. W. Robinson, Commun. Math. Phys. **7**, 337 (1968).
[10] V. E. Zobov, Preprint 518, Institute of Physics, Siberian Branch of the Academy of Sciences of the USSR, Krasnoyarsk, 1988.
[11] V. E. Zobov, Teor. Mat. Fiz. **84**, 111 (1990).
[12] T. Morita, J. Math. Phys. **12**, 2062 (1971).

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