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SOLIDS
Structure

On the Coordinate of a Singular Point of Time Correlation Functions for the System of Nuclear Magnetic Moments of a Crystal

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Abstract—The hypothesis concerning the existence of singular points on the imaginary time axis for a correlation function of a system with the dipole–dipole interaction of nuclear spins of a crystal is verified. Within the framework of the self-consistent fluctuating field theory taking into account the principal corrections related to the correlation of local fields, a result for this coordinate is obtained in terms of the ratios of lattice sums. Experimental values of this coordinate are calculated from the wings of the nuclear magnetic resonance absorption spectrum of a BaF_2 crystal for the magnetic field directions along the three crystallographic axes. Good agreement of the theoretical and experimental results justifies this hypothesis. © *2003 MAIK "Nauka/Interperiodica".*

1. INTRODUCTION

Nuclear magnetic systems of crystals are convenient objects for studying nonequilibrium statistical physics of many-particle systems. The point is that, first, the exact form of the interaction (dipole–dipole) is known; second, the magnetic system is well isolated from the lattice; and third, one can control the system state with the help of a resonant radio-frequency field and observe it using nuclear magnetic resonance (NMR) methods. An important characteristic of these systems is the rate of attaining equilibrium between the subsystems in the presence of a large mismatch of resonant frequencies determined by the wings of the spectra of the correlation functions. This fact stimulated the study of such systems. In a number of experimental studies, it was found that the frequency dependence of the wings of the spectra can be described by a simple exponential function (see, e.g., [1–3] and the analysis of other experiments in [4]) instead of the expected Gaussian function [5]. The peculiarity of this shape of the spectrum wing is that the corresponding correlation function must have a singular point on the imaginary time axis. In turn, this may indicate a new type of collective effects in such systems. Unfortunately, low accuracy of the registration of a weak signal on the spectrum wing makes the interpretation of its shape ambiguous.

Theoretical investigations [6] confirmed the possibility of the existence of singular points on the imaginary time axis for correlation functions of rigid spin lattices at high temperatures, at least for lattices of large dimension d. The divergence of the form of the spectrum wing from the Gauss distribution is caused by the time fluctuations of the local magnetic field on the spin due to the flips of the neighboring spins creating this field. In turn, these flips are caused by the internal interaction between the spins (dipole–dipole or exchange interaction). The coordinate of a singular point can be easily calculated [6–9] in the approximation of a self-consistent fluctuating local field for lattices of large dimension, i.e., in the case when the correlation of local fields can be neglected. The problem on the variation of this coordinate with decreasing space dimension remains so far unsolved.

In our earlier publications [10, 11], we found the first terms of the expansion in the inverse dimensionality of space for the coordinate of a singular point of the autocorrelation function (ACF) of the Heisenberg model with an isotropic interaction of nearest neighbors. The experimental data [1–3] were obtained for nuclear magnetic systems of crystals with the dipole–dipole interaction. This interaction is characterized by the anisotropy and necessitates the inclusion of distant neighbors. Both these factors are taken into account in this paper when determining the coordinate of a singular point.

In the approximation of a self-consistent fluctuating field described in Section 2, a simple nonlinear equation for the ACF taking into account the axial symmetry of the dipole–dipole interaction in the spin space is written out the coordinate of a singular point of the solution to this equation is determined, and a formula for the variation of this coordinate with a small variation in the coefficients of the power series in the time

for the ACF is derived. In Section 3, we calculate the first corrections to the singular point coordinate due to the local field correlation arising when the space dimension is decreased. In Section 4, theoretical results are compared with experimental data.

2. EQUATIONS FOR AUTOCORRELATION FUNCTIONS

We consider a system of nuclear magnetic moments with spin $I = 1/2$ that form a perfect lattice of dimension d. The spin dynamics in a strong constant magnetic field is determined by the secular part of the dipole–dipole interaction with the Hamiltonian [5]

$$\mathcal{H} = \sum_{i \neq j} b_{ij}\left[I_i^z I_j^z - \frac{1}{2}(I_i^x I_j^x + I_i^y I_j^y)\right], \quad (1)$$

where

$$b_{ij} = \frac{\gamma^2\hbar(1 - 3\cos^2\theta_{ij})}{2r_{ij}^3},$$

θ_{ij} is angle between the internuclear vector $\mathbf{r}_{ij}$ and the constant magnetic field, and I_i^α is the α component ($\alpha = x, y, z$) of the vector spin operator at the ith site. For a high temperature, the time-dependent correlation functions of two spins located at the ith and jth lattice sites are defined by the expression [5]

$$\Gamma_{\alpha ij}(t) = \frac{\mathrm{Tr}\{\exp(i\mathcal{H}t)I_i^\alpha \exp(-i\mathcal{H})I_j^\alpha\}}{\mathrm{Tr}\{(I_i^\alpha)^2\}}. \quad (2)$$

We obtain the cross correlation function for $i \neq j$ and the autocorrelation function for $i = j$. By virtue of the translation symmetry of the lattice, we omit subscript ii on the ACF. Taking into account the axial symmetry of the Hamiltonian with respect to spin components, we use the notation $\Gamma_x(t) = \Gamma_y(t) = X(t)$. Autocorrelation functions (2) can be expanded into power series,

$$\Gamma_\alpha(t) = \sum_{n=0}^{\infty} \frac{(-1)^n M_{2n\alpha} t^{2n}}{(2n)!}, \quad (3)$$

where the nth coefficient of the expansion is determined via the $2n$-fold commutator

$$M_{2n\alpha} = \frac{\mathrm{Tr}\{[\mathcal{H}, \ldots[\mathcal{H}, I_i^\alpha]\ldots]I_i^\alpha\}}{\mathrm{Tr}\{(I_i^\alpha)^2\}}. \quad (4)$$

It is known [5] that $M_{2n\alpha}$ is the $2n$-order moment of the spectral density of the corresponding ACF.

Up to now, exact equations for ACFs have not been obtained because of the complexity of description of a many-particle system with strong interactions. Many approximate versions of the equations have been proposed. In particular, the following system of nonlinear integral equations for ACF was derived in [12, 13]:

$$\frac{d}{dt}\Gamma_\alpha(t) = -\int_0^t G_\alpha(t - t_1)\Gamma_\alpha(t_1)dt. \quad (5)$$

The kernels of these equations are represented in the form of a series in irreducible dressed skeleton diagrams with an increasing number of vertices. Each term of the series can be expressed in terms of the multiple time integral of the product of functions $\Gamma_x(t)$ and $\Gamma_z(t)$. All contributions corresponding to the diagrams with two and four vertices are determined.

System of equations (5) has been investigated in [6] in the approximation of lattices of an infinite dimension that corresponds to the approximation of a self-consistent fluctuating local field. In this limit, the equations for ACF correspond to the averaged precession of the magnetic moment in a three-dimensional Gaussian random local field whose correlation functions are expressed via the spin ACFs as

$$\langle\omega_\alpha(t)\omega_\alpha(0)\rangle = \langle\omega_\alpha^2\rangle\Gamma_\alpha(t), \quad (6)$$

where

$$\langle\omega_x^2\rangle = \langle\omega_y^2\rangle = \frac{S_1}{4}, \quad \langle\omega_z^1\rangle = S_1, \quad S_1 = \sum_j b_{ij}^2.$$

For series $G_{\alpha 0}(t)$, majorizing series are found and the existence of singular points of the ACFs on the imaginary time axis is established. In the neighborhood of the nearest singular point with coordinate τ_0, the principal part has the form

$$\Gamma_\alpha(t) \approx A_\alpha(\tau_0 + it)^{-2}. \quad (7)$$

The coordinate of the singular point estimated by the spectral moments on the order from two to ten is

$$\tau_0 = \frac{2.77}{M_{2x}^{1/2}}, \quad (8)$$

where $M_{2x} = 5S_1/4$ is the second moment of the spectrum of function $\Gamma_x(t)$.

If the space has a finite dimension, in the series for the kernel, one should take into account the additional terms

$$\delta G_\alpha(t) = G_\alpha(t) - G_{\alpha 0}(t)$$

that contain coupling loops and multiple interactions of neighboring spins. These corrections reflecting the cor-

relation of the local fields vanish in the limit as $d \longrightarrow \infty$. It is natural to expect that, if the dimension of the space is sufficiently large, the relative variations of moments $M_{2n\alpha}$ of the ACFs and the coordinates of the singular point τ_c with additional terms taken into account are small (on the order of $\varepsilon \sim 1/d$); i.e.,

$$M_{2n\alpha} = M_{2n\alpha}^{(0)} - \varepsilon M_{2n\alpha}^{(1)} + \ldots, \quad \tau_c = \tau_0 + \varepsilon\delta\tau_c + \ldots$$

The coordinate τ_c of the singular point (equal to the convergence radius of the power series in time) can be determined as the limit of the ratio between the moments,

$$\tau_c^2 = \lim_{n\to\infty}\frac{M_{2(n-1)\alpha}}{M_{2n\alpha}}2n(n-1)$$
$$= \tau_0^2\lim_{n\to\infty}\frac{1-\varepsilon M_{2(n-1)\alpha}^{(1)}/M_{2(n-1)\alpha}^{(0)}+\ldots}{1-\varepsilon M_{2n\alpha}^{(1)}/M_{2n\alpha}^{(0)}+\ldots},$$

which gives

$$2\frac{\delta\tau_c}{\tau_0} = \lim_{n\to\infty}\left(\frac{M_{2n\alpha}^{(1)}}{M_{2n\alpha}^{(0)}} - \frac{M_{2(n-1)\alpha}^{(1)}}{M_{2(n-1)\alpha}^{(0)}}\right). \quad (9)$$

Due to the complexity of series $G_{\alpha 0}(t)$, even the first corrections $M_{2n}^{(1)}$ (linear in ε) can hardly be found. Therefore, to estimate $\delta\tau_c$, we take the approximate version of the equation for $\Gamma_\alpha(t)$ that allows one to determine high-order moments. In the case of dipole–dipole interaction (1), as a result of the efforts of many authors [3, 4, 8, 9, 14–18], it has been established that a good approximation is obtained if the (longitudinal) interaction between the z components of the spin is fully taken into account and the xx and yy (transverse) interactions are taken into account to the minimal required extent. For the ACF of the x component of the spin, we take the Anderson–Weiss equation [19] describing the spin precession in a Gaussian longitudinal field, renormalize this field to ensure the correct value of the second moment M_{2x}, and determine its correlation function (6) via the ACF of the z component of the spin [4, 8. 9]:

$$X(t) = \exp\left\{\int_0^t\int_0^{t_1}\Gamma_z(t_2)\,dt_1dt_2\right\}. \quad (10)$$

Here and below, in the formulas we pass to the imaginary dimensionless time $t \longrightarrow it(5S_1/4)^{-1/2}$, preserving its previous notation. After this substitution, the argument of the exponential function in expression (10) becomes positive and the coefficient M_{2x} of the integral becomes equal to unity. For the ACF of the z component, we use the equation

$$\Gamma_z(t) = 1 + \frac{2}{5}\int_0^t\int_0^{t_1}X^2(t_2)dt_1dt_2. \quad (11)$$

It will be shown below that, for the location of the singular point on the imaginary time axis, this equation gives an insignificant difference as compared with the equation used before [4, 8, 9],

$$\Gamma_z(t) = 1 + \frac{2}{5}\int_0^t\int_0^{t_1}X^2(t_2)\Gamma_z(t_1-t_2)dt_1dt_2, \quad (12)$$

but simplifies the calculations.

Since the kernel of Eq. (11) is $X^2(t)$, we denote the latter by $Y(t)$ and obtain, using formula (10), the differential equation

$$\frac{d}{dt}Y(t) = 2Y(t)\int_0^t\Gamma_z(t_1)dt_1$$
$$= 2Y(t)\left\{t + \frac{2}{5}\int_0^t\int_0^{t_1}\int_0^{t_2}Y(t_3)dt_1dt_2dt_3\right\}. \quad (13)$$

Substituting $Y(t)$ in the form of the series

$$Y(t) = \sum_{n=0}^{\infty}t^{2n}Y_{2n} \quad (14)$$

into Eq. (13) and equating the coefficients of the same powers of time, we obtain the recurrence equation

$$Y_{2n} = \frac{1}{n}Y_{2n-2} + \frac{2}{5n}\sum_{k=0}^{n-2}\frac{Y_{2k}Y_{2(n-k-2)}}{(2k+1)(2k+2)(2k+3)}. \quad (15)$$

The coordinate of the singular point (equal to the convergence radius of series (14)) can be determined (taking into account the order of pole (7)) as the limit of the ratio

$$\tau_0^2 = \lim_{n\to\infty}\frac{Y_{2n-2}(2n+2)(2n+3)}{Y_{2n}(2n-1)2n}. \quad (16)$$

Solving recurrence equation (15) and using formula (16), we find

$$\tau_0 = \frac{2.69}{M_{2x}^{1/2}},$$

whereas, using Eq. (12) with the convolution, we obtain

$$\tau_0 = \frac{2.68}{M_{2x}^{1/2}}.$$

Both these values differ from a more precise value (8) by 3%. This difference exerts no substantial influence on the values of corrections $\delta\tau_c$; therefore, for the calculation of these corrections, we will use the simplest equation.

3. CALCULATION OF THE CORRECTIONS TO THE COORDINATE OF THE SINGULAR POINT OF THE CORRELATION FUNCTION

Let us consider function $\Gamma_x(t)$ as the generating function of the lattice patterns formed by bonds b_{ij}. This can be justified by the structure of expression (4) for moments, where each commutator with $\mathcal{H}$ adds a bond b_{ij} to the constructed pattern. In more detail, the rules of constructing the patterns are considered in [6, 10, 11]. The solution to the system of equations (10) and (11) of the zeroth-order approximation is the generating function of the root trees constructed from the double bonds. On these trees, the double bonds caused by the *zz* interactions (*z* fields in Eq. (10)) alternate with the bonds caused by the *xx* and *yy* interactions (the variations of *z* fields described by Eq. (11)). An arbitrary number of branches which have no intersections can emerge from any node of this tree. This can hold as $d \longrightarrow \infty$. When constructing the patterns on finite-dimensional lattices, there is a probability that the branches intersect either directly near the node from which they emerge, which results in a multiple interaction of the neighbors, or near a far node, forming a loop of bonds. For a tree with such a fragment, the weighting factor obtained during the construction of the tree by calculating the initial multiple commutators (4) does not coincide with the factor obtained in the case of intersection due to the mechanical overlap of branches constructed independently by Eqs. (10) and (11) and located on a real lattice. Therefore, the latter should be eliminated and replaced by trees with a correct weight.

To theoretically estimate the variation of the coordinate of the singular point of the ACF caused by the described variations of the moments, we consider the dimension *d* of the space as a variable. If *d* is taken sufficiently large, then the intersection probability is low and we can consider only the simplest intersections, namely, the quadruple interaction of neighbors and loops in the form of a triangle formed by four bonds. Such contributions are contained even in the fourth moment of the ACF. The intersections in which more bonds are involved give a higher order of smallness in $1/d$ [9, 10]. In the case of the dipole–dipole interaction and $d = 3$, their smallness is confirmed by the ratio of the values of the lattice sums [2, 20, 21].

3.1. Quadruple Interaction of Neighbors

As is shown in [3], in the case when the number of neighbors is not very large, to improve the accuracy of the main approximate equation, one should replace the Anderson–Weiss function (10) by the product

$$P_i(t) = \prod_j F_{ij}(t), \tag{17}$$

$$F_{ij}(t) = 1 + \frac{b_{ij}^2}{S_1}\int_0^t\int_0^{t_1} F_{ij}(t_2)\Gamma_{zj/i}(t_1 - t_2)dt_1dt_2, \tag{18}$$

where $\Gamma_{zj/i}(t)$ is the ACF of *z* component of the *j*th spin disregarding the interaction with the *i*th spin on which the field is considered,

$$\Gamma_{zj/i}(t) = 1 + \frac{2}{5}\sum_{k\neq i,\,j}\frac{b_{jk}^2}{S_1} \times \int_0^t\int_0^{t_1}\frac{P_j(t_2)P_k(t_2)}{F_{ij}(t_2)F_{jk}^2(t_2)}\Gamma_{zj/i}(t_1 - t_2)dt_1dt_2. \tag{19}$$

In addition, recurrence of the interaction of the *j*th and *k*th spins is excluded in the kernel of this integral equation.

We differentiate the square of function $P_{ij}(t)$ (17) with respect to time:

$$\frac{d}{dt}P_i^2(t) = 2P_i^2(t)\sum_{j\neq i}\frac{1}{F_{ij}(t)}\frac{d}{dt}F_{ij}(t). \tag{20}$$

Taking into account relations (17)–(20), one can easily verify that, neglecting the contribution of separate interaction b_{ij}^2 in comparison with sum S_1, we return to the equation of zeroth-order approximation (13). To within the first correction from these contributions, we find that

$$Y(t) = P_i^2(t) = Y_0(t) - \frac{S_2}{S_1^2}Y_1(t).$$

Here,

$$S_2 = \sum_j b_{ij}^4$$

and $Y_1(t)$ is the solution to the equation

$$\frac{d}{dt}Y_1(t) = 2Y_1(t)\int_0^t \Gamma_z(t_1)dt_1 + \frac{4}{5}Y_0(t)\int_0^t\int_0^{t_1}\int_0^{t_2} Y_1(t_3)dt_1dt_2dt_3 + C\frac{dY_0(t)}{dt}\int_0^t\int_0^{t_1}\Gamma_z(t_2)dt_1dt_2$$
$$+ \frac{4}{5}DY_0(t)\int_0^t\int_0^{t_1}\int_0^{t_2} Y_0(t_3)dt_1dt_2dt_3 + \frac{8}{5}AY_0(t)\int_0^t\int_0^{t_1}\int_0^{t_2} Y_0(t_3)dt_1dt_2dt_3\int_0^{t_3}\int_0^{t_1}\Gamma_z(t_5)dt_4dt_5 \quad (21)$$
$$- 2BY_0(t)\int_0^t \Gamma_z(t-t_1)dt_1\int_0^{t_1}\int_0^{t_2}\Gamma_z(t_3)dt_2dt_3,$$

where $\Gamma_z(t)$ is determined via $Y_0(t)$ with the help of Eq. (11). The coefficients A, B, C, and D are introduced into Eq. (21) in order to separate the contributions of different kinds. For $A = 3/2$, $C = 1$, $D = 1$, and $B = 0$, we obtain the contribution corresponding to the exclusion of the quadruple interaction of neighbors due to the intersection of the tree branches emerging from the same node. For $A = 0$, $C = 0$, $D = 0$, and $B = 1$, we obtain the contribution of the quadruple interaction with the correct weight, which, therefore, appears with the opposite sign. This contribution stems from the second iteration in Eq. (18).

3.2. Triangle Composed of Four Bonds

There are two reasons for the formation of the simplest triangle-like loops: first, the contribution of the cross correlation function $\Gamma_{zjk}(t)$ to the correlator of the local field on the separated spin in expressions (10) and (17) and, second, the result of the simultaneous action of the field of the third spin on the two spins bonded by the transverse (flip–flop) interaction in the kernels of integral equations (11) and (19) for $\Gamma_z(t)$. In the one-loop approximation, we obtain

$$Y(t) = Y_0(t) - \frac{S_3}{S_1^2}Y_1(t),$$

where

$$S_3 = \sum_{i,j} b_{ij}^2 b_{ik}b_{jk},$$

$Y_0(t)$ is the zeroth-order approximation (13), and, for the first-order correction $Y_1(t)$, we obtain equations of the form (21) with the following values of the parameters: $A = 1$, $B = 0$, $C = 0$, and $D = 1$.

The structure of Eq. (21) becomes clear when interpreted in terms of generating functions of root trees having an embedded fragment with a branch intersection. The summands on the right-hand side with coefficients A, B, C, and D represent the contribution of the corresponding fragment with the intersection joined to the tree root. If, however, the intersection occurs at a far node of the tree, then the necessary chain of bonds from the root to the fragment is composed via iterations with the help of the first two terms on the right-hand side of the equation. Recall that we operate in the approximation linear in intersections; i.e., we assume that there is at most one intersection on the tree. By virtue of this assumption and the translation invariance of the lattice sites, the form of the expression for the fragment is independent of its location in the tree. However, its contribution to $Y_1(t)$ obviously depends on the length of the chain leading to this site.

3.3. Calculation of Corrections

Substituting series (14) for functions $Y_0(t)$ and $Y_1(t)$ into Eq. (21), we obtain the following recurrence equation for coefficients $Y_{2n}^{(1)}$ of function $Y_1(t)$:

$$Y_{2n}^{(1)} = \frac{1}{n}Y_{2n-2}^{(1)} + \frac{2}{5n}\sum_{k=0}^{n-2}\frac{Y_{2k}^{(0)}Y_{2(n-k-2)}^{(1)} + Y_{2k}^{(1)}Y_{2(n-k-2)}^{(0)}}{(2k+1)(2k+2)(2k+3)} + D\left(Y_{2n}^{(0)} - \frac{1}{n}Y_{2n-2}^{(0)}\right) + \frac{C}{2}\left(1-\frac{1}{n}\right)Y_{2n-2}^{(0)}$$
$$+ \frac{C}{5n}\sum_{k=0}^{n-2}\frac{2(n-k-2)Y_{2k}^{(0)}Y_{2(n-k-2)}^{(0)}}{(2k+1)(2k+2)(2k+3)(2k+4)} + \frac{2A}{5n}\sum_{k=0}^{n-3}\frac{Y_{2k}^{(0)}Y_{2(n-k-3)}^{(0)}}{(2k+3)(2k+4)(2k+5)} \quad (22)$$
$$+ \frac{8A}{25n}\sum_{k=0}^{n-4}\sum_{p=0}^{n-k-4}\frac{Y_{2p}^{(0)}Y_{2k}^{(0)}Y_{2(n-k-p-4)}^{(0)}}{(2p+1)(2p+2)(2p+3)(2p+4)(2k+2p+5)(2k+2p+6)(2k+2p+7)}$$

$$-\frac{B}{6n}Y^{(0)}_{2n-4}-\frac{4B}{5n}\sum_{k=0}^{n-3}\frac{(2k)!}{(2k+5)!}Y^{(0)}_{2k}Y^{(0)}_{2(n-k-3)}-\frac{4B}{25n}\sum_{k=0}^{n-4}\sum_{p=0}^{k}\frac{(2k-2p)!(2p)!}{(2k+7)!}Y^{(0)}_{2p}Y^{(0)}_{2(k-p)}Y^{(0)}_{2(n-k-4)}.$$

Using this equation, we determine coefficients $Y^{(1)}_{2n}$ for different contributions; then, by formula (9), we find the corresponding corrections to the coordinate of the singular point. The correction corresponding to the exclusion of the forbidden quadruple interaction of neighbors ($A = 3/2$, $B = 0$, $C = 1$, $D = 1$) is equal to

$$\frac{S_2}{S_1^2}\frac{\delta\tau_c}{\tau_0} = 1.507\frac{S_2}{S_1^2}, \tag{23}$$

the correction corresponding to the addition of the allowed quadruple interaction of neighbors ($A = 0$, $B = 1$, $C = 0$, $D = 0$) is

$$\frac{S_2}{S_1^2}\frac{\delta\tau_c}{\tau_0} = -0.124\frac{S_2}{S_1^2}, \tag{24}$$

and the correction corresponding to the inclusion of correlation of fields in the form of a triangle composed of four bonds ($A = 1$, $B = 0$, $C = 0$, $D = 1$) is

$$\frac{S_3}{S_1^2}\frac{\delta\tau_c}{\tau_0} = 0.55\frac{S_3}{S_1^2}. \tag{25}$$

4. COMPARISON WITH EXPERIMENT

In a neighborhood of the nearest singular point, principal part (7) determines the wing of the ACF spectrum,

$$g(\omega) \approx A_\alpha|\omega|\exp(-|\omega|\tau_c). \tag{26}$$

Moreover, since the singularities of all time correlation functions of the spin system under consideration must be located at the same point, the argument of the exponential function in formula (26) is the same (including the NMR absorption spectrum, i.e., the Fourier transform of the correlation function of the total spin of the system [5]).

The wing of the NMR absorption spectrum was experimentally investigated in [3] for a single crystal of BaF_2 with a magnetic field directed along the crystallographic axes [111], [110], and [100]. The frequency dependence of the spectrum for detuning from the spectrum center exceeding $2.2\sqrt{M_2}$ (for [100], even $2.1\sqrt{M_2}$), where $M_2 = 9S_1/4$, is well described by exponential function (26) (this is justified by the fact that the experimental points shown in Fig. 3 in [3] in the semilogarithmic coordinates lie on a straight line). The values of argument τ_e of the exponential function in formula (26), at which the best agreement with the experiment is achieved in the detuning interval from $2.2\sqrt{M_2}$ to $3\sqrt{M_2}$, are given in the table in the form of the ratio to the limiting theoretical value of τ_0 (8). The mean square error increases from 0.5% in orientation [111] to 2% in orientation [100] due to a decrease of the signal-to-noise ratio with increasing NMR line width. However, the actual accuracy of determining τ_e is lower, first, because of the systematic distortions in the wing introduced by the spectrometer, and second, since the simple dependence (26) is attained in the limit as $\omega \longrightarrow \infty$, i.e., in the spectral region that is inaccessible because of the noise. As the center of the spectrum is approached, the deviation of its shape from dependence (26) becomes noticeable.

Let us return to theoretical results. Collecting corrections (23)–(25), we obtain

$$\frac{\tau_c}{\tau_0} = 1 + 1.38\frac{S_2}{S_1^2} + 0.55\frac{S_3}{S_1^2}. \tag{27}$$

Substituting the values of the lattice sums for a simple cubic lattice from [2], we find the values of this ratio for the three main orientations of the magnetic field which are presented in the table. It is difficult to estimate the accuracy of these values, because expansion (27) is asymptotic in $1/d$. We estimate the error caused by the replacement of complete equation (5) with simplified equations (10) and (11), as well as the error in determining the convergence radius of the series by its coefficients, in the range of 2–3%.

The results presented in the table show good agreement between the theoretical and experimental values of the coordinates of singular points of the correlation functions for all three orientations of the field. It should be emphasized that the orientation dependence of the second moment, which is the frequency scale of the spectrum, does not affect the ratios presented in the table. Their values depend not on the mean square of local fields, but on the extent of correlation of these fields, which is expressed in formula (27) in terms of the ratio of different lattice sums. On the one hand, the coincidence of two independent estimates for the coordinate shows that the errors whose values were difficult

The ratios of the experimental τ_e and theoretical τ_c values of coordinates of the singular points of the correlation functions to limiting value τ_0 (8) for three directions of the magnetic field

Field direction	τ_e/τ_0	τ_c/τ_0
[111]	1.10	1.14
[110]	1.24	1.25
[100]	1.33	1.34

to estimate are small. On the other hand, the values of the coordinate ratios obtained may indicate that, with the decrease in the space dimension from $d = \infty$ to $d = 3$, the singular point moves but does not go to infinity. A final conclusion can be made after increasing the accuracy of theoretical calculations and experimental measurements.

Note in conclusion that result (27) can be applied to experiments performed on other crystals and for other field orientations after substituting the corresponding values of the lattice sums.

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