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MODERN PROBLEMS OF SPIN DYNAMICS

Proceedings of ITEP seminar
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UDK 539.1 M-16

MODERN PROBLEMS OF SPIN DYNAMICS.Proceedings of ITEP seminar on spin dynamics Extended abstracts: Preprint ITEP 35-98/

Editor F.S.Dzheparov - M., 1998 - 28p.

The issue contains extended abstracts of 13 reports (see Content) of the ITEP seminar on spin dynamics have been done during January-June 1998.

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Saturation of Dipole Energy under Rotation of the Sample. Slow Rotation

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An extension of the well known Nakajima-Zwanzig projection technique for considering time-dependent projection operator is presented. The present theory is adopted for quasiadiabatic evolution and saturation of dipole energy is studied in details.

It is known that, in static sample, a homonuclear dipole-coupled spin system can be settled in a quasiequilibrium state characterized by two inverse spin temperatures

$$\rho_{qs} \sim 1 - \beta_Z \omega_0 I_Z - \beta_D \mathcal{H}'_D \tag{1}$$

where $\mathcal{H}'_D$ is the secular homonuclear dipolar Hamiltonian. Under rotation of the sample, $\mathcal{H}'_D$ becomes time-dependent and doesn't commute with itself at different times : $[\mathcal{H}'_D(t), \mathcal{H}'_D(t')] \neq 0$ producing a saturation. If time-dependence of $\mathcal{H}'_D(t)$ is slow the relaxation theory can be based on the time dependent projection operator

$$\pi(t)A = \langle A \rangle + I_Z \frac{\langle A I_Z \rangle}{\langle I_Z^2 \rangle} + \mathcal{H}'_D(t) \frac{\langle A \mathcal{H}'_D(t) \rangle}{\langle \mathcal{H}'^2_D(t) \rangle}, \quad \langle \ldots \rangle = Tr[\ldots] \tag{2}$$

Using natural definitions

$$\beta_Z = -\frac{1}{\omega_0} \frac{\langle I_Z \pi \rho \rangle}{\langle I_Z^2 \rangle}, \quad \beta_D = -\frac{\langle \mathcal{H}'_D \pi \rho \rangle}{\langle \mathcal{H}'^2_D \rangle} \tag{3}$$

and starting from the Liouville equation

$$\frac{d\rho}{dt} = -i\,[\mathcal{H}'_D(t), \rho(t)] = -i\mathcal{L}_D(t)\rho(t) \tag{4}$$

one obtains after some calculations the exact master equations

$$\frac{d\beta_Z}{dt} = 0, \quad \frac{d\beta_D}{dt} = -\frac{\beta_D}{2}\frac{d}{dt}\left(\ln \langle \mathcal{H}'^2_D(t) \rangle\right) - \int_0^t M(t,\tau)\beta_D(\tau)d\tau \tag{5}$$

where the memory function $M(t,\tau)$ is

$$M(t,\tau) = \langle \dot{\mathcal{H}}'_D(t)\overline{\pi}(t)S(t,\tau)\overline{\pi}(\tau)\dot{\mathcal{H}}'_D(\tau) \rangle / \langle \mathcal{H}'^2_D(t) \rangle \tag{6}$$

$$S(t,\tau) = \widehat{T} \exp\left\{-i\int_t^\tau \left[\mathcal{L}_D(u) + i\dot{\pi}(u)\overline{\pi}(u)\right] du\right\}, \quad \overline{\pi}(t) = 1 - \pi(t) \tag{7}$$

For convenience, a slow variable $\beta_S(t)$ is introduced through

$$\beta_D(t) = \left[\langle \mathcal{H}'^2_D(0) \rangle / \langle \mathcal{H}'^2_D(t) \rangle\right]^{1/2} \beta_S(t) \tag{8}$$

which evolution is given by

$$\frac{d\beta_S}{dt} = -\int_0^t M_S(t, t-\tau)\beta_S(t-\tau)d\tau \tag{9}$$

$$M_S(t,\tau) = \left[\langle \mathcal{H}'^2_D(t) \rangle \langle \mathcal{H}'^2_D(\tau) \rangle\right]^{-1/2} \langle \dot{\mathcal{H}}'_D(t)\overline{\pi}(t)S(t,\tau)\overline{\pi}(\tau)\dot{\mathcal{H}}'_D(\tau) \rangle \tag{10}$$

The Eqs. 5-10 are exact. The contribution $\dot{\pi}\overline{\pi} \sim \omega_R$ can be neglected in the slow rotation regime with respect to $\mathcal{L}_D \sim \omega_l$ (where $\omega_l = \sqrt{M_2}$ is usual local frequency). Then

$$M_S(t, t-\tau) \approx \frac{1}{\langle \mathcal{H}'^2_D(t) \rangle} \langle \dot{\mathcal{H}}'_D(t) e^{-i\mathcal{L}_D(t)\tau} \dot{\mathcal{H}}'_D(t) \rangle \tag{11}$$

Finally one obtains

$$\beta_D(t) = \left[\langle \mathcal{H}'^2_D(0)\rangle / \langle \mathcal{H}'^2_D(t)\rangle\right]^{1/2} \beta_D(0) e^{-\overline{W}_S t} \tag{12}$$

where

$$\overline{W}_S = \frac{1}{T_R}\int_0^{T_R} W_S(t)dt \tag{13}$$

$$W_S(t) = \frac{1}{\langle \mathcal{H}'^2_D(t)\rangle}\int_0^{\infty} \langle \dot{\mathcal{H}}'_D(t) e^{-i\mathcal{L}_D(t)\tau} \dot{\mathcal{H}}'_D(t)\rangle d\tau \tag{14}$$

The results for $W_S(t)$ are very similar to usual forms of relaxation rate if $\dot{\mathcal{H}}'_D(t)$ is considered as the perturbation of the main Hamiltonian $\mathcal{H}'_D(t)$. It can be checked that $\overline{W}_S \sim \omega_R^2/\omega_l$.

An initial state with large dipole order can be produced in usual way by the well known Jeener-Broekaert pulse sequence.

We studied the saturation of dipole energy in experiment as well [2]. Measurements on adamantane for various orientations and values of the rotation spinning speed were carried out. As a result Eqs.12,13 give excellent description of the experiment for $\omega_R \ll \omega_l$.

Our theoretical treatment of the quasiadiabatic processes is quite general and it can be successfully applied, for example, to all problems discussed in [1].

The case of fast rotation is presented in a second contribution.

The work was fulfilled in the SCM laboratory at CEA Saclay (France), it was supported by a grant from CNRS.

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Saturation of Dipole Energy under Rotation of the Sample. Fast Rotation

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The creation and evolution of dipole order under fast sample rotation ($\omega_R \gg \omega_l$) is investigated for the first time. It is shown that the Jeener-Broekaert sequence is still efficient for creating a pseudodipolar order.

In static sample or in the limit of adiabatic rotation, a homonuclear dipole-coupled spin system can be prepared in the quasiequilibrium state

$$\rho_{qs} \sim 1 - \beta_Z \omega_0 I_Z - \beta_D \mathcal{H}'_D$$

where $\mathcal{H}'_D$ is the homonuclear dipolar Hamiltonian. Under fast rotation of the sample when ω_R is stronger than ω_l (where $\omega_l = \sqrt{M_2}$ is usual local frequency), the above expansion is no longer valid and an appropriate effective Hamiltonian, mastering corresponding quasiequilibrium and saturation can be constructed.

Under rotation of the sample, the dipole Hamiltonian may be expanded as

$$\mathcal{H}'_D(t) = H_0 + \sum_{m\neq 0} H_m e^{-im\omega_R t}. \tag{1}$$

It is possible to reduce the time-dependent part of the Hamiltonian by canonical transformations [1] by a factor $\epsilon = \omega_l/\omega_R \ll 1$ and handled it as a perturbation. The spin temperature approach can be applied then to estimate the saturation of dipole order. Let

$$S^{(1)}(t) = +i \sum_{m\neq 0} \frac{H_m}{m\omega_R} e^{-im\omega_R t} \tag{2}$$

The Liouville equation of $\tilde{\rho}(t) = e^{+iS^{(1)}(t)}\rho(t)e^{-iS^{(1)}(t)}$ is

$$i\frac{d\tilde{\rho}}{dt} = [H_s^{(1)} + H_f^{(1)}(t), \tilde{\rho}], \tag{3}$$

where to first order

$$H_s^{(1)} = H_0 + \sum_{m>0} \frac{1}{m\omega_R}[H_m, H_{-m}] + o(\epsilon^2), \tag{4}$$

$$H_f^{(1)} = \sum_{m\neq 0} \frac{1}{m\omega_R}[H_m, H_0]e^{-im\omega_R t} + \frac{1}{2}\sum_{0\neq m\neq n\neq 0} \frac{1}{m\omega_R}[H_m, H_{-n}]e^{-i(m+n)\omega_R t} + o(\epsilon^2).$$

The procedure Eqs. 1-4 can be iterated leading to a new fast oscillating Hamiltonian $H_f^{(2)} \sim \epsilon H_f^{(1)}$ and so on. The convergence of this expansion must be checked in calculation of the rate of saturation by comparison of rates and states calculated after n and $n+1$ iterations and the method works when difference is small, that corresponds to high rotation speed in leading terms.

The analysis of the behavior of the new effective dipole-dipole Hamiltonian $H_s^{(1)}$ with respect to 3d rotation in spin space reveals that $H_s^{(1)}$ is the sum of a zero and

second rank tensor. Then, the Jeener-Broekaert sequence is efficient for preparing the spin system with high dipole order corresponding to

$$\tilde{\rho}_{qs} = 1 - \beta_S H_s^{(1)}$$

By standard theoretical treatment in relaxation calculation, the saturation of this order by the time-dependent perturbation $H_f^{(1)}(t)$ can be easily obtained. Calculations lead to

$$\frac{d\beta_S}{dt} = -W_f \beta_S,$$

$$W_f = \sum_{m>0} \int_{-\infty}^{\infty} M_{m,m}(\tau) e^{-im\omega_R \tau} d\tau,$$

$$M_{m,n}(\tau) = \frac{1}{\langle H_s^2 \rangle} \langle [H_s, \widetilde{H}_{f,m}^{(1)}(\tau)][\widetilde{H}_{f,-n}^{(1)}(\tau), H_s] \rangle,$$

$$\widetilde{H}_{f,m}^{(1)}(\tau) = e^{iH_s\tau} H_{f,m}^{(1)}(\tau) e^{-iH_s\tau}.$$

According to modern point of view on high frequency asymptotics of spin correlation functions [2,3] we can expect, that $\log W_f \propto -\omega_R/\omega_l$, where $\omega_l^2 = \langle JJ^+ \rangle / \langle I_+ I_- \rangle$, $J = [I_+, H_s^{(1)}]$, and $\langle ... \rangle = Tr(...)/Tr1$.

Measurements on adamantane for various orientations and values of the rotations were carried out. High-spinning speed pseudodipolar spectra were obtained and the predicted decrease of saturation with respect to ω_R was observed [4].

The work was fulfilled in the SCM laboratory at CEA Saclay (France), it was supported by a grant from CNRS.

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From 10^{10} Spins To a Single Spin Using Scanning Tunneling Microscope.

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The possibilities to observe the ESR signal of a single spin with use scanning tunneling microscope (STM) and the probable mechanisms of this phenomenon are analysed.

The sensitivity of conventional ESR is about 10^{10} spins. The ordinary ways to improve it are both by icreasing the observed magnetization and improving the efficiency of detection by observing high energy photons.

The detection sensitivity can be extended to a single spin. In the optical methods of the magnetic resonance detecting the microwave irradiation changes the single molecule fluorescence. Perhaps the alternative approach to the single particle ESR study is the use of STM. So far as the scanning tunneling microscopy is the only possible method allowing us to study the structure of the conducting surfaces with atomic resolution [1], the joining one with ESR opens promising perspectives in surface science because the ESR is one of the most of powerful traditional techniques to explore the local characters of a condensed matter.

Recently some articles were published [2-5] contained, as suggested, results of experimental observing by STM of the ESR signals of a single local paramagnetic center located at a SI(111)7×7 surface which was thermally oxidizing. Unfortunately as mentioned by authors of Ref. [2-5] their results perhaps are not has one meaning. There is why the problem of the joining the STM and single spin ESR-spectroscopy actual still now.

We assume that at the room temperature and for the moderate external magnetic fields ($H_0 \approx 100 \div 1000$Oe) the most of perspective type of the paramagnetic center ESR of which affects the tunneling current are a pair of impurity atoms (ions) with nonzero spins coupling by appropriate exchange interaction. Let us mark, that one of the atoms can be situated at the tip of STM as well. Let us name these pairs as singlet-triplet scattering centers (STSC).

Probably there are some different concrete types of STSC in semiconductors. The first type of STSC what we should like to notice is the positive ion (e.g. Cr^+, Mn^{2+}, Ni^+,...) locates at the semiconductor surface. We can assume also that it confines one of the vacant electrons and so generates something like hydrogen atom. The radius of this atom varies from 30 up to 100 Å in dependence of the dielectric constant. The second one type we should like to notice appears if the pair of donor atoms (e.g. phosphorus atoms in silicon) located not so far one from another one. In this situation atoms forms something like a hydrogen molecule. The ESR spectra of this exchange coupled system was studied by Ch. Slichter [6]. So, the most of simple spin-Hamiltonian of the above STSC is

$$H = \hbar\omega_1 S_{z1} + \hbar\omega_2 S_{z2} + J S_1 S_2 + H_{int} \qquad (1)$$

In Eq. (1) S_1 and S_2 are electron (or atom) spins, ω_1 and ω_2 are their Zeeman

frequencies differs e.g. because of different values of g-factors or their anisotropy or the slope of constants of the crystal field and so on, J – is the exchange constant, H_{int} includes all other interactions i.e. hyperfine one. Though the constant of the hyperfine interaction sometimes exceeds the constant J, we shall suppose hyperfine constant to be weak. The strong one and it anisotropy will not affect the qualitative picture. Zero approximation for the Hamiltonian (1) means that spin singlet and triplet are right functions. But because of different Zeeman frequencies in Eq. (1) the above functions will be mixed with the parameter of mixture about: $\alpha \propto \hbar(\omega_1 - \omega_2)/J$. If the constant J is not too large the mixture is quite effective process. So, the natural ratio of populations of the singlet and triplet states 1:3 will change (to oscillate) with the time and whether there is the time-dependent magnetic field H_1 with the Larmor frequency this changing will become irreversible if the relaxation is omitted. As the difference in the scattering amplitudes of the tunneling electrons on the singlet and triplet states reaches 100%, the changing of populations can dramatically affects the resistance and thus acts on the tunneling current Our estimation demonsrates that we can achieve conditions needing to observe ESR effects with the experimental equipment described in Ref. [2-5].

At low temperatures and for a large amount of the external magnetic field H_0, anybody has more ordinary and simple situation to study ESR of a single spin by STM. As known at low temperatures the resistance basically depends on the scattering of the carriers by impurities and the dependence of the cross-section scattering on spins due to the mutual exhange interaction. So the spin polarizations of electrons and impurities act on the resistance:

$$\Delta\rho/\rho = (\rho_{ESR} - \rho)/\rho \propto \pi(a_s^2 - a_t^2)P_l P_e(s_l + s_e - s_l s_e)/\rho. \quad (2)$$

$P_{l,e} = th(\hbar\,\omega_{l,e}/2kT_{l,e})$ – are polarizations of the local paramagnetic centers (e) and of the free carriers (l), s_l and s_e are saturation factors, a_s and a_t are scattering lengths for the singlet and triplet scatterings. There is why the tunneling current will affects by microwave irradiation.

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Ergodic Theorem for Subsystem of Impurity Spins in a Crystal

F.S.Dzheparov

Ergodic hypothesis is one of the most important fragments of modern statistical physics. More than 30 years there coexist opposite points of view on the status of related proofs [1-7] and on possibility to construct the theory of irreversible processes within (quantum) mechanics and known interactions [6,7]. Terminological barriers between physics and mathematics are very high in the field. Therefore it is useful to find a simple enough and rich in context system to check and develop main ideas of ergodic theory. We studied the subsystem of impurity nuclear spins in a crystal as such simple and instructive example. As a realistic image a spin subsystem of ^{107}Ag can be considered in AgF, enriched by isotope ^{109}Ag. Other example is subsystem $^{8}Li - ^{6}Li$ in LiF [8], but main idealizations are not fulfilled here so well.

Subsystem of impurity spins I_k, $k = 1, ..., N$, isn't isolated and its dipole energy isn't conserved. But $z-$component of total subsystem spin $I_z = \sum_{k=1}^{N} I_k^z$ is an additive integral of motion in a strong external magnetic field $B = (0, 0, B_z)$ with very good accuracy. Therefore in typical conditions, when dipole temperature and heat capacity of matrix spins are infinite, we can expect, that, starting from any realizable state, subsystem will came to Gibbs equilibrium $\rho_G = \exp(\Phi - \xi I_z)$, according to ergodic hypothesis. Here Φ and ξ are defined, as usual, by the conditions: $Tr\rho_G = 1, TrI_z\rho_G = \langle I_z \rangle$.

The process is mastered by the equation [9]

$$\dot{\rho}_D = \frac{1}{2}\sum_{jk} w_{jk}[I_j^+ I_k^-, [I_j^- I_k^+, \rho_D]], \tag{1}$$

where $w_{jk} = a_{jk}^2 \tau_2 = w_{kj}$, $a_{jk} \propto r_{ij}^{-3}$ is usual dipole coefficient, and ρ_D is a diagonal part of ρ in the representation of eigenstates for operators I_k^z and all their products $C_m(j_1, ..., j_m) = \prod_{\alpha=1}^{m}{}' I_{j_\alpha}^z$. The prime indicates, that all j_α are different here. Eq.1 is valid if $R\tau_2 \ll 1$, $R\tau_c \ll 1$ [9], where correlation time τ_c is flip-flop time for matrix spins, $\tau_2 \propto T_2$, and T_2 and R are phase relaxation time and typical flip-flop rate for impurities. The inequalities are fulfilled very well if impurity concentration $c \leq 0.05$ [9]. Using the expansion

$$\rho_D(t) = \frac{1}{Tr1}\{1 + \sum_{m\geq 1}\sum_{j_1,...,j_m}{}' z_m C_m(j_1, ..., j_m) K_m(j_1, ..., j_m, t)\}, \tag{2}$$

$$K_m(j_1, ..., j_m, t) = < C_m(j_1, ..., j_m) > = TrC_m(j_1, ..., j_m)\rho_D(t),$$

(with $z_m^{-1} = Tr(C_m(j_1, ..., j_m))^2/Tr1$) we can obtain the equations:

$$\dot{K}_m(j_1, ..., j_m, t) = -\sum_{i\notin[m]}\sum_{l\in[m]} w_{il}(K_m(j_1, ..., j_m, t) - K_m(j_1, ..., j_m, t \mid j_l \to j_i)). \tag{3}$$

Here $[m] \equiv (j_1, ..., j_m), K_m(j_1, ..., j_m, t \mid j_l \to j_i)$ is the coefficient $K_m(j_1, ..., j_m, t)$ where j_l is substituted by j_i. Eq.3 is fulfilled if all $I_k = \frac{1}{2}$. For $m = 1$ Eq.3 coincides [9] with well known random walk equation.

The unique steady state solution of Eq.3 corresponds to uniform stirring of initial condition $K_m(j_1,...,j_m,t=0)$ on all $N_m = N!/(N-m)!$ different K_m, and

$$K_m(j_1,...,j_m,t\to\infty) = Q_m, \quad Q_m = \frac{1}{N_m}\sum_{j_1,...,j_m}{}' K_m(j_1,...,j_m,t=0). \tag{4}$$

If

$$\rho(t=0) = (1+\frac{3p_1^0}{I_1(I_1+1)}I_1^z)/Tr1, \quad p_1^0 = TrI_1^z\rho(t=0), \tag{5}$$

then all $K_m(t) \equiv 0$ for $m \geq 2$, and evolution isn't ergodic. Evolution of $^8Li - ^6Li$ system [8,9] (with $I_k \neq \frac{1}{2}$) isn't ergodic as well.

If initial state has quasiequilibrium form

$$\rho(t=0) = \exp(\Phi - \sum_{j=1}^{N}\xi_j I_j^z) = \frac{1}{Tr1}\prod_{j=1}^{N}(1+\frac{3p_j^0}{I_j(I_j+1)}I_j^z), \quad p_j^0 = -\tanh(\xi_j/2), \tag{6}$$

which corresponds to absolutely uncorrelated initial spin states, then

$$K_m(j_1,...,j_m,t=0) = \prod_{\alpha=1}^{m}{}' p_{j_\alpha}^0.$$

And if $\bar{p} = \frac{1}{N}\sum p_j^0 \propto N^0$, then $K_m(j_1,...,j_m,t\to\infty) = \bar{p}^m + O((m-1)/N)$. Therefore the final distribution coincides with Gibbs one within first m terms up to $O(\frac{m-1}{N})$.

If initial spin state has finite correlation radius, so that every spin is correlated with no more than N_c other spins, then $Q_m = \bar{p}^m + O((m-1)N_c/N)$, and the system is ergodic as well in leading order on $(m-1)N_c/N$.

If correlations in initial state are global ($N_c \neq o(N)$), then final state will not be Gibbs distribution.

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Nuclear Relaxation via Paramagnetic Centers

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Nuclear relaxation of spins 1/2 in dielectrics proceeds primarily via interaction with paramagnetic impurities. This process has been studied for years (in particular, in relation with nuclear dynamic polarization), nevertheless some interesting problems are not enough investigated up to now. For instance, in literature on spin dynamics the fact, that a long-time behavior in such systems is not an exponential one was not yet elucidated. There is no respective analysis even for $2d-$ and $1d-$systems, while experiments with fractal samples are under way now [1]. In continuous medium approximation the discussed process is described by a kinetic equation

$$\partial\tilde{p}(x,t)/\partial t = D\Delta\tilde{p}(x,t) - \sum_z n_z v_{xz}\tilde{p}(x,t), \quad \tilde{p}(x,0) = 1, \tag{1}$$

where $\tilde{p}(x,t)$ is a polarization of a nucleus, placed in a site x of a crystal, d is its dimension and D is a spin diffusion coefficient. $v_{xz} = v_0 r_0^6/|x-z|^6 = C/|x-z|^6$ is a relaxation rate of a nuclear spin x, interacting with an electronic paramagnetic center (acceptor), arranged in z. n_z is a corresponding occupation number, $\langle n_z\rangle_c = c \ll 1$, c is a concentration of impurity, $n = c/\Omega_c$ is its density and Ω_c is a volume of the crystal unit cell. The observable is a total nuclear polarization averaged over random distribution of paramagnetic centers: $p(t) = \Omega^{-1}\int d^d x\tilde{p}(x,t) = \langle 0|G(t)|0\rangle = \langle 0|\langle G(t)\rangle_c|0\rangle$. Here we introduced the propagator $G_{xy}(t)$, which is a solution of Eq.(1), but with another initial condition: $G_{xy}(t=0) = \delta(x-y)$. $|0\rangle$ stands for a normalized vector with components $\langle x|0\rangle = 1/\sqrt{\Omega}$, Ω is a volume of the crystal, and $\langle\ldots\rangle_c$ denotes the average over random positions of impurities. Expansion of $p(t)$ in a power series over impurity concentration starts as follows [2]:

$$p(t) = \langle 0|G(t)|0\rangle = \langle 0|G^{(0)}(t)|0\rangle + n\int d^d r\langle 0|[G^{(1)}(t,r) - G^{(0)}(t)]|0\rangle + O(n^2) =$$

$$= \exp[-M(t)(1+O(n^2)], \quad \text{where} \quad M(t) = n\int d^d r\langle 0|[G^{(0)}(t) - G^{(1)}(r,t)]|0\rangle. \tag{2}$$

Here $G^{(0)}(t)$ is the propagator without impurities, $G^{(1)}(t,r)$ denotes the propagator when only one impurity is located in the crystal in r. We also took into account that $\langle 0|G^{(0)}(t)|0\rangle = 1$. Due to translation invariance, one may rewrite $M(t)$ in the form: $M(t) = n\Omega\cdot\langle 0|[G^{(0)}(t) - G^{(1)}(0,t)|0\rangle$, or in Laplace transform ($f(\lambda) = \int_0^\infty \exp(-\lambda t)f(t)dt$):

$$M(\lambda) = n\Omega\langle 0|(\frac{1}{\lambda+A} - \frac{1}{\lambda+A+U_0})|0\rangle = \frac{n\Omega}{\lambda^2}\langle 0|T(\lambda)|0\rangle, \tag{3}$$

$$T(\lambda) = U_0\frac{1}{1+G^{(0)}U_0}, \quad G^{(0)}(\lambda) = \frac{1}{\lambda+A}, \quad A = -D\Delta, \quad (U_0)_{xy} = \delta_{xy}v_{x0}.$$

Here T–matrix $T(\lambda)$ does not depend on boundary conditions at $\Omega \to \infty$ due to a short-range action of the "potential" v_{x0}. For calculations it is more convenient to proceed with the next transformation:

$$M(\lambda) = \frac{n\Omega}{\lambda^2} < 0|U_0\frac{1}{\lambda+A+U_0}(\lambda+A)|0 >= \frac{n\Omega}{\lambda} < 0|U_0\frac{1}{\lambda+A+U_0}|0 >=$$

$$= \frac{n\Omega}{\lambda} < 0|U_0 \frac{1}{(A+U_0)(\lambda+A+U_0)}(A+U_0|0>=$$

$$= \frac{n\Omega}{\lambda} < 0|U_0 \frac{1}{(A+U_0)(\lambda+A+U_0)} U_0|0> = \frac{n\Omega}{\lambda} \sum_n \frac{|<n|U_0|0>|^2}{(\lambda+E_n)E_n}. \qquad (4)$$

where the eigen vectors $|n\rangle$ are determined by the equation $(A+U_0)|n\rangle = E_n|n\rangle$. Results equivalent to (2),(4) were published [3], but here we used another more straightforward and consistent approach [4]. Now we have to diagonalize the operator $A+U_0$. It is obvious, that $M(\lambda \to 0)$ depends mainly on small E_n. At small λ, following [3], one may apply an approach, known in the slow particle scattering theory as a scattering length theory. At large λ series expansion over diffusion coefficient [4] works well. The following interpolation relationship gives sufficient accuracy for all t

$$M(t) = M_F(t) + M_1(t), \quad M_F(t) = n\int d^d x(1-\exp(-v_{x0}t)) = (\beta_F t)^{d/6}. \qquad (5)$$

Here $M_F(t)$ describes initial (Förster) stage of relaxation and $M_1(t)$ has been calculated according to Eq.(4) in the frame of the scattering length theory. For arbitrary dimensionality d we obtained

$$M_1(t) = \vartheta(d>2)\sigma_d(d-2)nDtb^{d-2} + 2^{d-2}(d-2)^2\frac{\sigma_d}{\Gamma^2(2-\frac{d}{2})}b_0^d n \cdot \chi\left(\frac{Dt}{b^2}, d\right), \qquad (6)$$

$$\chi(a,d) = \int_0^\infty \frac{dx}{x^3} \cdot \frac{1-\exp(-ax^2)}{x^{d-2}+x^{2-d}-2\cos[\frac{\pi}{2}(d-2)]},$$

$$b_0 = \frac{b}{2}\left[\Gamma\left(2-\frac{d}{2}\right)\Big/\Gamma\left(\frac{d}{2}\right)\right]^{\frac{1}{d-2}}, \quad b = \left(\frac{C}{D}\right)^{\frac{1}{s-2}}\left[\frac{\Gamma(1-\frac{d-2}{s-2})}{\Gamma(1+\frac{d-2}{s-2})}\right]^{\frac{1}{d-2}} \cdot (s-2)^{-\frac{2}{s-2}}.$$

Here σ_d is an area of a unit d–dimensional sphere, b is the scattering length and $s=6$ is an exponent in the dependence of v_{x0} vs x. In case of $Dt/b^2 \gg 1$

$$M_1(t,d{=}1){=}4n\sqrt{\frac{Dt}{\pi}}, \quad M_1(t,d{=}2){=}\frac{4\pi Dnt}{\ln(Dt/b^2)}, \quad M_1(t,d{=}3){=}4\pi Dbnt. \qquad (8)$$

$M_1(d{=}1)$ does not depend on b. In $2d$–case this dependence is very week.

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New Effective Medium Approximation for Nuclear Relaxation via Paramagnetic Centers

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In [1] we developed a theory of nuclear relaxation of spins 1/2 in dielectrics for the case of interaction of the spins with paramagnetic centers (PC) under the presences of nuclear spin diffusion. The analysis was based on the expansion of the average nuclear polarization, $p(t)$, in power series on concentration c of PC. Such an approach allows to describe $p(t)$ in the samples with arbitrary dimensionality d, $d \geq 1$, within the first order of variation of $p(t)$. Final formulas are not applicable at long t. Indeed, let us consider a contribution to $p(t\to\infty)$ from large empty (without PC) region [2]. Polarization decays only on boundaries. Respective solution of a diffusion equation for a sphere with the radius R is proportional to $\exp(-\kappa Dt/R^2)$, where $\kappa \sim 1$, D is a spin diffusion coefficient. A probability to find such a sphere $\propto \exp(-nV(R))$, where $V(R) \propto R^d$. Thus

$$p(t\to\infty) \propto n\int_0^\infty dV(R)\exp\left[-nV(R) - \kappa DtR^{-2}\right] \propto \exp[-(Bt)^{\frac{d}{d+2}}], \tag{1}$$

where B is a constant, which depends on geometry, density of PC and the diffusion coefficient. Accurate proof of eq.(1) is given in [3]. A crossover from equations obtained in [1] to this asymptote is investigated rather poor. Numerical simulations [4] indicate that the asymptote (1) can be observed at $p(t) < 10^{-11}$. So we may expect that the intermediate region is rather wide and needs an appropriate theory. Mean field theories which is also called as a coherent potential method [5], or effective (or coherent) medium approximation [6] could be a natural candidates for that. They are formulated in Laplace transform for the propagator. However these methods, being applied to $1d-$ and $2d-$systems, give senseless results even in the leading order. To overcome this difficulty we developed a similar theory, but directly in t-representation. In this case the propagator $G(t)$ may be written as

$$G(t) = \langle\exp[-(A+U)t]\rangle_c = \exp[-B(t)], \quad B(t) = A\cdot t + M(t), \tag{2}$$

$$A = -D\Delta, \qquad U = \sum_z n_z U^z, \qquad U^z_{xq} = \delta_{xq} v_{xz}, \qquad v_{xz} = C/|x-z|^6. \tag{3}$$

Here v_{xz} is a relaxation rate of a nuclear spin x, interacting with the PC, arranged in z. n_z is a corresponding occupation number, $\langle n_z\rangle_c = c \ll 1$, $\langle\ldots\rangle_c$ denotes the average over random positions of PC. Let us rewrite unknown operator $M(t)$ in the form, similar to U: $M(t) = \sum_z M^z(t)$. It is possible to say, that operators $M^z(t)$ should adequately describe an influence of acceptors in a so-called "effective medium", which appears after taking average over acceptor configuration. Therefore, it is natural to require, that the average propagator $G(t)$ ought to be the same, if one of the lattice sites in the effective medium would be replaced by a real site together with the subsequent averaging over the distribution of PC:

$$G(t) = \langle\exp[-At - M(t) + M^z(t) - n_z U^z t]\rangle_c. \tag{4}$$

Eqs.(2-4) make up a full set of nonlinear operator equations. Now let us proceed with its solution. Taking an average over n_z we obtain

$$c[\exp(-B(t) - U^z t + M^z(t)) - \exp(-B(t) + M^z(t))] = e^{-B(t)} - e^{-B(t)+M^z(t)}. \quad (5)$$

The operator $M^z \propto c$ and therefore is small. Contrary $M = \sum_z M^z$ is not small, so keeping in both parts of eq.(5) leading terms on c, we arrive to

$$c[\exp(-B(t) - U^z t) - \exp(-B(t))] = -\int_0^1 d\xi e^{-\xi B(t)} M^z e^{-(1-\xi)B(t)}, \quad (6)$$

which gives

$$M(t)\exp(-B(t)) = c\sum_z [\exp(-B(t)) - \exp(-B(t) - U^z t)] \quad (7)$$

after summation over z and taking into account translation invariance. Let $M(t) = [m_0(t) + m_1(t)]t$, where $(m_0(t))_{xq} = \delta_{xq} m_0(t)$. In m_0 we have separated a part M, which is proportional to unity operator. Using Laplace transformation, it is possible now to rewrite eq.(7) as follows

$$[m_0(t) + m_1(t)]t \cdot e^{-(A+m_1(t))t} = c\int_{\epsilon-i\infty}^{\epsilon+i\infty} \frac{d\lambda e^{\lambda t}}{2\pi i} \sum_z \frac{1}{\lambda + A + m_1(t)} U^z \frac{1}{\lambda + A + m_1(t) + U^z}.$$

This equation is reduced to results obtained in [1] if $m_1 = 0$. When $m_1 \neq 0$ it is necessary to find a convenient way to calculate $M(\lambda)$ from eqs.(5-6) in [1], including terms $\sim O(k^2)$, when $|0\rangle \to |k\rangle$, where $\langle x|k\rangle = e^{ikx}/\sqrt{\Omega}$. Ω is a volume of the crystal. Within this accuracy $\langle k|m_1(t)|k\rangle = D_1(t)k^2$. Thus m_1 simply renormalizes the diffusion coefficient: $D \to D + D_1(t)$. Corrections to the effective medium propagator obtained in such a way could be calculated using $T-$matrix expansions [6], and the first non-zero terms will be $\sim T^4$. To our knowledge, it is an unique way, which allows to avoid senseless results in the leading order at small d. Moreover it enables, at least in principle, to calculate corrections to the leading order for all t and d.

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Spin Kinetics in Dilute Systems. Variations of Physical Predictions in Cluster Theory

F.S.Dzheparov, I.V.Kaganov

The main problems of spin dynamics theory in magnetically diluted systems (MDS) are produced by very broad distribution of energies there. Two characteristic energy constants — interaction of nearest neighbors via minimal distance and interaction $\overline{E}$ at average distances, which relation can exceed hundreds and thousands, create gigantic width of relaxation times distribution and regular two-temperature theory becomes insufficient for many processes [1]. Some problems can be solved using the concentration expansion [2], which is useful at $\overline{E}t \leq 1$.

New method of cluster separation was introduced [3] and developed [4,5] to describe evolution of MDS on medium ($\overline{E}t \sim 1 \div 10$) and large ($\overline{E}t > 10$) times. The clue of this theory is separation and exact calculation of singular part of interactions which is realized by compact clusters. The rest of interactions might be considered in Anderson — Weiss — Kubo (AWK) approximation (normal random process) because, after cluster separation, the local dipole field, produced on every spin by extra-clusters spins, is a sum of many terms of the same order of magnitude. After the clusters separation the characteristic time of flip-flop transitions in the rest of system is determined by interactions at average distances , so the ratio of flip-flop time of extra-clusters spins and time of phase relaxation is close to one in regular systems.

Cluster classification, based on comparison of intra- and extra-cluster interactions for every spin was used [5] to calculate the free induction decay (FID) and to estimate the function of local longitudinal field correlation. However, different methods of cluster separation might lead to different predictions and the best method is not evident. Therefore we studied the dependence of some theory predictions on some important details of cluster classification. We introduce a new classification, more natural than one, discussed early in [3-5]. It is based on comparison of intra-cluster dipole field and total extra-cluster one. Second moment of the distribution of local fields, produced on the cluster by extra-cluster spins, is used as corresponding measure. Our new construction, as well as theory [5], is based on separation of 2-spin clusters ant it produce a possibility to study the dependence of free induction decay on the quota κ of spins, contained in clusters.

We studied carefully the physical region of values for κ and we choose it as $\kappa = 0.4 \div 0.6$.

As an example of our results we suggest a new representation for FID:

$$G(t) = Tr(S_+(t)S_-)/Tr1 = G_2(t) + G_1(t), \tag{1}$$

$$G_2(t) = \frac{4D}{\pi^2}\int_0^\infty \frac{d\omega}{\omega^2}\int_{y_0(\omega)}^\infty \frac{dy}{y^2}\exp(-\frac{D^2}{\pi\omega^2} - I(t)\omega^2)\cos Dty,$$

$$G_1(t) = \exp(-2D\sqrt{\frac{I(t)}{\pi}}) - \frac{4D}{\pi^2}\int_0^\infty \frac{d\omega}{\omega^2}\int_{y_0(\omega)}^\infty \frac{dy}{y^2}\exp(-\frac{D^2}{\pi\omega^2} - I(t)\omega^2 - D^2y^2I(t)),$$

where $y_0(\omega) = 2\omega/(\pi\kappa D)$, $G_2(t)$ and $G_1(t)$ are FIDs of two-spin clusters and extra-clusters spins correspondingly, $D \simeq \overline{E}$ is Anderson line width, $I(t) = \int_0^t d\tau(t-\tau)K(\tau)$.

Correlation of local field $\omega_x(t)$ was taken as $\langle\omega_x(t)\omega_x\rangle = M_{2x}K(t)$ with exact value and distribution for local second moment M_{2x}, depending on position x of spin or cluster. $K(t) = \exp(-\sqrt{t/\tau_c})$ with $\tau_c \simeq 4/D$ were chosen for numerical estimations. General discussion of similar approximations is carried out in [4,5].

A generalizations of Eq.1 was developed to take into account diffferences in fluctuations of local fields on clusters and extra-clusters spins.

Results, obtained within different cluster approaches, developed in this work and in preceding article [5] are similar qualitatively. FID is close to Anderson exponential relaxation during first order of the decay, then it deviate to Foerster like behavior, predicted in Ref.2, but it is realized for very small values of $G(t)$ [5]. Dependence on κ and on the type of cluster expansion are studied for the first time and they have the same order of value. These results give the possibility of experimental verdict about type of cluster classification which is "actually realized", and, therefore, what kind of processes is more important in the spin dynamics.

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A New Semi-Phenomenological Theory for Problems of Spin Spectral Transport in Disordered Media

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The equations

$$\dot{P}_{xy} = -\sum_z (w_{zx} n_z P_{xy} - w_{xz} n_x P_{zy}), \quad P_{xy}(t=0) = \frac{n_x}{c_x}\delta_{xy} \tag{1}$$

describe random walks in disordered system with site disorder [1]. Here $P_{xy}(t)$ is a probability to find a walker at a moment t in a site $\mathbf{x}$ of a crystal if it was in $\mathbf{y}$ at initial moment, w_{zx} is a rate of transfer from $\mathbf{x}$ to $\mathbf{z}$, $w_{xx} = 0$, n_x is an occupational number, $n_x = 1$ or $n_x = 0$ relative to is or isn't site $\mathbf{x}$ occupied by a donor, that is an impurity, which can carry a walker. Strong disorder is realized when $c_x = \langle n_x \rangle \ll 1$, where $\langle \ldots \rangle$ means averaging over donors' distribution.

Dipole transport such as spin diffusion like processes [1,2] or localized electronic excitation hopping [3] are among the most important applications of Eq.1, and the problem to find the solution, averaged over random donors distribution in the crystal belongs to most complex and important in modern physics [2,3] due to wide applications and because the problem has no real small parameter and it is related with very complex field theories. Among many approaches developed to solve particular subproblems of the problem (see [1-4] and references therein), only semi-phenomenological theory (SPT) [1] gives an uniform approximation for all c_x and t if $c_x = c \leq 1$. But this kind of theories fails if c_x isn't a constant, that is very important for problems of spectral transport in optics [3], when $\mathbf{x}$ incorporates spatial and spectral coordinates. Our interest is stimulated as well by similar difficulties, related with the spin spectral transfer like one studied in [4].

We constructed a new SPT which has no defects, mentioned above. The theory reproduces known value of diffusion coefficient for spin delocalization [5] with satisfactory accuracy and it has (for the first time) right behavior for all important limiting situation in the spectral transport.

SPT is the simplest theory of mean field class. It starts from the fact, that

$$\mathcal{P}_{xy}(t) = \langle P_{xy}(t) \rangle$$

is mastered by the equation

$$\dot{\mathcal{P}}_{xy} = -\sum_z \int_0^t dt_1 (N^y_{zz}(t-t_1)\mathcal{P}_{xy}(t_1) - N^y_{zx}(t-t_1)\mathcal{P}_{zy}(t_1)), \tag{2}$$

and it uses an hypothesis, that we can choose some simple auxiliary process to calculate $N^y_{zz}(t)$ and then to solve general problem (2) using these kernels [1]. Exact kernels $N^y_{zz}(t)$ can depend or not depend on initial position $\mathbf{y}$ of the walker relative to what kind of memory is preferable for treatment: 1) geometrical, when $N^y_{zz}(t)$ depends on $\mathbf{y}$, but it decays fast with time t; or 2) temporal memory, when $N_{zz}(t)$ does not depend on $\mathbf{y}$, but time decay has slow diffusion like tail, which one-to-one defines the asymptotics $\mathcal{P}_{yy}(t \to \infty)$ if $c_x \ll 1$ [1]. First kind of kernels was justified within technique of Nakajima - Zwanzig projectors[1]. Second (temporal) type is connected

with projector $Af_x = (n_x/c_x)\langle n_x f_x\rangle$ for arbitrary f_x. Second kind of kernels is simpler and preferable for three dimensional systems, if we aren't looking for asymptotics of $\mathcal{P}_{yy}(t \to \infty)$, because SPT can not give $N_{xx}(t \to \infty)$ correctly. We studied both type of kernels, but only second will be discussed below for the sake of brevity, and label y will be canceled.

Next model task was chosen as auxiliary:

$$\lambda R_x = n_x - (n_z w_{zx} + \tilde{D}_x)R_x + n_x w_{xz} R_z, \ \lambda R_z = -(n_x w_{xz} + \tilde{D}_z)R_z + n_z w_{zx} R_x, \qquad (2)$$

where $\tilde{D}_q = \Lambda_q \sum_{r\neq x,z} w_{rq} n_r, \quad q = \{x, z\}$ and Eqs.2 are written in Laplace representation with $R_q(\lambda) = \int_0^\infty dt \exp(-\lambda t) R_q(t)$. Multiplier Λ_q takes into account that walker can go away and back. It is defined self-consistently below. According to SPT, $\mathcal{R}_x = \langle R_x\rangle$ is mastered by the equations:

$$\lambda \mathcal{R}_x = c_x - (N_{zx} + D_x)\mathcal{R}_x + N_{xz}\mathcal{R}_z, \quad \lambda \mathcal{R}_z = -(N_{xz} + D_z)\mathcal{R}_z + N_{zx}\mathcal{R}_x, \qquad (3)$$

with $D_q = \mu_q \sum_{r\neq q} N_{rq}$, $N_{xz}(\lambda) = \int_0^\infty dt \exp(-\lambda t) N_{xz}(t)$. Here μ_q is another multiplier, which is analogous to Λ_q and is not equal to it in general. The result for $c_q \ll 1$ is

$$N_{xz}(\lambda) = w_{xz}(Q_x Q_z)^{-1}\langle n_x[(\lambda + \tilde{D}_x)(\lambda + \tilde{D}_z) + w_{zx}(\lambda + \tilde{D}_x) + w_{xz}(\lambda + \tilde{D}_z)]^{-1}\rangle \qquad (4)$$

with condition of self-consistency $Q_x = (\lambda + D_x)^{-1} = \langle(\lambda + \tilde{D}_x)^{-1}\rangle$. The method (in difference of preceding SPT) is exact in first order in c_q, with the same accuracy we must average $\tilde{D}_x$ and $\tilde{D}_z$ in (4) independently. One condition of self-consistency is not enough to determine Λ_q and μ_q both. Another one is the condition that diagonal part of propagator, obtained using kernel (4) must be the same as the diagonal part of propagator, obtained using cumulant expansion in Laplace representation. We can formulate this demand because of exceptionally high precision of cumulant expansion in Laplace representation [1] in case of dipole interaction. Precision of this approach in case of interaction $w_{0x} \sim 1/x^s$ is shown in the next table:

s	6	10	12	15	20	30	40	50
γ	1.026	0.96	0.93	0.88	0.83	0.77	0.74	0.72

Here γ is ratio: correct third term of concentration expansion over third term of cumulant expansion [1] of diagonal part of propagator. The new SPT might be used for many kinetic problems of dipole transport in disordered systems, especially for the problems of spectral diffusion (relaxation) in diluted paramagnet, studied in experiments [4].

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Diffusion in a System of Impurity Centers with Dipole-Dipole Transition Rates

F.S. Dzheparov, D.V. L'vov, V.E. Shestopal

Transport of nuclear polarization in a system of impurity nuclei belongs to problems of random walks in disordered media (RWDM) with dipole interactions. Their experimental studies were performed by the methods of β-NMR [1], time dependent narrow band laser spectroscopy [2], depolarization of fluorescence [3] and degenerate four-wave mixing [4]. Various theoretical and numerical approaches were applied in research of these systems. However there is no agreement in resolution of the most important question about the form and parameters of the longtime asymptotics. First of all the diffusion coefficient values differ significantly. Although the diffusive behaviour of the asymptotics is generally accepted, its mathematical proof is not found.

Basing on a new theoretical method for studying of the longtime asymptotics in RWDM models [5] we investigate the migration on simple cubic (SC) and face centered cubic (FCC) lattices at arbitrary impurity concentration.

Incoherent transport in a system of randomly distributed impurity centers is described by the kinetic equation:

$$\dot{p}_{im} = -\sum_j (\nu_{ji} p_{im} - \nu_{ij} p_{jm}), \quad p_{im}(t=0) = \delta_{im},$$

where p_{jm} is the probability to find a walker at time t at the center with a number j (placed in site $\mathbf{x}_j$ of regular lattice L) if it was initially at the site m. In the standard model of dipole transport $\nu_{i\neq j} = \nu_0 r_0^6 |\mathbf{x}_i - \mathbf{x}_j|^{-6}$, $\nu_{ii} = 0$. Positions of impurities are assumed to be uncorrelated. In the limit of low concentrations the characteristic time scale is determined by Forster's constant $\beta = (16/9)\pi^3 (r_0^3/\Omega)^2 c^2 \nu_0$ where Ω is a prime cell volume and c is a dimensionless concentration of impurities. We consider random configurations with a large period $R\mathbf{e}_i$ where $\mathbf{e}_i$ are prime cell vectors of L and introduce the quantity $\rho_j(\mathbf{k},t) = \sum_m p_{jm}(t) \exp[i\mathbf{k}(\mathbf{x}_m - \mathbf{x}_j)]$. The quantity ρ_i is periodic: $\mathbf{x}_i - \mathbf{x}_j = R\mathbf{M}$, $\mathbf{M} \in L$, entails $\rho_i = \rho_j$. Thus we obtain the system of N equations on ρ_i (N is the number of impurities in the periodicity volume) and solve them numerically [5]. The quantity of interest is $P(\mathbf{k},t|N) = \frac{1}{N}\sum_{i=1}^{N} \rho_i$. Calculations show that $\ln P(\mathbf{k},\beta t >> 1|N)/(\beta t)$ tends to a finite positive value for all considered configurations where $N = 200 \div 2000$ and for small $k\bar{r}$ where $\bar{r} = (\Omega/c)^{1/3}$ is the average distance between impurities. As the result

$$P(\mathbf{k},\beta t >> 1|N) = a \exp(-Dk^2 t + \sigma k^3 t),$$

where the coefficient σ is known exactly [5]. It is convenient to write the diffusion

coefficient D in a form: $D = (\kappa / 6)\beta\bar{r}^2$.

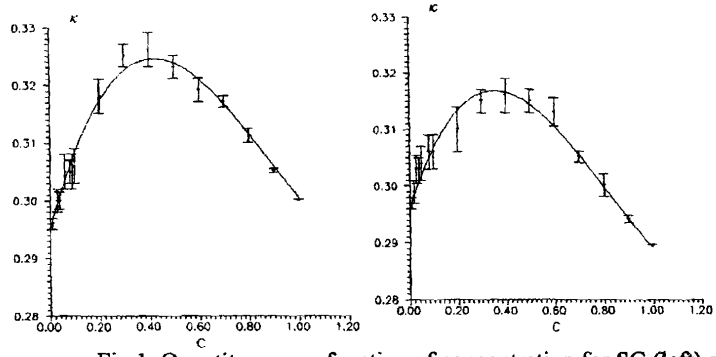

Fig.1. Quantity κ as a function of concentration for SC (left) and FCC (right) lattices and its analytical approximation.

When βt tends to 1000 the diffusion coefficient D monotonically decreases but remains within three percents from its value at $\beta t = 40$ for concentrations 1%<c<100%. For each value of c we considered from 3 to 5 various pseudo-random configurations of impurities to average obtained values. The results are presented in fig.1. The values of $\kappa_u \equiv \kappa(c=1)$ are well known: $\kappa_u(SC) = 0.2999$, $\kappa_u(FCC) = 0.2895$. The least square approximation with the expression $\kappa = \kappa_u + (\kappa_1 + \kappa_2 c + \kappa_3 c^2)(1-c)$ produces for the SC lattice the values $\kappa_1 = -0.0050 \pm 0.0006$, $\kappa_2 = 0.164 \pm 0.004$, $\kappa_3 = -0.11 \pm 0.04$. Quantity $\kappa_u + \kappa_1$ corresponds to the diffusion coefficient at $c \to 0$. In the case of FCC lattice $\kappa_1 = 0.0066 \pm 0.0007$, $\kappa_2 = 0.132 \pm 0.004$, $\kappa_3 = -0.09 \pm 0.04$. One can see that values of $\kappa_u + \kappa_1$ for FCC and SC lattices coincides within the accuracy of calculations. Such an agreement must take place because at small concentration average distance between the impurities is large, $\bar{r} >> r_0$, and therefore at $\nu_0 t >> 1$ the propagator should not depend on a lattice type.

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Tensor of Spin Diffusion for Polarization Transport on Rare Nuclei.

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A process of spin polarization transport has been under intense investigations for many years [1]. A theoretical description of the process at moderate times was given by a method of concentration expansion [2] and an autocorrelator $< \widetilde{P}_{00} >$ was measured in [3]. The measurements of the long-time asymptotics are carried out now for disordered system $^8Li-^6Li$ by β-NMR method. Numerical simulation [4] shows that in disordered system with isotropic transition rates of dipole type diffusion asymptotic realizes and dependence of diffusion coefficient on concentration was studied [5]. We consider here long-time asymptotic behaviour of the process of random walks with anisotropic transition rates which take place in real spin systems.

Spin migration in a system of impurity nuclei is described by the kinetic equation [1]:

$$\frac{d\widetilde{P}_{xy}}{dt} = -\sum_{z} n_x n_z \left(\nu_{zx}\widetilde{P}_{xy} - \nu_{xz}\widetilde{P}_{zy}\right), \qquad \widetilde{P}_{xy}(t=0) = \frac{n_y}{c}\delta_{xy}, \tag{1}$$

where $\widetilde{P}_{xy}$ is polarization in lattice site $\mathbf{x}$ at time t with initial condition of unit polarization in $\mathbf{y}$, n_x is the occupation number. Polarization transition rate

$$\nu_{xy} = \frac{\nu_0 r_0^6 (1 - 3\cos^2\vartheta_{xy})^2}{|\mathbf{x}-\mathbf{y}|^6}$$

where ϑ_{xy} is an angle between $\mathbf{H}\|OZ$ and $(\mathbf{x}-\mathbf{y})$, r_0 is a period of simple cubic lattice L. We study the limit of low concentrations c of impurities when the disorder of environment appears to be significant. The characteristic time scale is determined by the Förster's constant $\beta = (256/243)\pi^3 (r_0^3/\Omega)^2 c^2 \nu_0$ where Ω is the prime cell volume and c is the concentration of impurity nuclei. Lets introduce the quantity

$$\rho_x(\mathbf{k},t) = \sum_y \widetilde{P}_{xy}(t)\exp[i\mathbf{k}(\mathbf{y}-\mathbf{x})]$$

where the vector $\mathbf{k}$ is in Brillouin zone.

In the numerical simulation we placed pseudo-random configuration of impurities in cube with an edge Rr_0, $R \gg 1$ and then periodically continued this configuration (but not the initial condition for Eq.(1)) to the entire infinite lattice: $n_x = n_{x+RM}$, $\mathbf{M} \in L$. In this case $\rho_x = \rho_{x+RM}$ and we obtain the finite system of N equations which was solved numerically:

$$\dot{\rho}_x = -\sum_{x\in V} n_x n_z \left(W_{zx}(0)\rho_x - W_{xz}(\mathbf{k})\rho_z\right), \qquad \rho_x(\mathbf{k}, t=0) = n_x / c,$$

where $\mathbf{x},\mathbf{z}$ are the sites in the periodicity volume V and

$$W_{xz}(\mathbf{k}) = \sum_{\mathbf{M}\in L} \nu_{x,z+RM} \exp[i\mathbf{k}(\mathbf{z}-\mathbf{x}-\mathbf{M}R)].$$

The quantity of interest $P(\mathbf{k},t|N) = \frac{1}{N}\sum_{x\in V}\rho_x$ can be considered as a Fourier transform of propagator, which is averaged over all configurations that may be obtained from the given one changing its "initial" site within periodicity volume. In order to explain this statement we note that the generator in [1] is symmetric, i.e. $\widetilde{P}_{xy} = \widetilde{P}_{yx}$ and therefore the index $\mathbf{x}$ in ρ_x can be considered as a coordinate of the site which contained excitation at $t = 0$.

At long t we approximate $P(\mathbf{k},t|N)$ by the expression:

$$P(\mathbf{k},t|N) = a\exp\left(-\sum_{i=1}^{3} D_i k_i^2 t + \sigma(\mathbf{k})t\right),$$

where term $\sigma(\mathbf{k}) \sim |\mathbf{k}|^3$ can be calculated analytically by the Poisson-Evald method

$$\sigma(\mathbf{k}) = \frac{3\pi^2}{32}\frac{c}{\Omega}\nu_0 r_0^6\left(\frac{|\mathbf{k}|^3}{2} + \frac{k_3^2|\mathbf{k}|}{3} + \frac{k_3^4}{2|\mathbf{k}|}\right).$$

The quantities D_i are the components of the diffusion tensor which is diagonal in the basis. In order to display concentration dependence of D_i we write it in a form $D_i = \frac{\kappa_i}{6}\beta\bar{r}^2$ where $\bar{r} = r_0 c^{-1/3}$. From the calculations we see that the quantities D_i decrease monotonically with time and stabilizes with accuracy 5% at $\beta t = 40$. The system (4) was solved for various pseudo-random configurations of impurity nuclei at concentration $c = 1\% \div 6\%$ and $N \le 2000$. It was obtained that $\kappa_1 = \kappa_2 = 0.270 \pm 0.003$, $\kappa_3 = 0.510 \pm 0.003$. The value of κ_1/κ_3 is in a good agreement with the prediction of all theories considered in [1].

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Spin Dynamics in Diluted Systems. Testing of Cluster Based Theory with Direct Numerical Simulation

I.V.Kaganov

Main problems in the theory of spin dynamics in diluted spin system are in relation with huge range of characteristic energies there. Very large dispersion of relaxation times prevents the usual description for many situations [1]. Method of separation and exact consideration of singular part of interaction, generated by clusters of small number of close spins, was introduced [2] and developed [3,4]. Other interactions are considered in Anderson — Weiss — Kubo (AWK) approximation (normal random process). This approach was used [4] for calculation of free induction decay and function of local longitudinal field correlation in case of spin $S = 1/2$. The only serious test of model might be the experiment, at least numerical. Direct integration of equations of spin motion with calculation of correlators, averaging over different Gibbs ensembles and spatial configurations gives possibility of testing the theory (at least on small and medium times) and of determination of non-determined strictly parameters of theory (for example, characteristic time of flip-flops in system). today's computation possibilities demand the simulation of motion for classical spins. In the high-temperature approximation the transverse correlation function (free induction decay) has the form in standard notation $G(t) = \langle\langle S^+(t)S^-\rangle_0\rangle_c/\langle\langle S^+S^-\rangle_0\rangle_c$. Here $\langle\ldots\rangle_0 = \mathrm{Tr}(\ldots)/\mathrm{Tr}1$ is Gibbs averaging, $\langle\ldots\rangle_c$ is averaging over different spatial configurations of spins. Evolution goes under influence of secular part of dipole-dipole Hamiltonian. After separation of the clusters, the local fields on spins of mass and on the clusters is far closer to a normal process than before. Let separate the pairs from the system and neglect the dependence of the field induced by the system outside the pair from the position of point inside cluster [4]. Using techniques, analogous [4], one can obtain explicit expression for $G(t)$. Line width in Anderson model D_s is characteristic scale parameter in case of spin S. Let, further, consider longitudinal spin autocorrelation function, which determines behavior of $G(t)$, be $e^{-\sqrt{t/\tau_c}}$ on average times (Förster exponent) [4]. Parameter τ_c is characteristic time of flip-flop in system. Then $G(t)$ may be calculated directly for any spin S in considered model. In general, behavior is analogous for any spin and convergence of functional sequence $G(t) = G_s(t)$ when $S \to \infty$ is very quick, so case $S = 5$ or $S = 6$ already may be used for approximation of infinite spin with very good precision.

The main problem of any numerical experiment is problem of validity of results. There are two independent possibilities for testing of numerical results in considered case (except varying of concentration, number of spins and configurations): comparing with analytical results in Anderson model in case of Anderson Hamiltonian and comparing with exact results of concentration expanding. Note, that $G(t)$, calculated in theory has correct first non-trivial order. The computer simulation was done by direct integration (Runge-Kutta, method of 8th order by Dorman-Prince) of diluted in lattice system of classical spins $\vec{\mu}_j$, which move under influence of secular dipole-dipole interaction with periodic boundary conditions. Followed calculation of correlators $q_z(t) = \mu_0^z(t)\mu_0^z$, $q_x(t) = \mu_0^x(t)\mu_0^x$, $\mu_0^+(t)\mu^-$ ($\mu^\pm = \mu^x \pm i\mu^y$, $\mu^x = \sum_j \mu_j^x$, $\mu^y = \sum_j \mu_j^y$) and averaging of them over different spins, different Gibbs ensembles

(over random distribution of direction of $\vec{\mu}_j(0)$ with equal probability of each direction (high temperature)), and different configurations, gives final result. Testing of program showed that deviations are no more than 5% on considered interval of time ($D_\infty t \leq 3$). Functions $\langle\langle q_z(t)\rangle_0\rangle_c$, $\langle\langle q_x(t)\rangle_0\rangle_c$ and $G(t)$, obtained numerically are in exact agreement with cluster expanding. If to suppose $\langle\langle q_z(t)\rangle_0\rangle_c$ has form $e^{-(t/\tau_c)^\alpha}$, one can obtain from these results for $\langle\langle q_z(t)\rangle_0\rangle_c$ that $\alpha \approx 0.66$, $\tau_c \approx 9.0 D_\infty^{-1}$ using maximal considered time. Basic numerical results were received with number of spins 350, number of Gibbs ensembles 350, number of spatial configurations 30, relative concentration of spins 10^{-2}, local error of integration 10^{-6}. Substitution of τ_c, founded above, into our theoretical formulas was done and result was compared with $G(t)$, obtained numerically. These two curves are in precise agreement. Resulting curve damps like exponent, but some more slowly on considered interval of time. It is one of the most important predictions of theory [4].

We see that theory [4] describes behavior of free induction decay on average times rather precisely. $\langle\langle q_z(t)\rangle_0\rangle_c$ is really almost Förster function, but characteristic time of flip-flop is $\sim 10/D_\infty$ (in [4] it was considered $\tau_c D = 4$). Obtained results may be useful for more deep understanding of processes in disordered paramagnet.

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Asymptotic Similarity of Time-Correlation Functions and the Problem of NMR Line-Shape in Solids. Scaling Approach.

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The problem of the shape of the free-induction decay (FID) signal in a solid is solved analytically, on the basis of hypothesis advanced here that a similarity exists between the time-correlation functions (TCF) arising in an infinite chain of gearing differential equations for the NMR FID signal and the TCF which are associated with this signal, for crystals with a large number of equivavalent nearest neighbors surrounding any spin in the lattice. It is demonstrated that the similarity law is a consequence of scaling relations between the coefficients appearing in the chain of equations for TCF. Also the procedure of scaling transformation of the system of TCF is developed allowing to derive the explicit solutions for a FID signal. Moreover, the proposed similarity law is confirmed for the first two TCF by a direct numerical calculation for fragments of a simple cubic lattice with periodic boundary conditions and linear crystalline polyethylene.

Oscillations in the NMR FID signal (FID is the Fourier transformed NMR line-shape) in the solid CaF_2 were first observed experimentally in 1957 by Lowe and Norberg [1]. Despite the fact of numerous of articles (see e.g., [2,3] and references therein) have been devoted to this problem and to closed problems of spin dynamics this area is far from complete. There is great interest in this problem, on the one hand, as specific problem of nonequilibrium statistical mechanics – the problem of establishment of equilibrium in systems of many interacting bodies. On the other hand, the shape of magnetic-resonance spectra contains information about the crystal and electronic structure of the sample and about the mobility of atoms and atomic groups i.e., it contains a substantial fraction of information accessible to NMR and in solids part of this information is, as a rule, masked by the main broadening mechanism (the mutual dipole-dipole interaction of the nuclear spins). Let us mark also, that the NMR line-shape problem is related to spin-diffusion problems, the problem of calculating the magnetic part of neutron scattering by paramagnets and the spectra of Raman scattering from quadrupole solids and it has deep analogies with many other problems in the statistical physics of condensed matter.

The Hamiltonian of a spin system with the dipole-dipole interaction in ordinary notations is

$$H = H_{ZZ} + H_{ff} = \sum_{i>j} b_{ij} S_{Zi} S_{Zj} - (1/4) \sum_{i>j} b_{ij} (S_i^+ S_j^- + S_i^- S_j^+) . \quad (1)$$

In the coordinate system rotating with a Larmor frequency, the observed FID is proportional to the TCF

$$A_0(t) = (1/Sp(S_x^2)) Sp\{S_x(t) S_x\} = (1/Sp(S^+ S^-)) Sp\{S^+(t) S^-\}, \quad (2)$$

where $S_x = \sum_i S_{xi}$, is the x- component of the total spin of the system and $S_x(t)$ is the solution of the Heisenberg equation $\dot{S}_x = (i/\hbar)[H, S_x]$. As is shown in [4], the problem of calculating TCF (2) is equivalent to the solution of the infinite system of differential equations

$$\begin{aligned} \dot{A}_0 &= i\nu_0^2 A_1 \\ \dot{A}_1 &= i\left(A_0 + \nu_1^2 A_2\right) \\ &\cdots\cdots \\ \dot{A}_n &= i\left(A_{n-1} + \nu_n^2 A_{n+1}\right) \\ &\cdots\cdots \end{aligned} \qquad (3)$$

with the initial conditions $A_0(0)=1$, $A_n(0)=0$, $n>1$. The functions $\{ A_n(t)\}$ are "multicommutator" (multiparticle) TCF because every differentiation of FID (2) adds the commutation operation and thus, generally speaking, adds another operator with a new summation index over the lattice. The parameters $\{\nu_j\}$, whose properties determine the solution of the system, are related to the moments of absorption line [4].

Let us note that in accordance with the results of Ref. [5,6] the relation (3), which are, in principle, determined for the entire crystal, can be related only to the component of the FID that is due to the spins of a "cell" [5,6] which are, to say roughly, are the equivalent nearest neighbours of a spin in the lattice. The scaling relations between the constants $\{\nu_j\}$, resulting in the "freezing" of them with the number j (j marks the begining of freezing) defines the "fix point" of the symmetry group bring us to the similarity relation

$$A_2(t) \approx \alpha A_0 + \alpha \dot{A}_0(t)\tau(t), \; \tau(t) = 1/\nu_0^2 t \qquad (4)$$

which involves the equation for FID $\ddot{A}_0 + (\beta/t)\dot{A}_0 + (\beta+1)\nu_0^2 A_0 = 0$. $A_0(0)=1$ with the solution of it describes by the formula

$$A_0(t) = CJ_\lambda(\sqrt{\beta+1}\nu_0 t)/(\sqrt{\beta+1}\nu_0 t)^\lambda = CJ_\lambda(bt)/(bt)^\lambda \qquad (5)$$

being in the excellent agreement with the experimental results for the systems with the large number of spins in the "cell" and where the present theory only valid. Here are $\lambda = |\beta - 1|/2$, J_λ - is a Bessel function of order λ, and C is a normalization constant supports the initial conditions.

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New Exactly Soluble Models of Random Walk in Disordered Lattice Media

V.E.Shestopal

A lot of interesting physical systems are described in terms of lattice migrations with random jump rates between sites [2, 4, 5, 6]. These problems generated many mathematical [1, 7, 8], numerical [9], and heuristic investigations [9].

We give new asymptotically exactly soluble models of continuum time random walk on the lattice Z^d with stochastic jump rates. The following properties *for the first time combined in our models* are of great importance in many physically interesting systems: 1) translation invariance of jump rates distribution; 2) arbitrary large number of independent local stochastic parameters per site; 3) long-ranged interaction, e.g. power-like decreasing of rates at infinity; 4) the symmetry requirement: a jump rate from one site to another is the jump rate between them.

This work continues the investigations of exactly soluble models of random walk in disordered media [7, 8].

The first class of our new models is described by the equations:

$$d\tilde{P}^{mn}_{xy}/dt = -(\alpha A\beta P)^{mn}_{xy} = -\sum_z \sum_{i,j,l=1}^{N} \alpha^{mi}_x A^{ij}_{x-z}\beta^{jl}_z \tilde{P}^{ln}_{xy}, \ \tilde{P}^{mn}_{xy}(t=0) = \delta_{xy}\delta_{mn}, \qquad (15)$$

where x, y, z run the lattice Z^d formed by (fictitious centers of) elementary cells, and $i, j, l, m, n = 1 \div N$ enumerate site types within a cell. $P^{mn}_{xy}(t)$ is the probability of finding a migrant at time t at site $(x; m)$ if it was initially at $(y; n)$.

Our main task is obtaining of the longtime asymptotical expansion of mean propagator $P^{mn}_{xy}(t) = \prec \tilde{P}^{mn}_{xy}(t) \succ$ where averaging (denoted by $\prec f \succ$ or $E(f)$) is performed over the distribution of $\{(\alpha_x, \beta_x) \mid x \in Z^d\}$.

Our special conditions are:

C1) at different x's pairs of $N \times N$-matrices $(\alpha^{ij}_x, \beta^{ij}_x)$ are i.i.d. random matrices and $\beta_x\alpha_x$ has a fairly large number of moments: $\prec (\beta_x\alpha_x)^{-r} \succ$, $r > 0$;

C2) a resolvent of the operator $-A$ at $\lambda \to 0$, $Re(\lambda) \geq 0$ uniformly in $k \in [-\pi, \leq \pi]$ satisfies estimations: $|\sum_z e^{-ikz}((\prec \frac{\lambda}{\beta\alpha} \succ +A)^{-1})^{mn}_{z0}| = O(|\lambda^{-r_1}|)$, $\int_{-\pi}^{\pi} dk |\sum_z e^{-ikz}((\prec \frac{\lambda}{\beta\alpha} \succ +A)^{-1})^{mn}_{z0}| = O(|\lambda^{-r_1}|), r_1 + r_2 < 2$, $r_2 < 1$;

moreover, we need some of the moments $E(\alpha_x), E(\alpha_x^{-1}), E(\beta_x), E(\beta_x^{-1}), E(\alpha_x^+\alpha_x), E(\beta_x\beta_x^+)$ and one of the resolvent properties:

$$|(\frac{1}{\lambda + \beta^+A^+\alpha^+}\ \frac{1}{\lambda + \alpha A\beta})^{mm}_{zz}| \text{ or } |(\frac{1}{\lambda + \alpha A\beta}\ \frac{1}{\lambda + \beta^+A^+\alpha^+})^{mm}_{zz}| = O(|\lambda|^{-r_3}).$$

We use three different forms of development in $\lambda((\beta\alpha)^{-1} - \prec (\beta\alpha)^{-1} \succ)$.

In many interesting models we obtain the leading asymptotical terms (one or two) of resolvent $P(\lambda)$ at $\lambda \to 0$ from the approximations:

$$P(\lambda) \approx \prec \alpha G\alpha^{-1} \succ \text{ or } \approx \prec \beta^{-1}G\beta \succ \text{ or } \approx \prec \beta^{-1}\left[G + G\lambda\eta G\right]\alpha^{-1}] \succ,$$

$$G = (\lambda + A \prec \frac{1}{\beta\alpha} \succ^{-1})^{-1}.$$

The substantial (exactly soluble) generalization of (15) consists in an application of the more general operator valued functions:

$$d\tilde{P}^{mn}_{xy}/dt = -\sum_{v,w,z}\sum_{i,j,l=1}^{N} \alpha^{mi}_{xv} A^{ij}_{v-w} \beta^{jl}_{wz} \tilde{P}^{ln}_{zy}, \quad \tilde{P}^{mn}_{xy}(t=0) = \delta_{xy}\delta_{mn};$$

and the following main condition is supposed:

the independent (or correlated at finite distances) identically distributed random operators α and β have inverse operators of the type

$$(\alpha^{-1})^{mn}_{xy} = \sum_{j=1}^{J} \alpha^{mn|j}_{x} \delta_{x-y-a_j} \alpha^{mn|j+J}_{y}, \quad (\beta^{-1})^{mn}_{xy} = \sum_{j=1}^{J} \beta^{mn|j}_{x} \delta_{x-y-b_j} \beta^{mn|j+J}_{y};$$

the function $x \to (\alpha^1_x, \ldots, \alpha^{2J}_x; \beta^1_x \ldots, \beta^{2J}_x)$ contains all the disorder of medium.

Author is very grateful to Professors F.S.Dzheparov and R.A.Minlos for their interest to this work and several important remarks.

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