INSTITUTE OF THEORETICAL AND EXPERIMENTAL PHYSICS

ITEP-28-94

A. D. Gul'ko, F. S. Dzheparov, S. V. Stepanov, S. S. Trostin

FUNDAMENTAL PROBLEMS IN SPIN DYNAMICS, DISORDERED SYSTEMS AND β-NMR

MOSCOW 1994

UDK 539.143.43 M-16

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A.D.Gul'ko, F.S.Dzheparov, S.V.Stepanov, S.S.Trostin - M., 1994 - 8p.

Ref. - 22.

1. β-NMR is the magnetic resonance and/or (longitudinal) relaxation of polarized β-active nuclei. Conventional NMR and β-NMR differs in the way of production and detection of nuclear polarization. In β-NMR polarized β-active nuclei (β-nuclei) are created *in situ* by (n,γ)-reaction ($^7Li(\vec{n},\gamma)^8\vec{Li}$ or $^{19}F(\vec{n},\gamma)^{20}\vec{F}$, for example) with polarized or cold neutrons ($\vec{n}$). Polarization of this probe nuclei is detected via their angular β-irradiation distribution $W(\vartheta) = 1+\alpha\cdot p\cdot\cos\vartheta$, where $\vec{p}$ is β-nucleus polarization ($p \approx 1$, that is around six orders greater then thermal polarization at room temperature), ϑ is the angle between β-emission and $\vec{p}$ and, $\alpha \approx 0.05$ is a nuclear constant. Just after $(\vec{n},\gamma)$-reaction the spin density matrix of β-nucleus with spin I is

$$\rho_0 = \frac{1}{\mathrm{Tr}\,I}\cdot\left(1+\frac{3p_0}{I(I+1)}\,I_z\right), \quad p_0 = \mathrm{Tr}\,I_z\rho_0 . \qquad (1)$$

Therefore the studies of $W(\vartheta)$ versus time t, external static $\mathcal{H}_0$ and alternating $\mathcal{H}_1 \perp \mathcal{H}_0$ magnetic fields, temperature T, pressure etc. present an important information about microscopic processes and structure of the substance [1,2].

The method was suggested by F.L.Shapiro [3] just after the discovery of a parity violation. First experiments were carried out in [4,5]. This report contains a review of theoretical and experimental studies of some fundamental problems on spin dynamics related with β-NMR. They were done using ^{8}Li β-nuclei in LiF crystals.

2. The problem of phase relaxation or resonance form-function is one of the oldest in NMR. The famous Anderson-Weiss-Kubo model considers the local field evolution as normal stochastic process. Phase relaxation in this model is described by the first term of cumulant expansion for free induction decay $g(t) = \langle I_+(t)I_-\rangle_0/\langle I_+I_-\rangle_0$ in powers of the local field $\omega_1(t)$:

$$g(t) = \int_{-\infty}^{+\infty} d\omega\cdot e^{-i\omega t}g(\omega) = \langle T\ \exp(i\int_0^t d\tau(\omega_1(\tau))\rangle \approx$$

$$\approx \exp[-\int_0^t d\tau(t-\tau)K(\tau)],$$

$$K(\tau) = \langle\omega_1(\tau)\omega_1\rangle_0\ ,\ \langle\ldots\rangle_0 = \mathrm{Tr}(\ldots)/\mathrm{Tr}1. \tag{2}$$

This model gave an explanation for resonance line narrowing by motion. Nevertheless it was considered so far as no more then qualitative in the general problem of form function of impuritive nuclei owing to difficulties of calculation of correlation function

$$K(t) = \sum_A K_A(t),\ \ K_A(t) = \sum_{i,j} d_i^A G_{ij}^A(t) d_j^A\ ,$$

$$G_{ij}^A(t) = \langle A_i^z(t)A_j^z\rangle_0\ . \tag{3}$$

Here d_i^A is the usual dipole coefficient of the interaction between β-nucleus, placed in the origin, and z-component A_i^z of the host spin, placed at r_i. Basing on general principles of statistical mechanics, we obtained [6] .

$$K_A(t) = \tilde{K}_A(t_{eff}) =$$

$$= M_{2IA}\left[(1-\gamma_A)\cdot\exp(-\frac{\alpha_A t_{eff}^A}{\tau_{cA}}) + \frac{\gamma_A}{(1+\beta_A t_{eff}^A/\tau_{cA})^{3/2}}\right], \tag{4}$$

$$t^A_{eff} = \int_0^t (t-\tau) g_{cA}(\tau) \frac{d\tau}{T_{2A}}, \qquad T_{2A} = \int_0^\infty g_{cA}(\tau) d\tau .$$

Parameters M_{2IA}, α_A, β_A, γ_A and τ_{cA} were microscopically determined. Two-spin correlator $g_{cA}(t) \sim \langle A^+_i(t) A^-_j(t) A^+_j A^-_i \rangle_0$ was chosen as $\exp(-M_{2A}t^2)$, $\mathrm{ch}^{-2}\sqrt{M_{2A}}t$ or $(1+\frac{2}{3}\cdot M_{2A}t^2)^{-3/2}$ (M_{2A} is one-spin second moment of the host nuclei). This choice had very small influence on $g(\omega)$ [6]. An agreement between experimental data [6] obtained for the first time and *ab initio* calculations of $g(\omega)$, was found within the fifth orders of variation of $g(\omega)$. Thus, Anderson-Weiss-Kubo hypothesis combined with the theory of irreversible processes leads to a good and simple description of the phase relaxation of impurity nuclei.

3. ^{8}Li-^{6}Li spin system is an excellent model for studies of many fundamental processes of nonequilibrium quantum statistics, because flip-flop cross-relaxation among ^{8}Li and ^{6}Li nuclei is the dominant depolarization processes in LiF in a wide range of magnetic fields $\mathcal{H}_0$ and temperatures T. The influence of static random distribution of isotopic impurity of ^{6}Li nuclei, having small concentration $c \ll 1$, on the cross-relaxation is the question of special interest. This system was discovered in [7,8] and its first theoretical treatment was carried out in [9]. The most important and general among related problems is delocalization of polarization in ^{8}Li-^{6}Li system. This process consists in transfer of nuclear polarization from initially polarized ^{8}Li to the nearest nonpolarized ^{6}Li nuclei including subsequent polarization transport among ^{6}Li and back to ^{8}Li. From theoretical point of view the problem has two independent parts. The first one [10], is the microscopical derivation of the master equation :

$$\partial p_i/\partial t = -\sum_j (\nu_{ji}p_i - \nu_{ij}p_j)\ , \quad p_i = \delta_{i0}\ . \tag{5}$$

Here $p_i = \langle I_i^z \rangle_0$ is the polarization of i-th nucleus (i=0 corresponds to ^{8}Li, and i≠0 to ^{6}Li), and $\nu_{ij} \approx \nu_0 r_0^6/r_{ij}^6$ is the rate of polarization transfer (r_0 is the distance between nearest Li nuclei). The second part is the calculation of the propagator $P_{xy}(t)$, having the sense of probability to find polarization at $\vec{x}$, if only the site $\vec{y}$ was initially polarized. The propagator is averaged over a random distribution of impuritive nuclei. To realize the macroscopical description of this system in terms of $P_{xy}(t)$, eq.5 is considered as microscopical law. So in this theory the way from microscopical equations of motions to master equations for observables is travelled twice, contrary to the usual statistical dynamics.

The theory [10,11] allows to calculate $P_{00}(t)$ for small and intermediate times $\beta t \le 1$, $\beta \sim c^2\nu_0$, but great mathematical problems hold in studies of long-time asymptotics [10-13]. Nevertheless the theory [10] predicts

$$P_{00}(t) \approx Q(t) + (1-Q(t))\frac{\xi}{(\mu\beta(t+\tau))^{3/2}}\left[1+\frac{\varphi}{(\mu\beta(t+\tau))^{1/2}}\right]\ , \tag{6}$$

$$Q(t) = \langle \exp(-\sum_j \nu_{j0}t)\rangle = \exp(-\sqrt{\beta t})\ ,$$

with ab initio calculated parameters β, μ, τ, ξ and φ. Brakets $\langle \ldots \rangle$ denote the configuration average over random distribution of ^{6}Li. This prediction was partially checked experimentally in mathematically similar problem of delocalization of electron excitation in optics [14] for $\beta t \le 100$, and in ^{8}Li-^{6}Li system for $\beta t \le 15$ [15,16]. These experiments are in agreement with eq.(6).

4. Another interesting process takes place in ^{8}Li-^{6}Li system, if it is irradiated by external alternating field with the magni-

tude ω_1 and frequency $\omega = \omega_I + \omega_S \approx 2\omega_I$ (double spin resonance), where ω_I (ω_S) is Larmor frequency of ^{8}Li (^{6}Li). The process is described by the following equations [15,17]

$$\partial p_i/\partial t = -\sum_j (\nu_{ji}p_i - \nu_{ij}p_j) - \sum_j (\mu_{ji}p_i + \mu_{ij}p_j), \quad p_i = \delta_{i0} \ . \quad (7)$$

where, neglecting the angular dependence, $\gamma \sim \mu_{ij}/\nu_{ij} \sim (\omega_1/\omega_I)^2 \ll 1$. In rather wide range, where $P_{00}(t) > 0.15 \cdot P_{00}(0)$ we obtained $P_{00}(t) = \exp(-\sqrt{\beta_e t}/2)$. It is very interesting that the effective rate of this process $\beta_e = \beta \cdot (1 + 27/4\sqrt{\gamma})^2$ has nonanalytical dependence on the relative intensity γ of spin flip-flip process. The physical meaning of this enhancement is that two-spin resonance violates the conservation law $\sum p_i = 1$ of the intense cross-relaxation flip-flop process, and produces total depolarization in closely spaced ^{8}Li-^{6}Li pairs.

5. The influence of the spatial motion of the Li ions on delocalization of polarization in the ^{8}Li-^{6}Li system became significant at temperatures T>500K [15,18], when the spatial diffusion of Li began to overtake the spin-spin delocalization of polarization. In this case the relaxation consists in polarization transfer to the nearest ^{6}Li spins with the following escape away of these nuclei. In the principal order in c we obtain [15,18]

$$\langle p_0(t) \rangle = \exp(-M(t)), \quad M(t) = c \cdot \sum_r [1 - b_0^{(1)}(r,t)], \qquad (8)$$

where $b_0^{(1)}(r,t)$ is the polarization of the ^{8}Li nucleus interacting with only one ^{6}Li, which at the moment t is separated by $\vec{r}$ from ^{8}Li and if preceding translation motions of both spins are taken into account. If T increase M(t) varies from $M(t) = \sqrt{\beta t}/2$ to $M(t) = c\nu_0 t$, when time τ_h for hopping transport of nucleus at mean distance became of order of $1/\beta$. The method gives a possibility to measure ion motions with the hopping time $\tau_h \sim 1$ s [15, 18].

6. Eqs.(2-8) are rather strict theoretical predictions. They were partially checked in β-NMR experiments in our works [6, 15-18] and in optics by time-resolved narrow band spectroscopy [14]. There were no contradictions in investigated ranges of parameters. Nevertheless new, more precise explorations of the long-time asymptotics and measurements of spin-diffusion parameters in disordered media will be of great importance for general and theoretical physics. It is very interesting to know as well could Anderson-Weiss-Kubo hypotheses combined with proper calculation of $G_{ij}(t)$ give a quantitative expression for correlators $\langle I_i^+(t) I_j^\pm(t) I_j^\mp I_i^- \rangle_0$.

7. Another interesting field of statistical mechanics of disordered systems arises from experimental studies of spectral transport [19] and spin echo and spin nutation relaxation [20] in magnetically diluted solids. New theoretical methods were developed recently [21]. They substantially broaden the possibilities of classical researches outlined in [22].

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