Spin dynamics in disordered solids.

F.S.Dzheparov

Modern state of studies in spin dynamics of statically disordered media is presented. Next four fundamental problems are attended mainly:
1) delocalization of nuclear polarization in subsystem of impurity nuclei (it is exemplified in model nuclear spin system ^{8}Li-^{6}Li in the LiF single crystal);
2) nuclear relaxation via paramagnetic impurities in crystals of arbitrary space dimension d;
3) free induction decay and EPR line form function at $d \leq 3$; and
4) form function of the hole, burned on the wing of the dipolar EPR line.

Colleagues:

ITEP, Moscow
Yu.G.Abov,
A.D.Gul'ko
S.S.Trostin,
O.N.Ermakov,
D.V.L'vov,
S.V.Stepanov,
V.E.Shestopal

IRE, Moscow
V.A.Atsarkin,
V.V.Demidov

Inst. Chem.. Phys. Moscow
T.N.Khasanovich
A.A.Lundin

Perm University
E.K.Khenner
I.V.Kaganov

CEA Saclay
J.-F.Jacquinot

Main specifics of the theory of spin dynamics in disordered solids results from the fact, that calculation of observable values must start from the solution of equation of motion, and then they should be averaged over random distribution of spins in the sample. Nominally any problem in statistical physics looks analogously, but content of existing text books is formed by much more simple bypass ways to the results.

Important bypass classes:

1) quantum mechanics $\rightarrow$ Boltzmann equation $\rightarrow$ $\rightarrow$ hydrodynamics;

2) projection technic of Nakajima-Zwanzig for deriving of various master equations together with effective approximations for corresponding memory functions.

Both these bypass ways produce satisfactory predictions if the system have such small parameters as, for example, ratio of collision duration to time between collisions, or ratio of memory time to time of variation of substantial observables (the observables whereon the system evolution is projected). Similar small parameters are not exist in disordered solids after some beginning stage, or they are absent at all. Therefore other more refined methods are necessary to predict experimental results. They are partially presented below.

First correct solutions of the problems of disordered media kinetics, which are directly connected with the spin dynamics, were obtained by Forster (1949) and Anderson (1951).

The Forster's problem.

$$\dot{p}_j = -\sum\nolimits_{a=1,N}^{N} v_{aj} p_j = -\sum\nolimits_{\mathbf{r}} n_{\mathbf{r}} v_{\mathbf{r}j} p_j, \quad p_j(t=0) = 1. \qquad (1)$$

Here v_{aj} is the depolarization rate under influence of the $a-$th paramagnetic center (acceptor), N is total number of acceptors in the sample, $v_{\mathbf{r}j} = v_{aj}(\mathbf{r}_a = \mathbf{r})$, and $n_{\mathbf{r}}$ is occupation number of the site $\mathbf{r}$ by an acceptor ($n_{\mathbf{r}} = 1(0)$ if the site $\mathbf{r}$ is (not) occupied by an acceptor). Occupations of different sites will be assumed as independent and having no dependence on the $\mathbf{r}$ (with small probability of occupation $c \ll 1$ as a rule):

$$\langle n_{\mathbf{r}} \rangle_c = c, \quad \langle n_{\mathbf{r}} n_{\mathbf{x}} \rangle_c = c\delta_{\mathbf{rx}} + c^2(1-\delta_{\mathbf{rx}}), \quad \langle \prod\nolimits_{j=1}^{\prime m} n_{\mathbf{r}_j} \rangle_c = \prod\nolimits_{j=1}^{\prime m} \langle n_{\mathbf{r}_j} \rangle_c = c^m. \qquad (2)$$

All $\mathbf{r}_j$ are different in the last relation.

Coincidence in indexes can be treated using the identity $n_{\mathbf{r}}^2 = n_{\mathbf{r}}$. The problem consists in calculation of the observable polarization, averaged over all possible positions of acceptors in the sample. Ensemble averaging can be used for macroscopic samples: $p(t) = \langle p_j(t) \rangle_c$. Occupation number representation gives the simplest and general solution of the last problem. Indeed

$$p(t) = \langle p_j(t) \rangle_c = \langle \exp\left(- \sum\nolimits_{\mathbf{r}} n_{\mathbf{r}} v_{\mathbf{r}j} t \right) \rangle_c = \prod\nolimits_{\mathbf{r}} \langle \exp\left(-n_{\mathbf{r}} v_{\mathbf{r}j} t\right) \rangle_c =$$

$$= \prod\nolimits_{\mathbf{r}} \langle 1 + n_{\mathbf{r}} \left[\exp\left(-v_{\mathbf{r}j} t\right) - 1 \right] \rangle_c = \prod\nolimits_{\mathbf{r}} \langle 1 + c \left[\exp\left(-v_{\mathbf{r}j} t\right) - 1 \right] \rangle_c =$$

$$= \exp\left\{ \sum\nolimits_{\mathbf{r}} \ln\left[1 + c \left(\exp\left(-v_{\mathbf{r}j} t\right) - 1 \right) \right] \right\} .$$

The identity $f(n_{\mathbf{r}}) = f(0) + n_{\mathbf{r}}(f(1) - f(0))$ is applied here. It is valid for any realistic function $f(x)$. This relation is exact for any c.

Typical depolarization rate is of the form

$$v_{aj} = v_0 \bar{r}_0^6 \chi(\mathbf{r}_{aj}/r_{aj})/r_{aj}^6,$$

v_0 scales the transport at minimal distance $\bar{r}_0$, $\mathbf{r}_{aj} = \mathbf{r}_a - \mathbf{r}_j$, $\chi(\mathbf{n}) = |Y_{21}(\mathbf{n})|^2$, and $Y_{lm}(\mathbf{n})$ is the spherical harmonics. Additional simplification is possible for the continuum media approximation (CMA), when $c \to 0$, but $p(0) - p(t) \neq 0$:

$$p(t, c \to 0) = \exp\left(n \int d^d r \left(e^{-v_{\mathbf{r}j} t} - 1 \right) \right) = \exp(-(\beta_F t)^{d/6}),$$

$$\beta_F \propto n^{6/d} v_0 r_0^6.$$

Here arbitrary spatial dimension d is considered, and impurity density $n = c/\Omega_c$ is introduced together with the prime cell volume Ω_c.
Forster's parameter is proportional to transfer rate at average distance $\bar{r} = n^{-1/d}$:

$$\beta_F = const \cdot v_{\mathbf{r}j}(|\mathbf{r} - \mathbf{r}_j| = \bar{r}).$$

Anderson model for EPR line form function.

$S = 1/2$, spins are randomly distributed inside a sample.

$$H = \frac{1}{2}\sum_{\mathbf{r},\mathbf{q}} n_{\mathbf{q}} n_{\mathbf{r}} b_{\mathbf{rq}} \left(S^z_{\mathbf{r}} S^z_{\mathbf{q}} - \frac{1}{3}\mathbf{S}_{\mathbf{r}}\mathbf{S}_{\mathbf{q}} \right) \rightarrow H_A = \frac{1}{2}\sum_{\mathbf{r},\mathbf{q}} n_{\mathbf{q}} n_{\mathbf{r}} b_{\mathbf{rq}} S^z_{\mathbf{r}} S^z_{\mathbf{q}},$$

$$b_{\mathbf{rq}} = b_0 r_0^3 (1 - 3\cos^2\vartheta_{\mathbf{rq}})/|\mathbf{r} - \mathbf{q}|^3, \quad b_{\mathbf{rr}} = 0$$

Spectra of both Hamiltonian coincide for two spin problems, if $S = 1/2$.

Exact solution for arbitrary concentration:

$$n_{\mathbf{r}} S^+_{\mathbf{r}}(t) = n_{\mathbf{r}} S^+_{\mathbf{r}} \exp\left(i \sum\nolimits_{\mathbf{q}} n_{\mathbf{q}} b_{\mathbf{rq}} S^z_{\mathbf{q}} t \right), \quad \mathbf{S} = \sum_{\mathbf{r}} n_{\mathbf{r}} \mathbf{S}_{\mathbf{r}}.$$

Free induction decay (FID):

$$F(t) = \langle\langle S_+(t) S_- \rangle\rangle_c / \langle\langle S_+ S_- \rangle\rangle_c = \langle\langle \exp\left(i \sum\nolimits_{\mathbf{q}} n_{\mathbf{q}} b_{\mathbf{rq}} S^z_{\mathbf{q}} t \right) \rangle\rangle_c =$$

$$= \prod\nolimits_{\mathbf{q}} \langle \cos(n_{\mathbf{q}} b_{\mathbf{qr}} t/2) \rangle_c = \prod\nolimits_{\mathbf{q}} \left(1 + c\left(\cos(b_{\mathbf{qr}} t/2) - 1\right)\right) =$$

$$= \exp\left(\sum\nolimits_{\mathbf{q}} \ln\left(1 + c(\cos(b_{\mathbf{qr}} t/2) - 1)\right) \right).$$

Applying CMA we arrive to Anderson's result:

$$F(t, c \to 0) = \exp\left(-n \int d^d q \, (1 - \cos(b_{\mathbf{qr}} t/2))\right) = \exp\left(-(D_A t)^{d/3}\right).$$

D_A is proportional to the rate of the process taken at the average distance: $D_A \propto b_{\mathbf{qr}}(|\mathbf{q} - \mathbf{r}| = \bar{r})$.

1. Delocalization of nuclear polarization in disordered spin system.

Examples:

1) nuclei ^{6}Li in the single crystal ^{7}Li^{19}F,

2) nuclei ^{107}Ag in the single crystal ^{109}Ag^{19}F.

Experiment: ^{8}Li-^{6}Li in the single crystal ^{7}Li^{19}F, β-**NMR**.

Polarized neutrons $\rightarrow$ polarized β-active nuclei (β-nuclei):

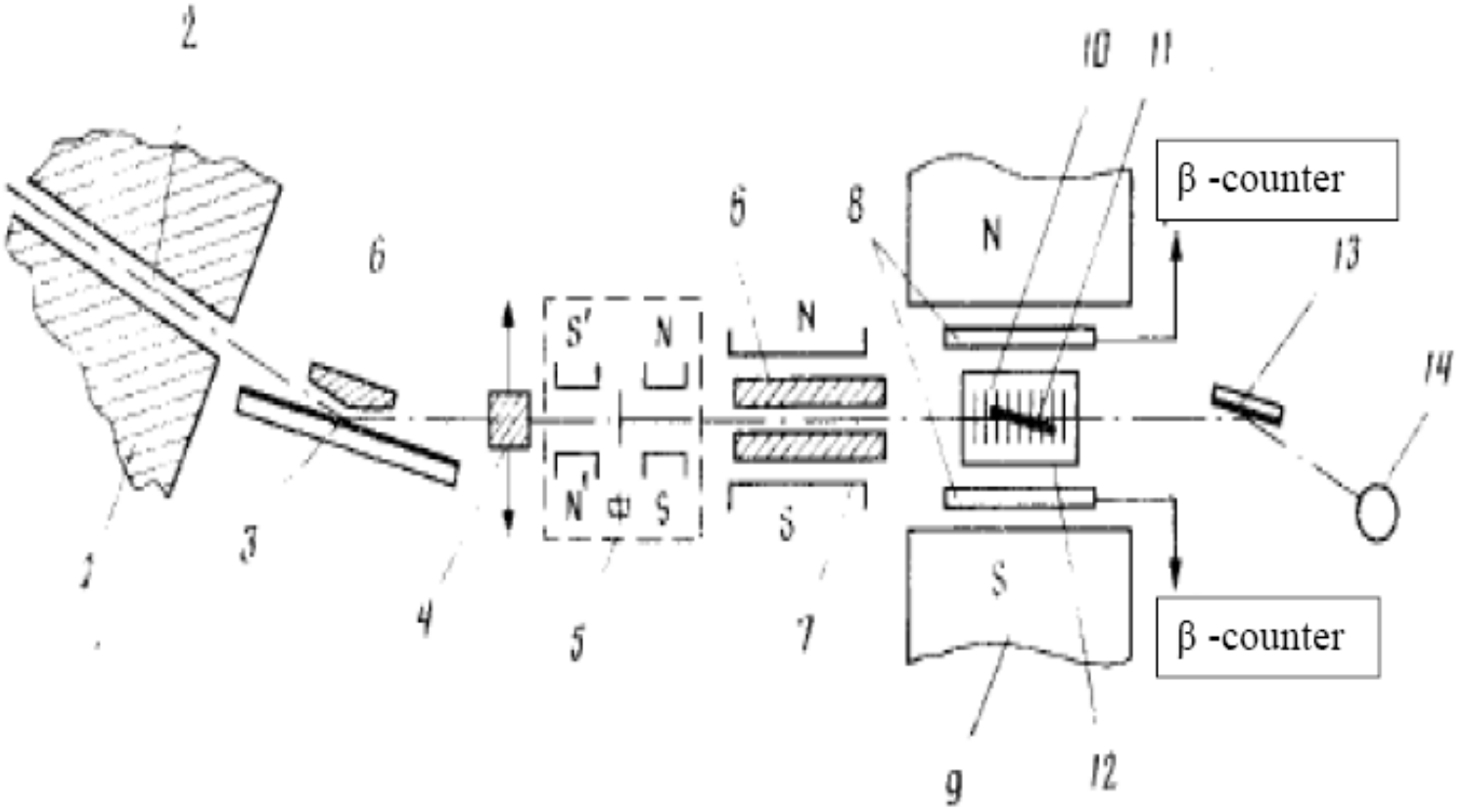
$$^{7}Li(\vec{n},\gamma)^{8}\overrightarrow{Li} \longleftrightarrow t = 0.$$

Angular distribution of β-radiation

$$W(\vartheta, t) \propto 1 + a \cdot p(t) \cdot \cos\vartheta.$$

Measurable value:

$$\varepsilon(t) = \frac{N(\vartheta = 0, t) - N(\vartheta = \pi, t)}{N(\vartheta = 0, t) + N(\vartheta = \pi, t)} \Longleftrightarrow a \cdot p(t).$$



Beta-NMR set up.
1- reactor shielding, 2 – collimator, 3 – cobalt polarizing mirror, 4 – chopper, 5 – spin-flipper, 6 – collimator, 7 - magnets for leading field, 8 – β-detectors, 9 – NMR-magnet, 10 – RF-coil, 11 – sample, 12 – cryostat, 13 – analyzer, 14 – neutron counter.

Spin dynamics.

Single crystal LiF, $\frac{g(^8Li)-g(^6Li)}{g(^8Li)} = 0.057.$

$H_0 = 200\text{G} \longleftrightarrow$ flip-flop ^{8}Li-^{6}Li has the same speed as flip-flop ^{6}Li-^{6}Li, other cross-relaxation transitions are forbidden.

$$\frac{\partial p_{i0}}{\partial t} = -\sum\nolimits_j (\nu_{ji} p_{i0} - \nu_{ij} p_{j0}), \qquad p_{i0}(t=0) = \delta_{i0},$$

$p_{i0}(t) = \langle I_i^z(t) \rangle$ is the quantum statistical average value of the z-component (polarization) of the i-th nucleus, placed at $\mathbf{r}_i$ ($i = 0$ corresponds to ^{8}Li, and $i \neq 0$ to ^{6}Li). The rates of polarization transfer:

$$\nu_{ji} = \xi_j \nu_{ji}^0 \cdot \left(\frac{1 - 3\cos^2\theta_{ji}}{(r_j/d)^3} \right)^2, \quad \nu_{ji}^0 = \frac{\pi}{6} S(S+1) \left(\frac{g_i g_j \beta_n^2}{\hbar d^3} \right)^2 g_{ij}(\omega_{ij}),$$

$\xi_j = I_j(I_j+1)/[S(S+1)]$, g_i — g-factor, β_n is nuclear magneton, θ_{ji} is the angle between $\mathbf{H}_0$ and $\mathbf{r}_{ji} = \mathbf{r}_j - \mathbf{r}_i$, $d = 2.01$Å is minimal Li-F distance, ω_{ij} is difference of the Larmor frequencies.

$$g_{ij}(\omega) \approx \exp(-\omega^2/(2M))/(2\pi M)^{1/2}, \quad M = 2M_2,$$

M_2 is second moment of the ^{8}Li NMR line. This approximation is correct quantitatively at least for $\omega^2 \leq 2M$. As a result ν^0_{ij} have two values only, $\nu^0_{ij} = \nu_0$ for transfer between ^{6}Li spins (at that $\omega_{ij} = 0$), and $\nu^0_{i0} = \nu_1$ for transfer between ^{8}Li and ^{6}Li (with $\omega_{ij} = \Delta$).

The way to

$$\frac{\partial p_{i0}}{\partial t} = -\sum\nolimits_j (\nu_{ji} p_{i0} - \nu_{ij} p_{j0}), \qquad p_{i0}(t=0) = \delta_{i0},$$

is long and complex, but disorder is not important here and standard small parameters were utilized. Roughly speaking the way is similar to derivation of hydrodynamics from quantum mechanics via Boltzmann equation.

The occupation number representation of the equation is of the form

$$\frac{\partial \tilde{P}_{\mathbf{x0}}}{\partial t} = -\sum\nolimits_{\mathbf{z}} (n_{\mathbf{z}} \nu_{\mathbf{zx}} \tilde{P}_{\mathbf{x0}} - n_{\mathbf{x}} \nu_{\mathbf{xz}} \tilde{P}_{\mathbf{z0}}), \qquad \tilde{P}_{\mathbf{x0}}(t=0) = n_{\mathbf{x}} \delta_{\mathbf{x0}}/c.$$

$$\frac{\partial \tilde{P}_{\mathbf{x0}}}{\partial t} = -\sum\nolimits_{\mathbf{z}} (n_{\mathbf{z}} \nu_{\mathbf{zx}} \tilde{P}_{\mathbf{x0}} - n_{\mathbf{x}} \nu_{\mathbf{xz}} \tilde{P}_{\mathbf{z0}}), \qquad \tilde{P}_{\mathbf{x0}}(t=0) = n_{\mathbf{x}} \delta_{\mathbf{x0}}/c.$$

The propagator $\tilde{P}_{\mathbf{x0}}$ gives polarization of the lattice site $\mathbf{x}$ when initially the site $\mathbf{0}$ was polarized, and $\nu_{\mathbf{zx}} = \nu_{ij}(\mathbf{r}_i = \mathbf{z}, \mathbf{r}_j = \mathbf{x})$.

The measurable value: $P_{\mathbf{00}}(t) = \langle p_{00} \rangle_c = \langle \tilde{P}_{\mathbf{00}} \rangle_c$.

Random walks in disordered media (RWDM) $\Longleftrightarrow$ one of the most complex modern field of the statistical physics.

The path integral:

$$\mathcal{P}_{\mathbf{xy}}(t) = \int_{\mathbf{q}(0)=\mathbf{x}}^{\mathbf{q}(1)=\mathbf{y}} D\mathbf{p}(\tau) D\mathbf{q}(\tau) \exp(I[p,q]),$$

$$I[p,q] = i \int_{\mathbf{x}}^{\mathbf{y}} \mathbf{p} d\mathbf{q} + n \int d^3 z \left(e^{-t \int_0^1 d\tau A^z(\mathbf{q}(\tau), \mathbf{p}(\tau))} - 1 \right),$$

$A^z(\mathbf{q}, \mathbf{p}) = \nu_{\mathbf{zq}} \left(1 - e^{-i\mathbf{p}(\mathbf{z}-\mathbf{q})}\right)$. The representation is similar to, but more complex than path integrals in famous polaron problems. Superfield path integral representations for $P_{\mathbf{xy}}(t) = \langle \tilde{P}_{\mathbf{xy}} \rangle_c$ exist as well.

These representations demonstrate the relation of the RWDM to general problems of the modern field theory, but they are too complex, and real calculations now are based on concentration expansion (real parameter: $c^m \to (\beta t)^{m/2}$) for $\beta t \lesssim 1$, and numerical simulation (giving diffusion tensor) for $\beta t \gg 1$.
The theory had produced the interpolating formula (without experimental fitting parameters)

$$P_{\mathbf{00}}(t) = F(t) = \exp(-\sqrt{\beta_1 t}) + \xi \frac{1-\exp(-\sqrt{\beta_1 t})}{(\mu\beta(t+\tau))^{3/2}} \left(1 + \frac{\varphi}{\sqrt{\mu\beta(t+\tau)}}\right),$$

$$\xi = \xi_0 = I(I{+}1)/[S(S{+}1)] = 3, \quad \mu\beta = 4\pi\,(c/\Omega_c)^{2/3} \left(\prod\nolimits_{\alpha=1}^{3} D_\alpha\right)^{1/3} = 0.71,$$

$$\varphi = 2.09,\ \ \mu\beta\tau = 5.11,\ \ \beta = (256/243)\pi^3 c^2 \nu_0 r_0^6/\Omega_c^2,\ \ \beta_1 = \beta{\cdot}\nu_1/\nu_0,\ \ c \ll 1.$$

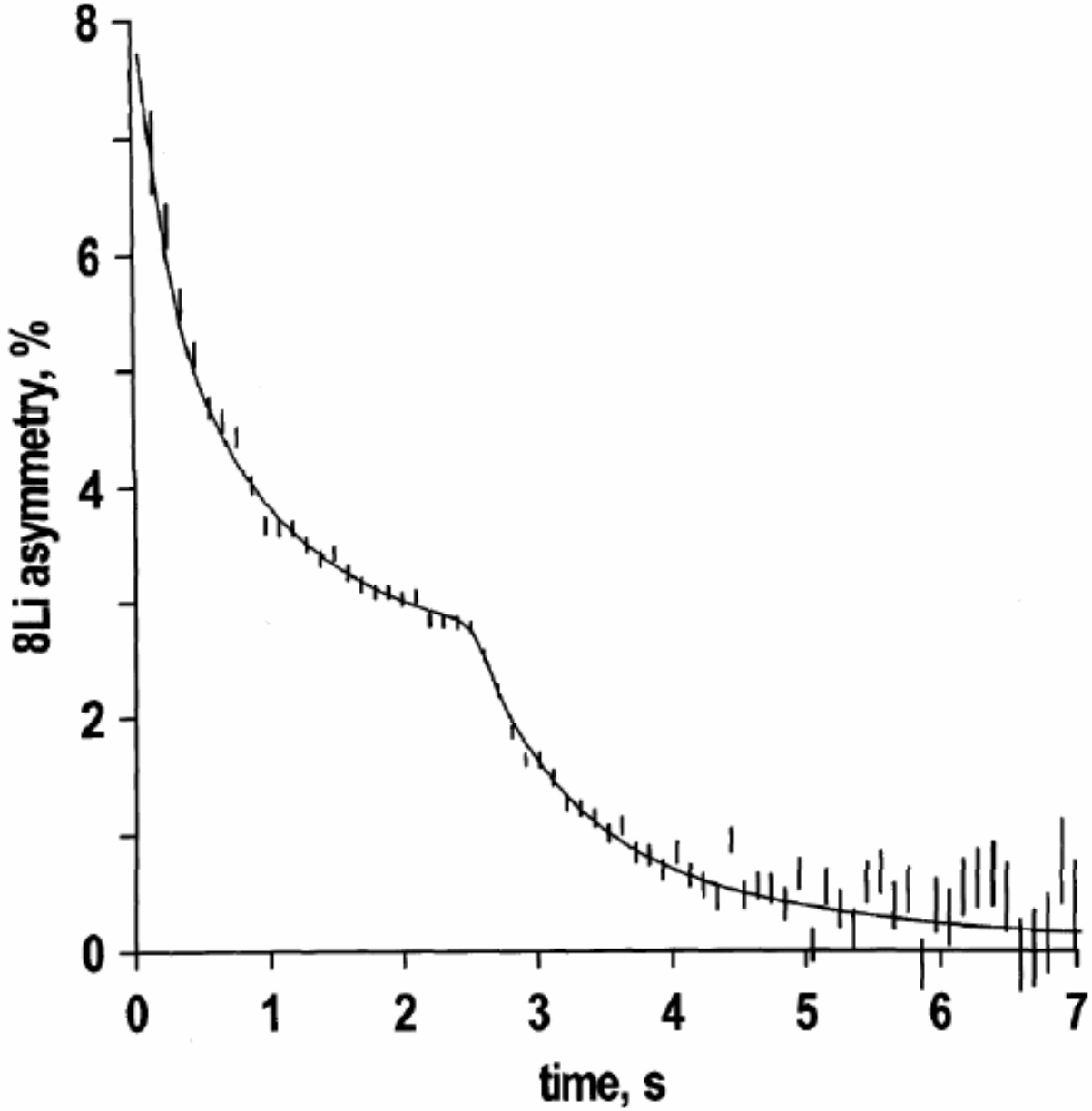
$P_{\mathbf{00}}(t)$ holds to within $(\beta t)^{1/2}$ at small βt, and it holds to within $(\beta t)^{-2}$ at large βt.

Last results of the ITEP group indicate that at $\beta_1 t \sim 25$ some correction is necessary. It can be introduced as

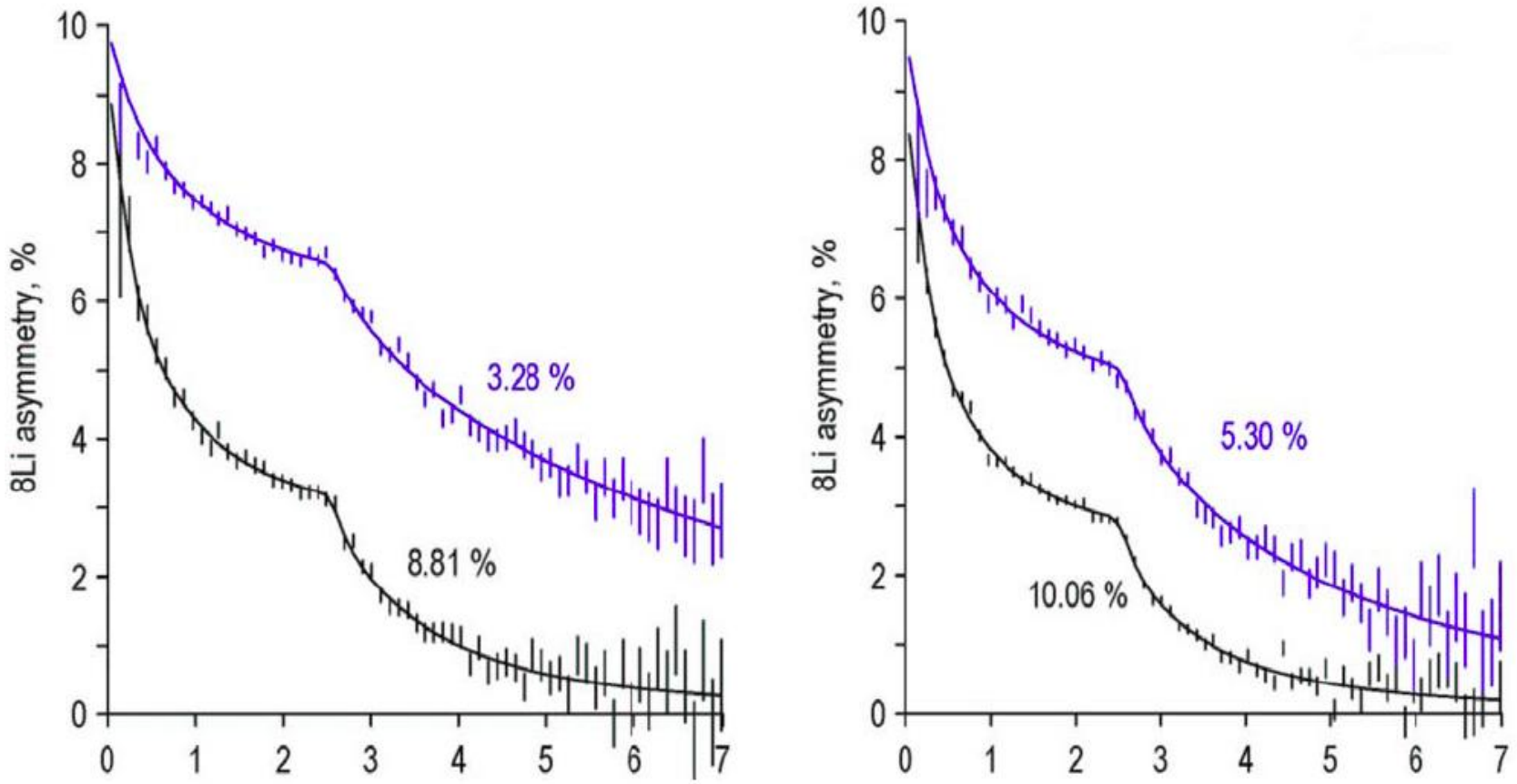
$$P_{\mathbf{00}}(t) = F(t)\left(1 - \frac{(\frac{1}{8}+\alpha)\beta_1 t - u(\beta_1 t)^2}{(1+v\beta t)^3}\right).$$

$$F(t) = \exp(-\sqrt{\beta_1 t}) + \xi\frac{1-\exp(-\sqrt{\beta_1 t})}{(\mu\beta(t+\tau))^{3/2}}\left(1 + \frac{\varphi}{\sqrt{\mu\beta(t+\tau)}}\right),$$

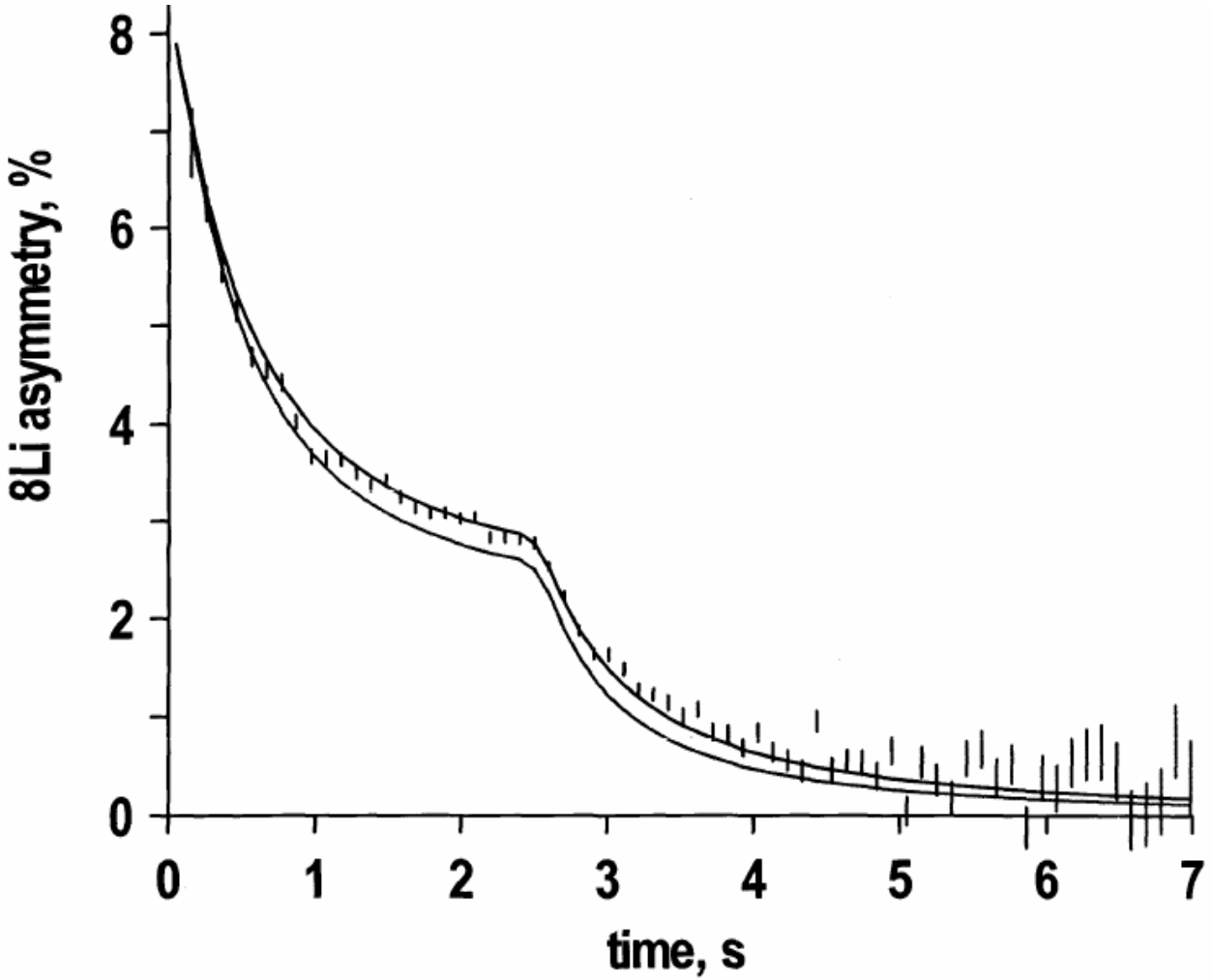
Here $F(t)$ is old relation, $\alpha = \alpha(\Delta)$ have been tabulated basing on the short time asymptotics, and fitting parameters u and v should be determined by experimental data. New relation holds to within βt at small βt, and it holds to within $(\beta t)^{-2}$ at large βt. The fitting produces $u \approx 0.06$ and $v \approx 0.12$. Direct numerical simulation of the $P_{\mathbf{00}}(t)$ is expected now as a natural way for more detail comparison of the experiment and theory.



c=10.06(4)%, β_0*=10.80s*$^{-1}$*,* β_1*=10.18s*$^{-1}$*, H*$_0$*=200G,* μ*=0.761, u=0.054(3), v=0.111(6).*



Depolarization kinetics of ^{8}Li β-nuclei in LiF crystals, having various concentration of ^{6}Li isotope. External magnetic field is equal to 200 G. It is parallel to the [111] axis of the crystal. Error bars indicate the statistical uncertainties only. Solid lines are the result of the fitting with simplest correction $G_{exp}(t)$.



Observable time dependence of the β-decay asymmetry for the ^{8}Li-^{6}Li system in LiF single crystal. Orientation: [111]||$\mathbf{H}_0$; ^{6}Li concentration c=10.06(4)%. The neutron pulse duration t_p=*2.5 c*. Lower line presents the calculation result without fitting parameters. Upper line includes simplest correction function $G_{exp}(t)$ with fitting parameters *u=0.054(3)* and *v=0.111(6)*.

2. Nuclear relaxation via paramagnetic impurities.

Other important generalization of the Forster's process is presented by nuclear relaxation via paramagnetic impurities, which is main relaxation channel in isolators if nuclear spin $I = 1/2$. The fundamental studies [Khutsushvili 1965, Alexandrov 1975, Atsarkin 1980, Abragam & Goldman 1982] were based on calculation of the linear (in impurity concentration c) term of the time dependence of the sample magnetization $P(t) = 1 - cQ(t)$ (for 3d-systems) with following substitution $P(t) = \exp(-cQ(t))$. Analysis of two- and one-dimensional problems was absent whereas experiments are already aimed at fractal objects [Tabti et al. 1997]. Therefore new theory was constructed [Dzheparov, Jacquinot, Stepanov 2002]. It produce the relation $P(t) = \exp(-cQ(t))$ as main approximation, and the function $Q(t)$ is calculated for arbitrary $d \leq 3$.

The process is used to be described by the kinetic equation

$$\frac{\partial p(\mathbf{x},t)}{\partial t} = D\Delta p(\mathbf{x},t) - \sum\nolimits_{\mathbf{z}} n_{\mathbf{z}} v_{\mathbf{zx}} p(\mathbf{x},t), \quad v_{\mathbf{zx}} = \frac{v_0 r_0^6}{|\mathbf{x}-\mathbf{z}|^6} = \frac{C}{|\mathbf{x}-\mathbf{z}|^6},$$

with initial condition $p(\mathbf{x},t) = p_0$. Here $p(\mathbf{x},t)$ is polarization of the nucleus, placed at the crystal site $\mathbf{x}$, D is spin-diffusion coefficient, and the angular dependence of $v_{\mathbf{zx}}$ is neglected. The observable nuclear polarization (normalized to $\bar{p}(t=0)=1$) is

$$\bar{p}(t) = \frac{1}{\Omega}\int d^d x p(\mathbf{x},t) = \langle 0|G(t)|0\rangle = \langle 0|\langle G(t)\rangle_c|0\rangle.$$

Here d is the space dimensionality, Ω is the crystal volume, the symbol $|0\rangle$ presents a vector having components $\langle \mathbf{x}|0\rangle = 1/\sqrt{\Omega}$, and the propagator $G_{\mathbf{xy}}(t) = \langle \mathbf{x}|G(t)|\mathbf{y}\rangle$ obey the same equation, but for initial condition

$$G_{\mathbf{xy}}(t=0) = \delta(\mathbf{x}-\mathbf{y})$$

Expansion of the observable $\bar{p}(t)$ in concentration powers:

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

$$= \exp\left(-M_0(t)(1+O(n^2)\right),$$

$$M_0(t) = n\int d^d r \langle 0|[G^{(0)}(t) - G^{(1)}(t,\mathbf{r})]|0\rangle.$$

The propagator $G^{(0)}(t)$ corresponds to evolution in the absence of acceptors, and $G^{(1)}(t,\mathbf{r})$ is the propagator of the system, having only one acceptor, placed at $\mathbf{r}$. Then, using operator transformations, we have

$$M_0(\lambda) = \int_0^\infty dt e^{-\lambda t} M_0(t) = \frac{n\Omega}{\lambda}\langle 0|U_0 \frac{1}{\lambda + A + U_0}|0\rangle =$$

$$= \frac{n\Omega}{\lambda}\langle 0|U_0 \frac{1}{(A+U_0)(\lambda + A + U_0)} U_0|0\rangle = \frac{n\Omega}{\lambda}\sum_n \frac{|\langle n|U_0|0\rangle|^2}{(\lambda + E_n)E_n}.$$

$$A = -D\Delta, \quad \langle \mathbf{x}|U_0|\mathbf{z}\rangle = \delta_{\mathbf{xz}} v_{\mathbf{x0}}, \quad (A+U_0)|n\rangle = E_n|n\rangle.$$

Obtained representation is too complex for direct calculations, but it is useful for different asymptotical treatments. Most important of them are short time and long time studies, because a satisfactory precision can be achieved using the representation

$$M_0(t) = M_F(t) + M_1(t).$$

$$M_F(t) = n \int d^d x (1 - \exp(-v_{\mathbf{x0}} t)) = (\beta_F t)^{d/s}.$$

$v_{\mathbf{x0}} = v_0 r_0^s / x^s$ is applied to clarify some parametrical dependencies.
$M_F(t)$ describes the initial (Forster's) part of relaxation, while $M_1(t)$ is the longtime asymptotic expression, formally continued to arbitrary time t. The results, obtained for $M_1(t)$ at arbitrary $d \leq 3$ are not short. They are presented in details in the article.

Satisfactory precision can be achieved using the representation

$$M_0(t) = M_F(t) + M_1(t).$$

$$M_F(t) = n \int d^d x (1 - \exp(-v_{\mathbf{x0}} t)) = (\beta_F t)^{d/s}.$$

In particular, in main asymptitics,

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

$$M_1(t, d = 3) = 4\pi Dbnt,$$

$b \propto (C/D)^{1/(s-2)}$ is a "scattering length", which incorporate all dependence on the "potential" $v_{\mathbf{x0}}$. It is evident, that at $d = 1$ the dependence on b is absent here, and for $d = 2$ is is rather weak.

New mean field theory.

In order to find argumentation for regrouping of the concentration expansion,

$$1 - M_0(t) \to \exp(-M_0(t))$$

we represent the propagator $G(t)$ in the form (no approximations!)

$$G(t) = \langle \exp(-(A+U)t) \rangle_c = \exp(-B(t)), \quad B(t) = At + M(t),$$

$$U = \sum\nolimits_{\mathbf{z}} n_{\mathbf{z}} U^{\mathbf{z}}, \quad U^{\mathbf{z}}_{\mathbf{xq}} = \delta_{\mathbf{xq}} v_{\mathbf{xz}}, \quad M(t) = \sum\nolimits_{\mathbf{z}} M_{\mathbf{z}}(t).$$

It can be said that the operators $M_{\mathbf{z}}(t)$ must adequately describe the effect of acceptors in the so-called effective medium that appears upon averaging over the configurations of acceptors. It is therefore **natural to assume** that, on average, the propagator $G(t)$ undergoes no changes if one of the sites of the effective medium is replaced by an actual one and if the result is thereupon averaged over the distribution of acceptors; that is,

$$G(t) = \langle \exp(-At - M(t) + M^z(t) - n_z U^z t) \rangle_c.$$

The relations, formulated above, gave a closed set of nonlinear operator equations. The solution practically coincides with

$$P(t) = \exp(-M_0(t)),$$

if $cQ(t) = M_0(t) \sim 1$ and $c \ll 1$.
Corrections are important for longer time.

It should be stressed, that
1) to clarify the influence of corrections to this solution in more details we can calculate next ($\propto c^2$) term of the concentration expansion, and
2) there exist physical [Balagurov & Waks 1973] and mathematical studies, giving the law

$$p(t \to \infty)) \propto \exp\left(-(t/T)^{d/(d+2)}\right),$$

which is expected to be valid at $\bar{p}(t) \lesssim 10^{-12}$.

3. Resonance line form function for magnetically diluted solids with arbitrary space dimension.

The line shape and the Fourier-transform-related free induction decay (FID) belong to the most important observable values in physics of magnetic resonance. It is well known, that in the study of nuclear spin systems forming a crystal lattice the first ($\propto t^2$ and $\propto t^4$) terms of the expansion of FID in powers of time carry highly important information. In the theory of the line shape of disordered (magnetically diluted) electron spin systems, the first ($\propto c$ and $\propto c^2$) terms in the expansion in powers of the concentration c of paramagnetic centers plays the same role [Dzheparov, Lundin, Khazanovich 1987]. The third ($\propto c^2$) term was calculated in a recent study [Dzheparov & Kaganov 2002] for the first time. The consideration is particularly topical in connection with the new experiments on measuring the EPR spectra of paramagnetic impurities distributed at the solid surface [Atsarkin et al. 2000, 2001].

Let the paramagnetic centers (PCs) be randomly distributed in a d-dimensional crystal lattice with the prime-cell volume Ω_c. The free induction decay in the high temperature approximation is given by

$$G(t) = \langle\langle S^+(t)S^-\rangle_0\rangle_c / \langle\langle S^+S^-\rangle_0\rangle_c \ ,$$

where $S^\pm = \sum_{\mathbf{r}} n_{\mathbf{r}} S^\pm_{\mathbf{r}}$, $S^\pm_{\mathbf{r}} = S^x_{\mathbf{r}} \pm iS^y_{\mathbf{r}}$, $S^+(t) = e^{iHt}S^+e^{-iHt}$, $S_{\mathbf{r}} = 1/2$, $n_{\mathbf{r}}$ is the occupation number, $\langle\cdots\rangle_0 = \mathrm{Tr}(\cdots)/\mathrm{Tr}1$, $\langle\cdots\rangle_c$ stands for the averaging over the spatial spin distributions (over occupation numbers), and H is the secular part of dipole-dipole interactions:

$$H = \frac{3}{4}\sum\nolimits_{rq} n_r n_q A(\mathbf{r},\mathbf{q})(S^z_r S^z_q - \frac{a}{3}\mathbf{S}_r\mathbf{S}_q).$$

Here $A(\mathbf{r},\mathbf{q}) = \hbar\gamma^2(1-3\cos^2\vartheta_{rq})/|\mathbf{r}-\mathbf{q}|^3$, γ is the gyromagnetic ratio, and ϑ_{rq} is the angle between $\mathbf{r}-\mathbf{q}$ and external static field $\mathbf{H}_0$. Parameter $a = 0$ in the Anderson model and $a = 1$ for pure dipole interaction.

For other a values the Hamiltonian corresponds to a system with the anisotropic axisymmetric g-factor. In what follows, $S = 1/2$ for all PCs. Concentration expansion:

$$G(t) = 1 + n \int d^d r_1 (2K_{01}(t) - 1) +$$

$$+\frac{n^2}{2} \int d^d r_1 d^d r_2 (2K_{012}(t) - 2K_{01}(t) - 2K_{02}(t) + 1) + O(n^3),$$

where $n = c/\Omega_c$ is the d-dimensional PC density, and

$$K_{01}(t) = \langle e^{iH_{01}t} S_0^+ e^{-iH_{01}t} (S_0^- + S_1^-) \rangle_0 \ ,$$

$$K_{012}(t) = \langle e^{iH_{012}t} S_0^+ e^{-iH_{012}t} (S_0^- + S_1^- + S_2^-) \rangle_0 \ .$$

$$H_{ij} = \frac{1}{2} A_{ij} (3 S_i^z S_j^z - a \mathbf{S}_i \mathbf{S}_j), \quad H_{012} = H_{01} + H_{02} + H_{12},$$

with $A_{ij} = A(\mathbf{r}_i, \mathbf{r}_j)$. The interaction $A_{ij} \propto |\mathbf{r}_i - \mathbf{r}_j|^{-3}$. Therefore substitution of integration variables $\mathbf{r}_i \to t^{1/3} \mathbf{r}_i$ excludes time from the integrands and reveals that n^m-term is $\propto (n t^{d/3})^m$.

Real parameter is

$$(D_d t)^{d/3} = n \int d^d r_1 (1 - 2K_{01}(t)) \ .$$

Therefore

$$G(t) = 1 + (D_d t)^{d/3} + \frac{1}{2}\xi_d(a)(D_d t)^{2d/3} + O((D_d t)^d),$$

The functions $\xi_d(a)$ were calculated numerically basing on diagonalization of the three-spin Hamiltonian. It was supposed, that at $d \leq 2$ all field directions are equally probable, then

$$\bar{G}(t) = 1 - (\bar{D}_d t)^{\frac{d}{3}} + \frac{\bar{\xi}_d(a)}{2}(\bar{D}_d t)^{\frac{2d}{3}} + O((\bar{D}_d t)^d),$$

and

$$D_d = \beta_d n^{d/3} \gamma^2 \hbar, \quad \beta_3 = \frac{2\pi^2}{3\sqrt{3}}, \quad \beta_2 = 4.647, \quad \beta_1 = 6.348.$$

D_3 coincides with the Anderson's result by construction.

The results are presented in the table:

a	0	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6
ξ_3	1	1.01	1.03	1.05	1.08	1.11	1.13	1.15	1.18
$\bar{\xi}_2$	1.027	1.07	1.11	1.15	1.19	1.22	1.25	1.27	1.29
$\bar{\xi}_1$	1.062	1.16	1.20	1.25	1.28	1.32	1.35	1.37	1.40

Obtained relations can be used directly for analysis of the wings of experimental EPR lines. But treatment of the full line or FID requires to regroup the concentration expansion in such a way to receive physically adopted result for all t. One of the simplest approaches [Galiullin et al. 1981, Dzheparov et al 1993, 1997] was generalized for this aim. The approach introduces the most essential properties of the disordered systems into the Anderson-Weiss-Kubo (AWK) theory, which was originally developed for the description of motional line narrowing.

The result is of the form

$$G(t) = \exp\left(-\left(2B_d^2 \int_0^t d\tau (t-\tau) F(B_d \tau)\right)^{d/6}\right),$$

$$F(x) = \exp(-(q_d x)^{d/3}).$$

Being approximative this representation nevertheless reproduces the structure of the concentration expansion, nonnegativity of the resonance line shape and parameters B_d and q_d can be defined using D_d and ξ_d, that gives

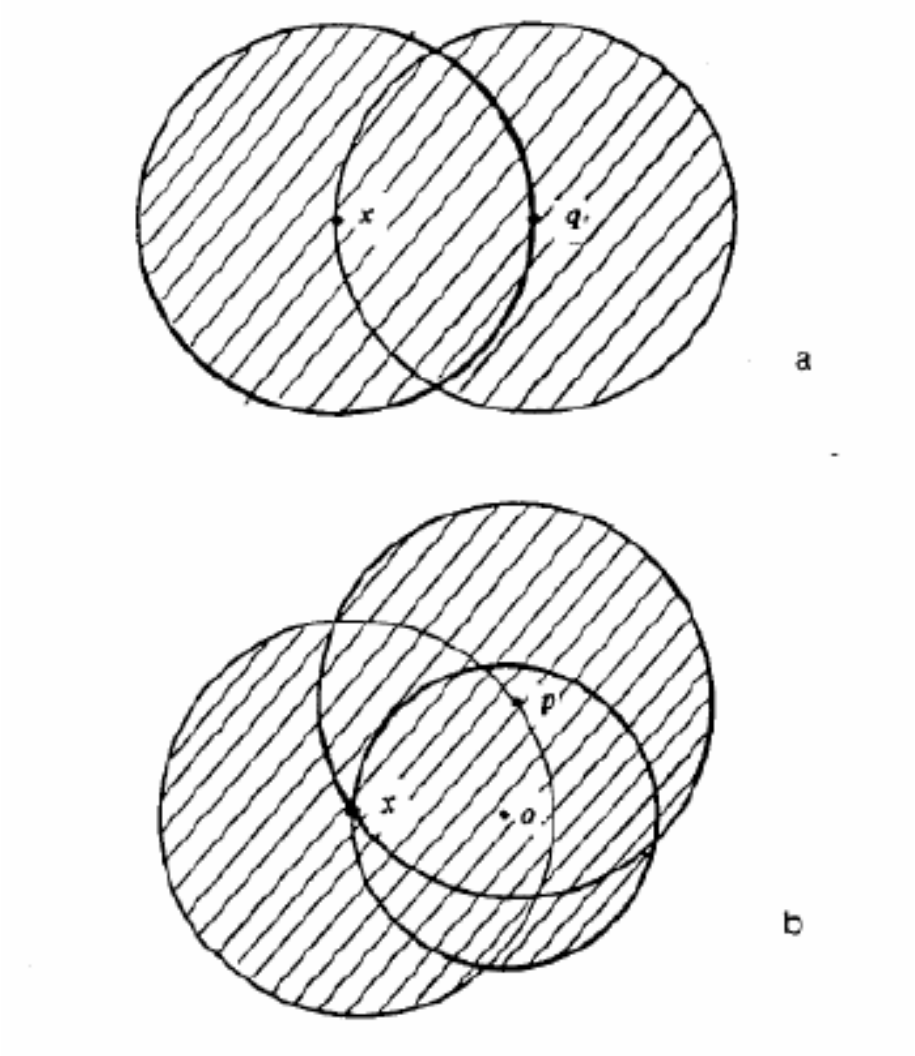
$$B_3 = D_3, \quad B_2 = \bar{D}_2, \quad q_3 = 3(\xi_3 - 1), \quad q_2 = ((10/3)(\bar{\xi}_2 - 1))^{3/2}.$$

The dimensionality $d = 1$ requires more refined treatment, because system orientations near the "magic" direction $\theta = \arccos(1/\sqrt{3})$ produce a singularity $g_1(\omega \to 0) \propto \ln(1/\omega)$.

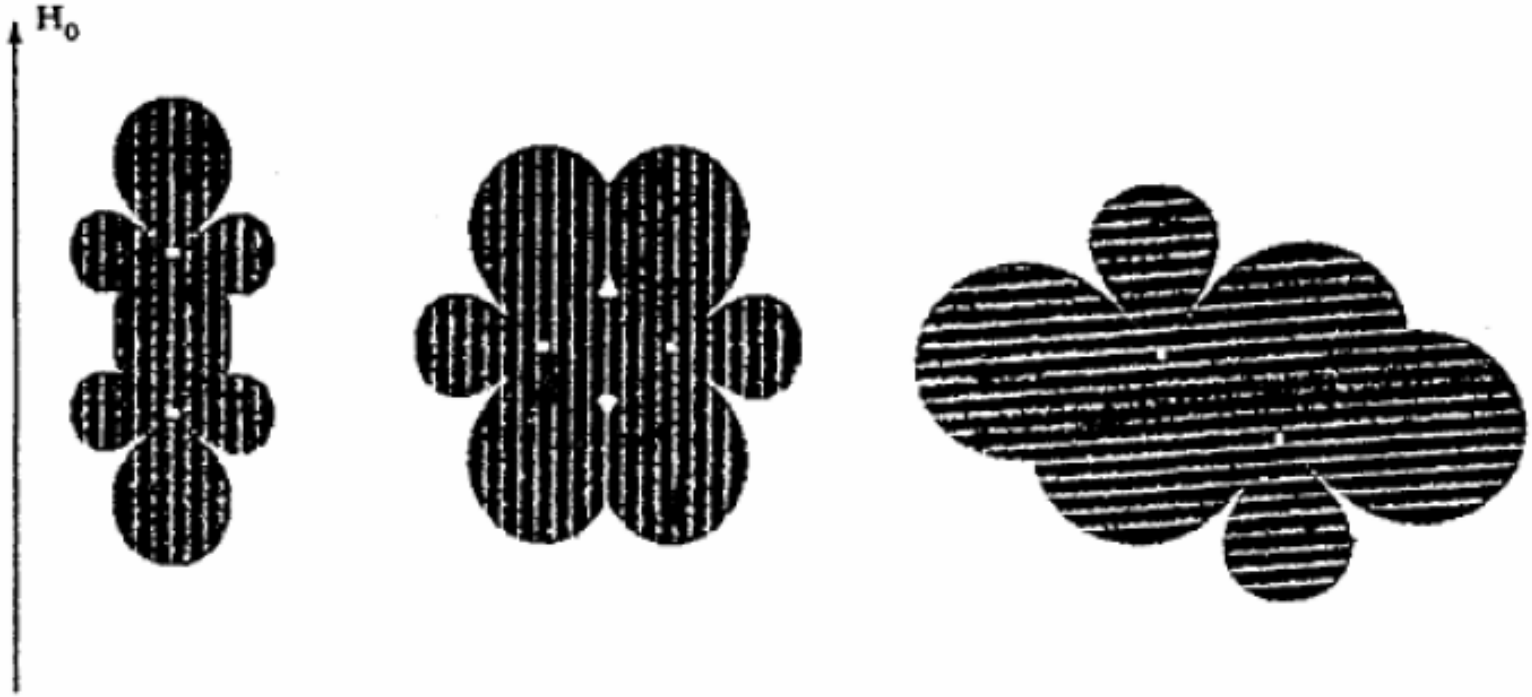
For pure dipole interaction with $a = 1$ our results give $q_3 = 0.33$ and $q_2 = 0.63$. Fitting of the experimental data [Atsarkin et al. 2000] in the region, where the samples were considered as two-dimensional, gives $q_2 = q_2^{exp} \approx 0.05$ with significant distinctions from both $q_2 = 0$, and $q_2 = 0.63$. Additional studies are necessary to clarify the nature of this deviation from pure dipole evolution.

4. Saturation on the wing of a dipole-broadened EPR line and cluster expansions.

One of bright demonstration of peculiarities of the spin dynamics in disordered media is realized in the shape of the hole burned on the wing of the EPR line. The EPR spectrum in dipole broadened $3d$ solids has Lorentz wing, but the experiment [Atsarkin et al. 1986] revealed that wing of the hole falls down exponentially contrary to the expectation, that dipole broadened line should be homogeneous. To solve this contradiction new method of cluster expansions [Dzheparov, Khenner, Kaganov 1993,1997] was constructed, which gives an alternative to both concentration expansion, discussed in p.3, and spin pockets conception [Porter 1953], used by Atsarkin et al. for interpretation of the data.



Forbidden volume of space clusters.
a) 2-cluster, b) 3-cluster; • denotes the position of the spin



Forbidden volume of energy 2-clusters for different orientation with respect to $\mathbf{H}_0$. The figure shows sections cut by the plane in which the spins forming the cluster lie.
□ - position of the spin.

If interaction inside a pare of spins exceeds interactions with any other spin, then the spectrum of the pare is similar to discrete one, broadened by small interaction with surrounding spins. The pare forms two-spin cluster (2-cluster). Analogically we can define 3- and other many-spin clusters. It is sufficient for many tasks to divide all spins in tree groups: 2- and 3-clusters and all others "mass" spins. Numerical analysis [Dzheparov, Khenner 1993] shows, that 2- and 3-clusters contains 51(1)% and 11(1)% of all spins correspondingly, but 2-clusters define all Lorentz wing of the EPR line. Mass spins (similar to nuclear spins in a crystal) have finite heat capacity, which is defined by interaction at average distance. They produce fluctuating fields, which gave main broadening of the clusters spectra. Transitions between states of the cluster take place due to interactions with other clusters and with mass spins, and they are slow.

As a result saturation at the EPR line wing induce transitions between states of the 2-cluster, and line shape of the hole is defined by interaction of the cluster with mass spins. If this interaction is estimated within the AWK model, then any mass configuration produce exponential wings of the hole

$$g(\Delta) \propto \exp(-\Delta/\mu),$$

where Δ is detuning of the saturating field from the cluster transition frequency, and μ is defined by magnitude of the fields produced by other spins on the cluster, and by the rate of their fluctuations. After configurational averaging the wings became

$$\langle g(\Delta) \rangle_c \propto \Delta^{-4},$$

Averaged hole shape describe the transitions for small magnitude ω_1 of the saturating field only.

In general case of exponential hole line wing the observable area of the hole σ should be averaged, and for $t_p\omega_1^2/\mu \gg 1$

$$\sigma \propto \ln\left(t_p\omega_1^2/\mu\right).$$

where t_p is the duration of the saturating pulse. Logarithm is slow function, therefore

$$\langle\sigma\rangle_c \propto \ln\left(t_p\omega_1^2/\langle\mu\rangle_c\right),$$

that was observed by Atsarkin et al. and was interpreted as exponential wing of Porter's pockets. Described theory produce microscopic picture of the phenomenon and indicate, that Porter's pockets have limited relation to the problem, because they are homogeneous by definitions, i.e.

$$g(\Delta) = \langle g(\Delta)\rangle_c,$$

while in the more microscopical theory this relation isn't fulfilled.

Conclusions

Four problems of the spin dynamics in disordered solids were discussed:
1) delocalization of nuclear polarization in subsystem of impurity nuclei (it is exemplified in model nuclear spin system ^{8}Li-^{6}Li in the LiF single crystal);
2) nuclear relaxation via paramagnetic impurities in crystals of arbitrary space dimension d;
3) free induction decay and EPR line form function at $d \leq 3$; and
4) form function of the hole, burned on the wing of the dipolar EPR line.

Occupation number representation was effective tool in all these problems at least for direct calculation of short time asymptotics basing on concentration expansions.

Special efforts are necessary for transformation of these expansions into results, physically adopted for all times. Important information for such activity was obtained by numerical simulation. New mean field theory gives important insight for similar transformations. Cluster expansions can be useful for better understanding of many problems.

New studies are necessary in order to improve the theoretical and experimental tools for future investigations.