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ORDER, DISORDER, AND PHASE TRANSITION IN CONDENSED SYSTEM

Exponential Bound for the Heating Rate of Periodically Driven Spin Systems

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Abstract—For the nuclear spin system of a solid in the presence of an inhomogeneous magnetic field, we have found a rigorous bound for the heating rate of the system under the action of a high-frequency magnetic field, which is applied, for example, to create effective Hamiltonians. We consider the autocorrelation function (ACF) of a spin rotating in a local field whose fluctuations are specified by a Gaussian random process. The correlation function of a random field is taken as the sum of a static inhomogeneous contribution and a time-dependent contribution expressed self-consistently via the spin ACF. The ACF singularities on the imaginary time axis whose coordinates determine the exponents of exponential asymptotics in the high-frequency domain are investigated. The dependences of the coordinates on field inhomogeneity for various approximations have been derived. The wing of the ACF spectrum in the cumulant approximation is shown to serve as a rigorous upper bound for the wing of the ACF spectrum and, consequently, for the heating rate of the system when subjected to variable magnetic fields. We have established that randomly distributed inhomogeneous magnetic fields increase the wings of the ACF spectra and, thus, speed up the system's heating.

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1. INTRODUCTION

A promising way of studying complex quantum systems is their simulation on other quantum systems [1–3]. The rapid development of this direction is currently related to the development of experimental methods for coherent control of quantum systems [2–7], such as ions and atoms in traps, electron paramagnetic centers in solids, and superconducting systems. To obtain an effective Hamiltonian needed for simulations, strong periodic driving, for example, laser pulses and radio-frequency or microwave field pulses, is applied to a quantum system. The Floquet or Magnus theory is used to describe the evolution of systems [8–11]. The required evolution of a system under the action of an average Hamiltonian is accompanied by its parasitic heating by higher harmonics. The duration of the simulation stage and, thus, the efficiency of the method depend on the heating rate. Qualitative estimates for the bound of the heating rate were found in [12–17], which showed its exponential slowdown as the oscillation frequency increased.

A practical application of the transformation of Hamiltonians by radio-frequency field pulses was realized back in the 1970s to obtain high-resolution NMR spectra in solids [18, 19] and was named "spin alchemy." A thermodynamic theory of the formation of a quasi-equilibrium state in a system on short time scales and its subsequent heating was developed in [20, 21] and explained the results of experiments. The formulas expressing them via the spin time correlation functions were derived for the heating rate, although these functions themselves were not calculated. The advantage of nuclear spin systems as compared with other quantum systems lies in known interactions, sufficient isolation from other subsystems, and the possibility of control and observation by NMR methods. Therefore, in such systems it is possible to pass from qualitative estimates of the bounds for the heating rate to quantitative estimates. In this paper we will find a rigorous estimate expressed, as is customary, via the second moment of the NMR spectrum.

The representation of a time-fluctuating local field on spins by a Gaussian random process well proven in such systems is used as the basis for our work. This approximation was suggested by Anderson [22] and Kubo [23] and is determined by a large number of independent contributions from the spins surrounding each spin. This approach was effectively applied to the solution of spin-dynamics problems, for example, in [22–26]. In these papers the correlation function of a Gaussian field was chosen from physical considerations. Following [27, 28], we will specify this function

self-consistently via the spin autocorrelation functions (ACFs) [29–31]. Previously, we applied this approach to explaining the exponential wings of the spectra of various correlation functions for homonuclear systems [32–34], heteronuclear systems [35], magnetically diluted systems [36, 37], and spin packets [38]. Using this method, we will now find rigorous bounds for the energy absorption rate of a high-frequency field in the presence of an inhomogeneous magnetic field. Such a field changes significantly the dynamics of spin systems; for example, in the opinion of many authors (for a review, see [39]), it can cause the transition of a system from a thermalized state to a many-body localized state characterized by a slowdown of the energy propagation inside the system. On the other hand, it follows from the qualitative estimates made in [16, 38] that an inhomogeneous magnetic field causes the high-frequency ACF asymptotics to grow. The problem of the influence of an inhomogeneous magnetic field on the dynamics of spin systems needs a further study.

This paper is structured as follows. In Section 2 we consider the motion of the magnetic moment in a Gaussian random field and analyze the relation between the ACFs derived using various approximations. In Section 3 we study the influence of an inhomogeneous magnetic field on the ACFs. The coordinates of their nearest singularities on the imaginary time axis are calculated via the radii of convergence of the series for the ACFs in powers of time. The dependences of these coordinates on inhomogeneous broadening are compared for the solutions of different equations. The results obtained are discussed in Section 4. Finally, the approximating functions for these dependences of the coordinates calculated numerically are derived in the Appendix.

2. A GAUSSIAN RANDOM LOCAL FIELD

Consider the rotation of the magnetic moment $\boldsymbol{\mu}(t)$ in a Gaussian random magnetic field $\mathbf{h}(t)$. The equation of motion can be written as [30, 31]

$$\frac{d}{dt}\boldsymbol{\mu}(t) = \hat{h}(t)\boldsymbol{\mu}(t), \tag{1}$$

where the matrix of the operator $\hat{h}(t)$ has the same form,

$$\hat{h}(t) = \begin{pmatrix} 0 & -h^z(t) & h^y(t) \\ h^z(t) & 0 & -h^x(t) \\ -h^y(t) & h^x(t) & 0 \end{pmatrix}, \tag{2}$$

for both ordinary vectors $\boldsymbol{\mu}$ and vector operators $\boldsymbol{\mu} = \gamma\mathbf{S}$ in the quantum-mechanical case.

We will seek a solution of Eq. (1) in the form of a series in the number of field operators (matrices). In this way, for the ACF we obtain

$$\Gamma_\alpha(t) = \sum_{n=0}^{\infty}\int_0^t dt_1\int_0^{t_1} dt_2 \ldots \int_0^{t_{2n-1}} dt_{2n}\langle\hat{h}(t_1)\hat{h}(t_2)\ldots\hat{h}(t_{2n})\rangle_{\alpha\alpha}, \tag{3}$$

where the brackets $\langle\ldots\rangle$ denote an averaging over the Gaussian random field realizations, while the subscript $\alpha\alpha$ is the matrix element of the product of matrices. For example, for the product of two matrices we obtain

$$\langle\hat{h}(t_1)\hat{h}(t_2)\rangle_{xx} = -g_z(t_1 - t_2) - g_y(t_1 - t_2),$$

where for the correlation function of the field projection at different instants of time we introduced the notation

$$\langle h^\alpha(t_1)h^\alpha(t_2)\rangle = g_\alpha(t_1 - t_2). \tag{4}$$

The mean of the product of an odd number of Gaussian variables becomes zero, while the mean of the product of an even number of such variables is the sum over all possible pairings of like projections. Generally, the averaging result depends on the set of projections and the sequence of their arrangement in the product. This complication is related to the fact that the rotations around different axes are non-permutable.

The special case of a field directed along one axis constitutes an exception. If, for example, $h^z \neq 0$ and $h^x = h^y = 0$, then the series (3) is easily summed into an exponential function

$$\Gamma_{0x}(t) = \exp\left\{-\int_0^t\int_0^{t'} g_z(t'')dt'\,dt''\right\}. \tag{5}$$

This result is attributable to the dependence of the term in (3) not on the mutual arrangement of different pairs, but only on the time interval between the action times of paired projections. In the so-called cumulant approximation this condition is extended to a three-component field, which leads to the result

$$\Gamma_{cx}(t) = \exp\left\{-\int_0^t\int_0^{t'} (g_z(t'') + g_y(t''))dt'\,dt''\right\}. \tag{6}$$

Generally, grouping the terms of the series obtained after the averaging in (3) over various pairing schemes and performing a partial summation, as described in [27, 30, 31], for the ACF we obtain the following system of integral equations:

$$\frac{d}{dt}\Gamma_\alpha(t) = -\int_0^t G_\alpha(t - t_1)\Gamma_\alpha(t_1)dt_1, \tag{7}$$

where the memory function is represented as a series in the number of pairs with different pairing schemes. The expressions for the contributions in $G_\alpha(t)$ contain-

ing from 2 to 4 pairs are given in [31]. For example, in the simplest case of one pair, we have the equation

$$\frac{d}{dt}\Gamma_{1x}(t) = -\int_0^t \{g_z(t-t_1)\Gamma_{1y}(t-t_1) + g_y(t-t_1)\Gamma_{1z}(t-t_1)\}\Gamma_{1x}(t_1)dt_1. \quad (8)$$

Otherwise, the ACF (3) can be represented as a series in powers of time:

$$\Gamma_\alpha(t) = \sum_{n=0}^{\infty}\frac{(-1)^n}{(2n)!}M_{2n\alpha}t^{2n}. \quad (9)$$

The coefficients $M_{2n\alpha}$ are the moments of the spectrum of ACF (3) [40]. In the case of static Gaussian fields,

$$g_\alpha(t) = \langle h_\alpha^2\rangle \equiv \Delta_\alpha^2 \quad (10)$$

the coefficients of the series (3) and (9) coincide, while, generally, this is not the case. Each term of the series (3) is the product of series in powers of time of the functions $g_\alpha(t)$.

Let us illustrate the relation for the coefficients of the series for (6) and (8) and the solution of Eq. (7) using an isotropic constant Gaussian field $g_x(t) = g_y(t) = g_z(t) = \Delta^2$ as an example. In this case, we find

$$M_{c2n} = \frac{(2n)!}{n!}\Delta^{2n}, \quad M_{1,2n} = \frac{(2n)!}{n!(n+1)!}2^n\Delta^{2n},$$

while the exact values for the series (3) in this case [23, 30, 31] are

$$M_{2n} = \frac{2(2n+1)!}{2^n n!3}\Delta^{2n}.$$

The following relation holds (at $n > 1$):

$$M_{c2n} > M_{2n} > M_{1,2n}, \quad (11)$$

which reflects the conditions for the derivation of the corresponding expressions. In Eq. (8) we summed part of the series (3), while in the cumulant expression (6) we took all pairing variants, but with overestimated coefficients.

Let us return to the time-dependent Gaussian field and specify it in a self-consistent approximation. In this approximation [27, 31, 32] we will express the field correlation functions via the spin ACFs as

$$g_\alpha(t) = \Delta_\alpha^2\Gamma_\alpha(t). \quad (12)$$

It is convenient to compare the time series (9) for different functions after passing to the imaginary time $t = i\tau$, when these series become series with positive terms. To be specific, let us choose the directions of the coordinate axes in such a way that the following condition is satisfied:

$$\Delta_z^2 \geq \Delta_y^2 \geq \Delta_x^2. \quad (13)$$

For the guaranteed derivation of an approximation with maximum coefficients for the ACF, $X(t)$, in the cumulant approximation (6) we should then take the same function $X(t)$ for the field in a self-consistent way, i.e., write the equation

$$X(t) = \exp\left\{-(\Delta_z^2+\Delta_y^2)\int_0^t\int_0^{t'}X(t'')dt'\,dt''\right\}. \quad (14)$$

The derived Blume–Hubbard equation [28] has the solution

$$X(t) = \frac{1}{\cosh^2(t\sqrt{(\Delta_z^2+\Delta_y^2)/2})} = \frac{1}{\cos^2(it\sqrt{(\Delta_z^2+\Delta_y^2)/2})}. \quad (15)$$

On the other hand, to obtain the function $Z(t)$ with guaranteed smaller coefficients, we should take the solution of the equation

$$\frac{d}{dt}Z(t) = -(\Delta_x^2+\Delta_y^2)\int_0^t Z^2(t-t_1)Z(t_1)dt_1. \quad (16)$$

The solutions of Eqs. (14) and (16) have singularities on the imaginary time axis [29–32] in the neighborhood of which the ACF is

$$\Gamma_\alpha(t) \approx \frac{A_\alpha}{(it\pm\tau_0)^2}. \quad (17)$$

For Eq. (14) this follows from its solution (15), while for Eqs. (16) and (7) this can be made sure after substituting the principal part of the solutions (17) into them (see the Appendix).

The coordinate of the singularity nearest to the coordinate origin determines the radius of convergence of the series (9). Therefore, this coordinate can be found via the ratio of high-order moments as the limit of the following quantity when $n \to \infty$:

$$\tau_{0n}^2 = \frac{2n(2n+1)M_{2(n-1)}}{M_{2n}}. \quad (18)$$

This formula is analogous to the d'Alembert formula for the radius of convergence of a series, where we replaced the coefficient $2n(2n-1)$ by $2n(2n+1)$, because we know the singularity index in (17) equal to two.

The relation between the coefficients of the series (9) for the solutions of Eqs. (7) and (14), which are positive on the imaginary time axis, leads to a relation between these functions themselves and, consequently, between the coordinates of the nearest singularities:

$$\tau_0 > \tau_c = \pi/\sqrt{2(\Delta_z^2+\Delta_y^2)}. \quad (19)$$

3. AN INHOMOGENEOUS MAGNETIC FIELD

The self-consistent time-fluctuating field considered above is produced by the spin–spin interaction between spins with identical Larmor frequencies. Let us investigate the influence of a random distribution of spin Larmor frequencies on the dynamics. Suppose that such a variation was caused by an inhomogeneous local magnetic field directed along the z axis and specified by a Gaussian distribution with a density

$$P(\omega_i) = \frac{1}{\sqrt{2\pi W^2}}\exp\left(-\frac{(\omega_i - \omega_0)^2}{2W^2}\right), \qquad (20)$$

where ω_0 is the mean frequency and W^2 is the variance.

There can be many reasons for the difference of resonance frequencies. In particular, this can be due to the interaction with a system of spins of a different kind in heteronuclear crystals. We considered this case in [35] using a LiF crystal as an example. The general formulas derived there allow the expressions for the first five coefficients of the series (moments) (9) to be derived in the axisymmetric case $\Delta_x^2 = \Delta_y^2 = \Delta_X^2$. Setting $\Delta_{FL}^2 = W^2$ and $\Delta_{LL}^2 = \Delta_{XL}^2 = 0$ in the formulas[1] from [35], we find in our case

$$M_{2X} = W^2 + \Delta_z^2 + \Delta_X^2, \qquad (21)$$

$$M_{4X} = 3W^4 + 3\Delta_z^4 + (4\Delta_X^2 + 6\Delta_z^2)W^2 + 5\Delta_X^4 + 6\Delta_z^2\Delta_X^2,$$

$$\begin{aligned} M_{6X} &= 15W^6 + 15\Delta_z^6 + (21\Delta_X^2 + 45\Delta_z^2)W^4 \\ &+ 51\Delta_X^6 + 73\Delta_z^2\Delta_X^4 + 55\Delta_z^4\Delta_X^2 \\ &+ (45\Delta_X^4 + 45\Delta_z^4 + 76\Delta_z^2\Delta_X^2)W^2, \end{aligned}$$

$$\begin{aligned} M_{8X} &= 105W^8 + (144\Delta_X^2 + 420\Delta_z^2)W^6 \\ &+ (448\Delta_X^4 + 630\Delta_z^4 + 988\Delta_z^2\Delta_X^2)W^4 \\ &+ \{1678\Delta_z^2\Delta_X^4 + 1544\Delta_z^4\Delta_X^2 + 420\Delta_z^6 \\ &+ 914\Delta_X^6\}W^2 + 1470\Delta_z^2\Delta_X^6 + 861\Delta_X^8 \\ &+ 105\Delta_z^8 + 1378\Delta_z^4\Delta_X^4 + 700\Delta_z^6\Delta_X^2, \end{aligned} \qquad (22)$$

$$\begin{aligned} M_{10X} &= 945W^{10} + (1245\Delta_X^2 + 4725\Delta_z^2)W^8 \\ &+ (5856\Delta_X^4 + 9450\Delta_z^4 + 15120\Delta_z^2\Delta_X^2)W^6 \\ &+ \{36858\Delta_z^2\Delta_X^4 + 37890\Delta_z^4\Delta_X^2 \\ &+ 9450\Delta_z^6 + 16676\Delta_X^6\}W^4 \\ &+ \{27643\Delta_X^8 + 57858\Delta_X^6\Delta_z^2 \\ &+ 64744\Delta_X^4\Delta_z^4 + 35400\Delta_X^2\Delta_z^6 \\ &+ 4725\Delta_z^8\}W^2 + 43989\Delta_z^2\Delta_X^8 \\ &+ 21847\Delta_X^{10} + 945\Delta_z^{10} + 48498\Delta_z^4\Delta_X^6 \\ &+ 33742\Delta_z^6\Delta_X^4 + 11385\Delta_z^8\Delta_X^2. \end{aligned}$$

Let us express the moments in units of the second moment by taking, for definiteness, $\Delta_z^2 = 4\Delta_X^2$, as for dipole–dipole interactions. Let us introduce the notation:

$$\begin{aligned} M_2 = M_{2X} = B^2 + W^2, \quad B^2 = \Delta_z^2 + \Delta_x^2, \\ w^2 = \frac{W^2}{M_2}, \quad b^2 = \frac{B^2}{M_2}, \\ \frac{\Delta_z^2}{M_2} = \frac{4b^2}{5}, \quad \frac{\Delta_x^2}{M_2} = \frac{b^2}{5}. \end{aligned} \qquad (23)$$

We find

$$\begin{aligned} \frac{M_{4X}}{M_2^2} &= 3 + \frac{2b^4}{5^2} - \frac{2b^2w^2}{5}, \\ \frac{M_{6X}}{M_2^3} &= 15 - \frac{24b^2}{5}w^4 - \frac{56b^4w^2}{5^2} + \frac{308b^6}{5^3}, \\ \frac{M_{8X}}{M_2^4} &= 160.7504b^8 + 473.68b^6w^2 + 579.2b^4w^4 \\ &+ 364.8b^2w^6 + 105w^8, \\ \frac{M_{10X}}{M_2^5} &= 2244.96b^{10} + 7632.286b^8w^2 \\ &+ 11001.18b^6w^4 + 8701.44b^4w^6 + 4029b^2w^8 + 945w^{10}. \end{aligned} \qquad (24)$$

From the derived formulas (23) and (24) we calculated M_{8X} and M_{10X} at various values of W^2 and estimated the radius of convergence of the series in powers of time from their ratio using Eq. (18). The result is shown in Fig. 1; τ_0^2 increases with W^2 at small W^2. At large W^2 the increase ceases, because the low-order moments in this limit are determined by the inhomogeneous field. For the Gaussian function $M_{10}/M_8 = 9M_2$ and, therefore, we observe a limiting value of $110/9 = 12.22$. If we increased the orders of the moments in Eq. (18), then for the Gaussian function the estimate of the radius of convergence would grow proportionally to the order, while the growth would stop when the dipole–dipole interactions are taken into account. Thus, whereas in spin systems without an inhomogeneous field [29–35] we managed to estimate the radius of convergence from the tenth moment with an accuracy of a few percent, higher-order moments are needed in the case of a large inhomogeneous field. Unfortunately, they are not known

[1] In Eq. (A.1) from [35] there is an erratum for $M_{8X}^{(F)}$: the correct fourth term in braces is $420\Delta_{FF}^6$ rather than $420\Delta_{XL}^6$.

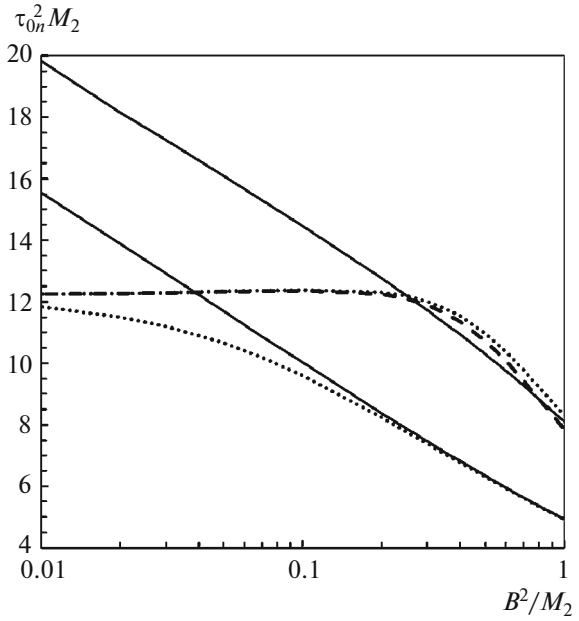

Fig. 1. Coordinates of the singularities calculated from Eq. (18) versus ratio B^2/M_2. The upper solid line is the result of our calculation for Eq. (31) at $n = 70$. The lower solid line is the result of our calculation for Eq. (25) at $n = 70$. The upper and lower dotted curves were calculated for the same equations, but at $n = 5$. The dashed curve was calculated from the ratio of the total moments M_{8X}/M_{10X} (24).

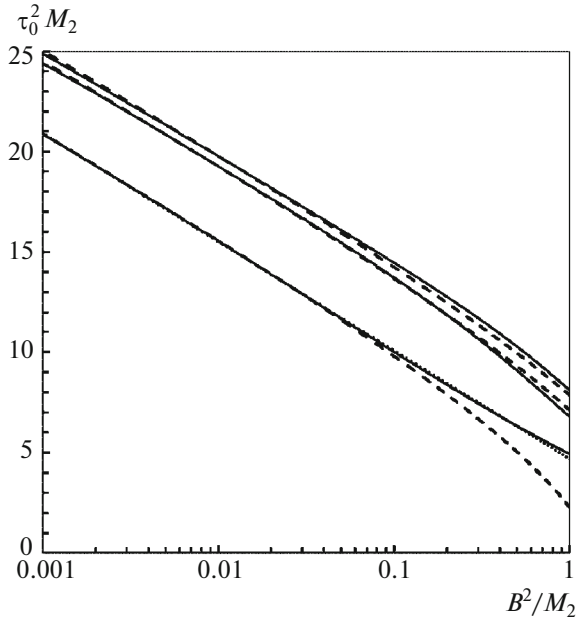

Fig. 2. Coordinates of the singularities of the solutions of Eq. (31) with (32), the simplified version (35), and Eq. (25) versus B^2/M_2, respectively, from top to bottom. The solid lines are the results of our calculations based on Eq. (A.11). The dashed curves are the results from Eqs. (34), (A.12), and (A.14), respectively. The dotted line is drawn using Eq. (27).

to us, because their calculation is a very complex problem that has not yet been solved. Since for the complete equation (7) we cannot calculate the high-order moments, let us turn to the approximate equations described in the previous section.

In the cumulant approximation the rotations in different fields are taken into account as independent ones. Therefore, in Eq. (14) we will simply add a new term from the inhomogeneous magnetic field and obtain the equation

$$D(t) = \exp\left\{-B^2\int_0^t\int_0^{t'} D(t'')dt'dt'' - W^2t^2/2\right\}. \qquad (25)$$

At $W^2 \neq 0$ we do not know the solution of this equation. However, we can calculate the coordinate of the singularity τ_{c0} via the radius of convergence of the series in powers of time:

$$D(t) = \sum_{n=0}^{\infty}\frac{(-1)^n}{(2n)!}D_n t^{2n}, \qquad (26)$$

for its coefficients we derive the following recurrence equation from (25):

$$D_{n+1} = B^2\sum_{k=0}^{n}\binom{2n+1}{2k}D_{n-k}D_k + (2n+1)W^2D_n.$$

The results of our calculation of τ_{c0}^2 from Eq. (18) are shown in Fig. 1. This dependence is well fitted (see Fig. 2) by the function

$$\tau_{c0}^2 M_2 = 2.35\ln\left\{\frac{2M_2}{B^2}\right\} + 3.05. \qquad (27)$$

τ_{c0}^2 gives a lower bound for τ_0^2:

$$\tau_0^2 > \tau_{c0}^2. \qquad (28)$$

The bound (27) is mathematically rigorous, but fairly rough, because it disregards the rotation anisotropy in systems with dipole–dipole interactions due to the rotation around one of the axes, the z axis, being preferential. For the secular part of the dipole–dipole interactions in a strong magnetic field $\Delta_x^2 = \Delta_y^2$ and $\Delta_z^2 = 4\Delta_x^2$. In this case, to increase the accuracy of the approximation, at the first stage it was suggested to take into account only the rotation around the z axis [32]. Since the rotations around the local z fields from the dipole–dipole-interactions and from the inhomogeneous magnetic z field add up, we obtain the propagator

$$G_0(t) = \exp\left\{-\Delta_z^2\int_0^t\int_0^{t'}\Gamma_z(t'')dt'dt'' - \frac{W^2t^2}{2}\right\}. \qquad (29)$$

The z-field correlation function in a self-consistent approximation is defined by the equation

$$\frac{d}{dt}\Gamma_z(t) = -aB^2\int_0^t \Gamma_x^2(t_1)\Gamma_z(t-t_1)dt_1 \tag{30}$$

via the ACF of the spin x component, for which, following [32], we write the equation

$$\Gamma_x(t) = G_0(t) - \varepsilon\int_0^t G_0(t-t_1) \times\int_0^{t_1}\Gamma_z(t_1-t_2)\Gamma_x(t_1-t_2)\Gamma_x(t_2)dt_1dt_2. \tag{31}$$

Equations (30) and (31) were derived in the approximation that the interactions with the x and y fields divide the interval of evolution into segments between which there is no correlation of the fields (pairing). The constants in the equations are determined by the transverse fields:

$$\varepsilon = \frac{B^2}{5} = \Delta_y^2, \quad aB^2 = \frac{2B^2}{5} = \Delta_y^2 + \Delta_x^2, \quad \Delta_z^2 = \frac{4B^2}{5}. \tag{32}$$

To calculate the coefficients of the time series, from (29)–(31) we derive the following system of recurrence equations:

$$G_{n+1} = \frac{4}{5}B^2\sum_{k=0}^{n}\binom{2n+1}{2k}G_kZ_{n-k} + (2n+1)W^2G_n,$$
$$Z_{n+1} = aB^2\sum_{k=0}^{n}Z_{n-k}\sum_{m=0}^{k}X_{k-m}X_m, \tag{33}$$
$$X_{n+1} = G_{n+1} + \varepsilon\sum_{k=0}^{n}G_{n-k}\sum_{m=0}^{k}X_{k-m}\sum_{p=0}^{m}\binom{2m}{2p}Z_{m-p}X_p,$$

where G_n, Z_n, and X_n are the coefficients of the series (26) for the functions $G_0(t)$, $\Gamma_z(t)$, and $\Gamma_x(t)$, respectively. The coordinates of the singularities calculated from these coefficients are presented in Fig. 1. The dependence of τ_0^2 on B^2/M_2 is well described (see the Appendix) by the function

$$\tau_0^2M_2 = 2\ln\left\{\frac{10M_2}{B^2}\ln\left(\frac{5M_2}{B^2}\right)\right\} + 2.3. \tag{34}$$

Apart from the result obtained from the coefficients with $n = 70$, for comparison, Fig. 1 presents the result for $n = 5$. The result for Eq. (31) is seen to be actually close to the result for the moments M_{10} of the complete equation (7). Previously, in [38] we investigated the simplified version of the equation derived from Eq. (31) at

$$\varepsilon = 0, \quad a = 1/2, \quad B^2 = \Delta_z^2. \tag{35}$$

The corresponding dependence (A.7) passes slightly below (34) (see Fig. 2).

4. DISCUSSION

The ACF form in the neighborhood of the singularities (17) closest to the coordinate origin determines the form of the high-frequency ACF asymptotics at $\tau_0|\omega| \gg 1$:

$$g_x(\omega) \approx A_x|\omega|\exp(-\tau_0|\omega|). \tag{36}$$

A relation between the winds of the spectra follows from the relation between the coordinates of the singularities (28):

$$g_x(\omega) \approx A_x|\omega|\exp(-\tau_0|\omega|) < A_{cx}|\omega|\exp(-\tau_{c0}|\omega|) \cong g_{cx}(\omega). \tag{37}$$

Thus, the wing of the spectrum for the function of the cumulant approximation $g_{cx}(\omega)$ serves as an upper bound for the wing of the spectrum of ACF (3).

Other time correlation functions of the spin system under consideration will have singularities at the same points of the imaginary time axis. Therefore, the wings of their spectra will have the same exponential cofactor and will differ only by the preexponential factors. For all these functions the wing of the function $g_{cx}(\omega)$ will serve as an upper bound, including that for the NMR absorption spectrum and the heating rate of the system by high harmonics under periodic driving. In both cases, the energy absorption rates are expressed via the Fourier transform of the correlation function of the system's total spin multiplied by the square of the amplitude of the radio-frequency field [40] or the square of the amplitude of the corresponding periodic driving harmonic [16, 20, 21].

Formula (36) shows that the energy absorption on the wing is exponentially small, i.e., it decays exponentially with increasing frequency. The results obtained in this paper allow the dependence of the process rate on inhomogeneous broadening W to be investigated. According to (27) and (34), the coefficient τ_0 in front of the frequency in the exponent in (36) decreases with increasing W due to an increase in $\sqrt{M_2}$ (23). If, however, the frequency is measured in units of $\sqrt{M_2}$, then the absorption drops, because $\tau_0^2M_2$ increases logarithmically, while the scale of $\sqrt{M_2}$ itself grows proportionally to W. The reason is that high frequencies on the wing of the ACF spectrum are formed due to a modulation of the local field from the surrounding spins oscillating in a transverse field (flip–flop rotations). The amplitude of these oscillations drops with increasing W, but the frequency grows. The logarithmic cofactor in τ_0 reflects this decrease in amplitude. At the same time, it expresses the obvious property of the system that there will be no exponential wing without dipole–dipole interactions. Note in this connection that there is no such logarithmic

cofactor in the estimation formula for the exponent derived in [16]. This suggests that although the estimate of the bound suggested in [16] is correct, it is rough and was obtained with a large margin.

The approximation of a Gaussian random field applied above disregards the correlation between the contributions in the field from various surrounding spins, which gives rise to loops of couplings on the lattice and multiple couplings. In the case of a nearest-neighbor interaction, the correlation contribution was shown to be small for lattices of a high space dimension [33]. Estimates show them to be also small in three-dimensional lattices with dipole–dipole interactions [16, 34]. In both cases, the correlation effects weaken the field action and lead to an increase in τ_0. Consequently, the function of the cumulant approximation $g_{cx}(\omega)$ (37) will remain a rigorous bound for the heating rate in real spin systems.

APPENDIX

Let us investigate the ACF behavior in the neighborhood of the nearest singularities on the imaginary time axis. The form (17) for the ACF in the neighborhood of a singularity follows from the form of the nonlinear equations for them. This can be made sure by a method similar to the Painlev'e method for analyzing the movable singularities of nonlinear ordinary differential equations [41]. Let us take an ACF near a singularity in the form

$$\Gamma_\alpha(t) \approx -A_\alpha(t - i\tau_0)^{-p} \tag{A.1}$$

and substitute it into Eq. (8) under the condition (12). Calculating the most divergent part of the integral on the right-hand side of Eq. (8) and performing differentiation on its left-hand side, we find

$$\frac{A_x p}{(t - i\tau_0)^{p+1}} \approx \frac{A_z A_y(\Delta_z^2 + \Delta_y^2)}{(2p-1)(t - i\tau_0)^{2p-1}}. \tag{A.2}$$

For the equality in (A.2) to hold, the exponents and coefficients must coincide:

$$p + 1 = 2p - 1, \quad A_x p(2p-1) = A_z A_y(\Delta_z^2 + \Delta_y^2). \tag{A.3}$$

It follows from the first equation in (A.3) that $p = 2$. The nonlinear equations of the same approximation as (8) for the ACF of two other spin components give two more equalities:

$$6A_y = A_z A_x M_{2y}, \quad 6A_z = A_y A_x M_{2z}, \tag{A.4}$$

where $M_{2x} = (\Delta_z^2 + \Delta_y^2)$, $M_{2y} = (\Delta_z^2 + \Delta_x^2)$, and $M_{2z} = (\Delta_x^2 + \Delta_y^2)$. From the system of three equations for the amplitudes (A.3) and (A.4) we find

$$A_\alpha = 6\sqrt{M_{2\alpha}/(M_{2x}M_{2y}M_{2z})}. \tag{A.5}$$

Let us turn to the general nonlinear equation for the ACF (7). The cofactor $g_\beta(t_k - t_q) = \Delta_\beta^2\Gamma_\beta(t_k - t_q)$ and simultaneously the integration over the time variables t_k and t_q are added in the series for the memory function $G_\alpha(t)$ when passing from the term with m pairs to the term with $m + 1$ pairs. Consequently, the form (17) of the singularity (A.1) with $p = 2$ will also be retained when the remaining terms of the series for the memory function are included, although the values of A_α and τ_0 themselves will change in this case.

Let us now investigate the ACF behavior in the neighborhood of the nearest singularities on the imaginary time axis in the presence of an inhomogeneous magnetic field using the solution of the nonlinear equations (29)–(31) as an example. Let us substitute the singular parts in the form (17) of the corresponding functions into Eqs. (29)–(31). Solving the equations for the coefficients of the singular parts, we find

$$\Gamma_z(t) \approx \frac{2/\Delta_z^2}{(it \pm \tau_0)^2}, \quad \Gamma_x(t) \approx \frac{\sqrt{12/aB^2\Delta_z^2}}{(it \pm \tau_0)^2},$$
$$G_0(t) \approx \left(1 - \frac{\varepsilon}{3\Delta_z^2}\right)\frac{\sqrt{12/aB^2\Delta_z^2}}{(it \pm \tau_0)^2}. \tag{A.6}$$

Let us find an estimate for τ_0^2 at $W^2/B^2 \gg 1$. Consider a linearized version of the system of equations (29)–(31) on the axis of imaginary time $t = i\tau$:

$$\Gamma_z(i\tau) = 1 + aB^2\int_0^\tau\int_0^{\tau_1}\Gamma_x^2(i\tau_2)d\tau_1 d\tau_2$$
$$\approx \frac{aB^2}{4M_2^2\tau^2}\exp(M_2\tau^2), \tag{A.7}$$

$$G_0(i\tau) = \exp\left\{\frac{(M_2 - \varepsilon)\tau^2}{2}\right\},$$
$$\Gamma_x(i\tau) = \exp\left(\frac{M_2\tau^2}{2}\right), \tag{A.8}$$

where $M_2 = B^2 + W^2$, and the asymptotic value is taken for the integral of the error function of an imaginary argument. The functions (A.7) and (A.8) have no singularities at a finite distance from the coordinate origin. The nonlinearity of Eqs. (29)–(31) is responsible for the appearance of such singularities. The nonlinearity will manifest itself at those values of the imaginary time at which the nonlinear contribution from $\Gamma_z(t)$ in the exponent for $G_0(i\tau)$ (29) exceeds the linear one (A.8). Hence we obtain the condition

$$\frac{aB^2\Delta_z^2}{16M_2^3\tau^2}\exp(M_2\tau^2) \geq \frac{(M_2 - \varepsilon)\tau^2}{2},$$

which leads to the following equation for estimating τ_0 after the substitution of parameters (32):

$$M_2\tau_0^2 = 2\ln\left(\frac{5M_2}{B^2}M_2\tau_0^2\right) + \ln\left(1 - \frac{B^2}{5M_2}\right). \quad (A.9)$$

From (A.9) we find the sought-for estimate

$$\tau_0^2 M_2 = 2\ln\left\{\frac{10M_2}{B^2}\ln\left(\frac{5M_2}{B^2}\right)\right\} + c_1. \quad (A.10)$$

The corresponding dependence at $c_1 = 2.3$ (34) is presented in Fig. 2 and describes well the results of our numerical calculation of τ_0 based on the formula

$$\tau_{0n}^2 = n(2n+1)\{X_{n-1}/X_n + Z_{n-1}/Z_n\} \quad (A.11)$$

at $n = 85$. This formula allowed the τ_{0n} oscillations at $B^2/M_2 < 0.01$ attributable to the anisotropy of dipole–dipole interactions to be smoothed.

For the simplified version of Eq. (31) with parameters (35) in [38][2] we found the dependence of the coordinate of a singularity

$$\tau_0^2 M_2 = 2\ln\left\{\frac{8M_2}{B^2}\ln\left(\frac{4M_2}{B^2}\right)\right\} + 2.3, \quad (A.12)$$

which, as can be seen from Fig. 2, passes slightly below (A.10).

In a similar way, for Eq. (25) we find

$$D(t) \approx \frac{2/B^2}{(it \pm \tau_{c0})^2}, \quad (A.13)$$

while for τ_{c0}^2 at $W^2/B^2 \gg 1$ we obtain an estimate

$$\tau_0^2 M_2 = 2\ln\left\{\frac{2M_2}{B^2}\ln\left(\frac{2M_2}{B^2}\right)\right\} + c_2, \quad (A.14)$$

which is presented in Fig. 2 and agrees well with the results of our numerical calculation at $c_2 = 1.62$ in the interval $B^2/W^2 < 0.1$. The approximating function (27) that conveys better the behavior of τ_{c0} for weak inhomogeneous fields is also shown there.

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