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CONDENSED MATTER

On the Effect of an Inhomogeneous Magnetic Field on High-Frequency Asymptotic Behaviors of Correlation Functions of Spin Lattices

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Singular points of spin autocorrelation functions on the imaginary time axis, which determine the arguments of exponential high-frequency asymptotic behaviors, have been analyzed. It has been shown that randomly distributed inhomogeneous magnetic fields expand the wings of spectra of autocorrelation functions and, thereby, intensify the heating of a system subjected to variable magnetic fields, which are used to create effective Hamiltonians or at the saturation of inhomogeneously broadened EPR lines.

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Study of the high-frequency behavior of dynamic correlation functions has currently become of particular interest [1–6] because of the possibility of creating new states of matter by applying a time-dependent external action [7–13]. Such studies are topical for the creation of topological states [8, 9, 11, 13], time crystals [12], and simulation of certain quantum systems using other quantum systems [7]. To increase the time of existence of created states, it is necessary to estimate the dependence of the rate of heating of a system on the parameters of the external action. Such an estimate for the high-frequency asymptotic behavior of the rate was performed in [1–6], where an exponential dependence on the frequency of the external action was obtained.

The exponential frequency dependence of high-frequency asymptotic behaviors of spin correlation functions is due to the existence of singular points of these functions on the imaginary time axis; the theory of these singular points was developed in [14–22]. The coordinate τ_0 of the nearest singular point determines the argument of the exponent $\exp(-\tau_0|\omega|)$. We analyze the dependence of the coordinate of a singular point on the dimension of space for systems with interaction between nearest neighbors [17, 18] and with dipole–dipole interaction [19, 20]. In one-dimensional spin systems, singular points are absent [23] and correlation functions have stronger frequency dependences $\sim\exp(-\omega^2)$ for the *XY* model [24] and $\sim\exp(-|\omega|\ln|\omega|)$ for the *XXZ* model [25]. Theoretical results obtained for three-dimensional lattices are in good agreement with experimental data for both homonuclear [19] and heteronuclear [20] systems. Finally, in [21, 22], we studied the concentration dependence of τ_0 in magnetically dilute spin lattices.

In the cited works, we considered spin systems in a homogeneous magnetic field. However, the dynamics of spin systems in an inhomogeneous magnetic field is of no less interest. First, an increase in inhomogeneity is accompanied by a transition from a thermalized state to a many-body localized one [26] with a significant change in many properties of spin systems [27–31]. Second, in magnetically dilute systems of electron spins with inhomogeneously broadened EPR lines, the absorption of the energy of the variable magnetic field and the establishment of spin temperature make a difference with that in homogeneous systems [32]. The description of these processes widely involves the concept of a spin packet, i.e., a set of spins having the same Larmor frequency [32, 33]. From experimental data on the saturation of the EPR line, it was found in [33] that the wings of the spectrum of the spin packet decrease exponentially. In this work, we study the effect of the inhomogeneous magnetic field on the coordinates of the nearest singular points of correlation functions on the imaginary time axis, which determine the high-frequency asymptotic behaviors of correlation functions and, thereby, slow relaxation processes and the wings of the spectrum of the spin packet.

We consider the system of spins with the secular part of the dipole–dipole interaction and inhomogeneous Zeeman interaction

$$H = \sum_i \omega_i S_{zi} + \sum_{i\neq j} b_{ij} S_{zi} S_{zj} - \frac{1}{2}\sum_{i\neq j} b_{ij} S_{+i} S_{-j}, \quad (1)$$

where $b_{ij} = \gamma^2\hbar(1 - 3\cos^2\theta_{ij})/2r_{ij}^3$ is the dipole–dipole coupling constant, $\mathbf{r}_{ij}$ is the vector connecting the ith and jth spins, θ_{ij} is the angle between the vector $\mathbf{r}_{ij}$ and static external magnetic field, $S_{\alpha i}$ is the αth component ($\alpha = x, y, z$) of the vector spin operator at the ith site, and $S_{\pm j} = S_{xj} \pm iS_{yj}$. Here and below, the energy is given in frequency units. We assume that the Larmor frequencies of spins ω_i are random variables. The following two distributions are most often used.

(i) The normal distribution

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

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

(ii) The uniform distribution in the interval $[-W\sqrt{3}, W\sqrt{3}]$ with the same variance.

The autocorrelation function of the spin at the jth site of the lattice is specified in the high-temperature approximation by the formula

$$\Gamma_{\alpha j}(t) = \mathrm{Tr}\{\exp(iH_j t)S_{\alpha j}\exp(-iH_j t)S_{\alpha j}\}/\mathrm{Tr}\{(S_{\alpha j})^2\}, \quad (3)$$

where $H_j = H - \omega_j S_{zj}$ is the Hamiltonian in the reference frame rotating at the Larmor frequency of the jth spin [34]. For the autocorrelation function, we use the system of equations from [16]:

$$\Gamma_x(t) = \exp\left\{-B^2 \int_0^t\int_0^{t'} \Gamma_z(t'')dt'dt''\right\}, \quad (4)$$

$$\frac{d}{dt}\Gamma_z(t) = -\frac{1}{2}B^2\int_0^t D^2(t_1)\Gamma_z(t - t_1)dt_1, \quad (5)$$

where $B^2 = \frac{1}{N}\sum_{i\neq j} b_{ij}^2$ and $\Gamma_\alpha(t) = \langle\Gamma_{\alpha j}(t)\rangle$ is the autocorrelation function averaged over the distribution of Larmor frequencies. For the normal distribution,

$$D(t) = \exp(-W^2t^2/2)\Gamma_x(t); \quad (6)$$

and for the uniform distribution,

$$D(t) = \frac{\sin\sqrt{3}Wt}{\sqrt{3}Wt}\Gamma_x(t). \quad (7)$$

The system of equations was obtained in the approximation of self-consistent fluctuating local field. Equation (4) describes the average precession of the spin in the field specified by a Gaussian random process whose correlation function is determined by Eq. (5) in terms of flip-flop transitions of spins with different Larmor frequencies.

Pairs of spins located at neighboring sites of the lattice at the minimum distance play an important role in magnetically dilute systems of nuclear spins. For example, a signal from such pairs was seen in the ^{29}Si NMR spectrum in a silicon crystal [35, 36] and the contribution from such pairs is responsible for the concentration dependence of the wings of the NMP spectrum [22]. The situation in magnetically dilute systems of electron spins is different. The electron magnetic moment is three orders of magnitude larger than the nuclear magnetic moment. For this reason, resonance frequencies of pairs of electron spins located at the minimum distance can exceed not only the width of EPR lines but also the average Larmor frequency ω_0 [37], in particular, because these frequencies are specified not only by dipole–dipole interaction but also by exchange interactions. For this reason, we calculate the spectrum of EPR lines disregarding such pairs of spins. We introduce the distance R above which the spectrum of pairs is within the spectrum of EPR lines and the parameter $\delta^2 = \sum_{|r_{ij}|>R} b_{ij}^2$, which is considered as an empirical parameter. For such systems, in Eqs. (4) and (5), we set $B^2 = c\delta^2$, where c is the concentration of spins, which is the ratio of the number of magnetic atoms (spins) to the total number of sites of the lattice. Then, $\Gamma_\alpha(t) = \langle\Gamma_{\alpha j}(t)\rangle$ is the autocorrelation function averaged not only over the distribution of Larmor frequencies but also over the independent distribution of spins over the sites of the lattice with the probability c.

Previous studies [15, 16] of nonlinear equations (4) and (5) for autocorrelation functions without inhomogeneous broadening ($W^2 = 0$) revealed singular points on the imaginary time axis. Near the singular points closest to the coordinate origin, the autocorrelation function has the form

$$\Gamma_\alpha(t) \approx \frac{A_\alpha}{(it \pm \tau_0)^2}. \quad (8)$$

The coordinate of the nearest singular point $\tau_0 = 2.61/B$ was found in [16]. At $W^2 \neq 0$, substituting Eq. (8) into Eqs. (4) and (5) and equating the coefficients of singular terms, we obtain

$$A_z = 2/B^2, \quad A_x = \exp(-W^2\tau_0^2/2)\sqrt{24}/B^2, \quad A_D = \sqrt{24}/B^2 \quad (9)$$

for the normal distribution given by Eq. (6) and

$$A_z = 2/B^2, \quad A_x = \frac{6\sqrt{2}W\tau_0}{B^2 \sinh\sqrt{3}W\tau_0}, \quad A_D = \sqrt{24}/B^2 \tag{10}$$

for the uniform distribution given by Eq. (7).

We first estimate τ_0^2 at $W^2/B^2 \gg 1$ for the normal distribution (6). The linearized variant of the system of Eqs. (4)–(6) on the imaginary time axis $t = i\tau$ has the form

$$\Gamma_z(i\tau) = 1 + \frac{1}{2}B^2 \int_0^{\tau}\int_0^{\tau_1} D^2(i\tau_2)d\tau_1 d\tau_2 \approx \frac{B^2}{8M_2^2\tau^2}\exp(M_2\tau^2), \tag{11}$$

$$D(i\tau) = \exp(M_2\tau^2/2), \tag{12}$$

where $M_2 = B^2 + W^2$ and the asymptotic value is taken for the integral of the error function. Functions (11) and (12) do not have singular points at a finite distance from the coordinate origin. Such singular points appear because of the nonlinearity of Eqs. (4)–(6). Nonlinearity is manifested at imaginary time values for which the nonlinear contribution from $\Gamma_x(t)$ in the exponent in Eq. (6) for $D(i\tau)$ becomes larger than the linear contribution in Eq. (12). This condition gives

$$\frac{B^4}{32M_2^3\tau^2}\exp(M_2\tau^2) \geq \frac{M_2\tau^2}{2}, \tag{13}$$

which provides the following equation for estimate of τ_0:

$$M_2\tau_0^2 = 2\ln\left(\frac{4M_2}{B^2}M_2\tau_0^2\right). \tag{14}$$

Formula (14) gives the desired estimate

$$M_2\tau_0^2 = 2\ln\left\{\frac{8M_2}{B^2}\ln\left(\frac{4M_2}{B^2}\right)\right\} + b_1. \tag{15}$$

Here, b_1 is a constant, which will be determined below from comparison with the numerical calculation.

For the uniform distribution (7), the equation for estimate of τ_0 is similarly obtained in the form

$$2\sqrt{3}W\tau_0 = 2\ln\left(\frac{12W^2}{B^2}\right) + 3\ln\left(2\sqrt{3}W\tau_0\right). \tag{16}$$

After the substitution of $M_2 = B^2 + W^2$ for W^2 in Eq. (16), which does not change the asymptotic behavior at $W^2/B^2 \gg 1$ but removes nonphysical divergence at $W^2 = 0$, the desired estimate is obtained from Eq. (16) as

$$\tau_0\sqrt{M_2} = \frac{1}{\sqrt{3}}\ln\left\{\frac{12M_2}{B^2}\left(2\ln\frac{12M_2}{B^2}\right)^{3/2}\right\} + b_2. \tag{17}$$

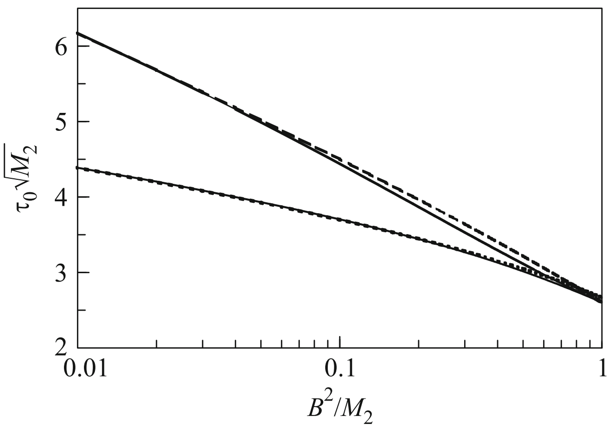

Fig. 1. Coordinates of singular points $\tau_0\sqrt{M_2}$ versus the ratio B^2/M_2. The solid lines are numerical calculations by Eq. (19) for the (lower line) normal distribution and (upper line) uniform distribution. The dotted line is obtained by Eq. (15) at $b_1 = 2.3$ and the dashed line is obtained by Eq. (17) at $b_2 = -0.22$.

The exact coordinate of the singular point τ_0 is determined in terms of the radius of convergence of power series in time for the autocorrelation function

$$\Gamma_z(t) = \sum_{n=0}^{\infty}(-1)^n Z_n t^{2n}/(2n)!, \quad D(t) = \sum_{n=0}^{\infty}(-1)^n D_n t^{2n}/(2n)! \tag{18}$$

by the formula

$$\tau_0^2 = \lim_{n\to\infty}\frac{2n(2n+1)Z_{n-1}}{Z_n}. \tag{19}$$

The recurrence relations for the coefficients are obtained by substituting series (18) into Eqs. (4) and (5) and equating the coefficients of equal powers of time on both sides:

$$X_{n+1} = B^2\sum_{k=0}^{n}\binom{2n+1}{2k}X_n Z_{n-k},$$

$$D_n = \sum_{k=0}^{n}\binom{2n}{2k}X_{n-k}P_k, \tag{20}$$

$$D_n^{(2)} = \sum_{k=0}^{n}\binom{2n}{2k}D_{n-k}D_k, \quad Z_{n+1} = B^2\frac{1}{2}\sum_{k=0}^{n}D_{n-k}^{(2)}Z_k,$$

where $P_k = (W^2/2)^k (2k)!/k!$ for the normal distribution and $P_k = (3W^2)^k/(2k+1)$ for the uniform distribution. The results of the calculation are shown in Fig. 1.

As is seen in Fig. 1, Eqs. (15) and (17) obtained above to estimate τ_0 reproduce well the calculated dependences at $b_1 = 2.3$ and $b_2 = -0.22$, respectively. These formulas describe the dependences of the coordinate of a singular point on the inhomogeneous broadening and concentration.

After the Fourier transform of the function $\Gamma_x(t)$ given by Eqs. (8)–(10), the high-frequency asymptotic behavior of the spectrum of the spin autocorrelation function is obtained in the form

$$g_x(\omega) \cong A_x|\omega|\exp(-\tau_0|\omega|), \tag{21}$$

where the coordinate of the singular point τ_0 can be taken from Eqs. (15) and (17) or the calculations shown in Fig. 1.

Formula (21) at $B^2 = c\delta^2$ describes the wings of the spectrum of the spin packet in magnetically dilute systems with inhomogeneously broadened EPR lines. The wing decreases exponentially. The scale of the frequency dependence is determined by inhomogeneous broadening; i.e., the length of the wings of the spin packet increases with inhomogeneous broadening. The reason is that the shape of a wing is determined by the modulation of the local field on the spin because of the flip-flop interaction between surrounding spins creating this field through the zz interaction. The large difference between the Larmor frequencies of flipping spins makes a large contribution to the frequency of such modulation. This means that the absorption of the energy of the microwave field with the frequency Ω on the wing of the spin packet with the resonance (Larmor) frequency ω_j is accompanied by flip-flop transitions of surrounding spins. In this case, the detuning energy $\omega = \Omega - \omega_j$ is transformed to the energy of the so-called reservoir of local fields [32, 38], which is formed by the dipole–dipole interaction and differences between the Zeeman energies of spins with different Larmor frequencies. Thus, the theory presented above explains why the long wings of the spectra of spin packets responsible for quite fast experimentally observed establishment of a common spin temperature in the reservoir of local fields [32] hold at large inhomogeneous broadening. Moreover, this theory explains the experimentally observed exponential shape of wings of the spectra of spin packets [33].

The theory can be applied to estimate the heating of spin systems subjected to a periodically varying magnetic field or periodic sequences of pulses of a variable magnetic field. The necessary relations of rates of processes to spin correlation functions were derived in [39]. The results obtained above make it possible to estimate the dependence of high-frequency asymptotic behaviors on the inhomogeneous magnetic field. The used approximation of self-consistent fluctuating local field is strict for infinite-dimensional lattices [18]. For three-dimensional lattices, the effect of excluded volume and the inclusion of loops of links [17–20] will increase the coordinate of a singular point on the imaginary time axis. The result obtained in this work should be considered as an approximate upper estimate for the high-frequency behavior of the correlation function (to obtain a more accurate bound, one should consider more complex equations derived in [15, 16]). Finally, for the complete description of the absorption of the energy of the high-frequency field and the transition from the thermalized state to the many-body localized state, it is necessary to estimate the rate of energy propagation in an inhomogeneous spin system (diffusion or cross relaxation) and to derive the corresponding kinetic equations.

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