Scientific session of the Division of General Physics and Astronomy of the Academy of Sciences of the USSR (27 March 1991)

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A scientific session of the Division of General Physics and Astronomy of the Academy of Sciences of the USSR was held on 27 March 1991 at the P. L. Kapitza Institute of Physics Problems of the Academy of Sciences of the USSR. The papers listed below were presented at this session.

1. Yu. G. Abov, A. D. Gul'ko, F. S. Dzheparov, and S. S. Trostin. Beta-NMR spectroscopy and investigations of random walks in disordered systems.

2. A. V. Inyushkin, A. N. Taldenkov, and V. V. Florent'ev. Heat conductivity of single crystals.

A brief summary of the papers is presented below.

Yu. G. Abov, A. D. Gul'ko, F. S. Dzheparov, and S. S. Trostin. *Beta-NMR spectroscopy and investigations of random walks in disordered systems.*

1. β-NMR spectroscopy (magnetic resonance and relaxation of polarized β-active nuclei (β-nuclei)) appeared after the discovery of nonconservation of parity in weak interactions.[1] If it is based on the fact that the probability of a β-particle emission at an angle ϑ to polarization p_0 of β-nuclei obeys the law $w(\vartheta) \sim 1 + ap_0\cos\vartheta$, where a is a nuclear constant. Therefore, creating β-nuclei in a substance and investigating the dependence of their emission distribution on time, external constant magnetic field and variable magnetic fields, temperature and pressure, we can study the processes determined by hyperfine and dipole interactions.

Such experiments were first used for studying spins and dipole moments of β-nuclei in Refs. 2 and 3. Later the method was mainly applied in investigations of condensed media, since β-NMR possesses considerable advantages as compared with classical methods such as NMR and EPR, and also with other nuclear methods (perturbed angular correlations and distributions of γ-radiation, Mössbauer effect) in analyzing some phenomena.

This review outlines the β-NMR investigations carried out using the reactor of the Institute of Theoretical and Experimental Physics. For detailed information see Refs. 4–6. Reviews of work carried out abroad are available in Refs. 7 and 8.

β-nuclei are obtained either in (n, γ)-reactions involving thermal polarized neutrons from a nuclear reactor or in nuclear reactions involving accelerators. In both cases polarization of β-nuclei at the moment of their formation is independent of temperature and is close to maximum. The spin matrix of the β-nuclei density has the following form immediately after the (n, γ)-reaction:

$$\rho_0 = \frac{1}{\mathrm{Sp}1}\left[1 + \frac{3p_0}{I(I+1)} I_z\right], \quad p_0 = \mathrm{Sp}I_z\rho_0 \sim 1. \tag{1}$$

Experiments with β-nuclei are divided into two classes: relaxation and resonance.

2. Let us consider a plan of a relaxation experiment taking β-nuclei depolarization of ^{8}Li($T_{1/2} = 0.84$ s, $I = 2$, $g = 0.8267$) in LiF as an example.[4,9] A crystal is placed in a constant field $\vec{\mathscr{H}}_0 // \vec{p}_0 // 0z$. When a neutron is captured by a ^{7}Li nucleus, a ^{8}Li nucleus is formed in an excited state. Passing to the ground state, it emits one or two γ-quanta and acquires recoil energy of about 300 eV, which is sufficient to form near it several pairs of radiation defects of a vacancy-interstice type. Measuring the polarization at times $t \sim T_{1/2}$ yields that

$$p_0(t) = p_0(0)\exp(-t/T_1(\mathscr{H}_0, T)), \tag{2}$$

where T is the temperature of the sample, with the preexponential term also depending on $\mathscr{H}_0$ and T, i.e. it is a remanent polarization for the processes occurring during the times $t \ll T_1$. The most important processes are depolarization under the effect of quadrupole electrical interaction with the defects mentioned above and cross relaxation with the nuclei of the stable rare isotope ^{6}Li. Investigation of the relation p_0 $(0, \mathscr{H}_0, T)$ yields information on the constants of hyperfine interactions and annealing of defects. The conclusion that cross relaxation ^{8}Li-^{6}Li is nonexponential was also drawn on the basis of this relation.[9] If in an (n, γ)-reaction internal conversion electrons are emitted, then a paramagnetic electron shell arises near β-nuclei or on them, which also contributes to a fast depolarization.[4]

3. Resonance experiments are usually conducted in a sufficiently strong field $\mathscr{H}_0$ so that the processes of fast relaxation can be neglected. Here the information on hyperfine and dipole-dipole interactions is obtained from the dependence of the polarization of the β-nuclei on the parameters of external (constant and variable) fields and on the temperature.

Among such investigations we note the detailed measurement of the shape function of the NMR line of ^{8}Li nuclei in LiF over the record-setting broad range of its variation by five orders,[10] and also the study in this substance of radiation defects,[11] multispin and multiquantum processes,[12–14] and the manifestation of dislocations in the resonance at a double Larmor frequency.[15]

4. Cross relaxation of ^{8}Li-^{6}Li is interesting because it is a unique example of the process of delocalization of polarization in a spatially-disordered spin system, which can be experimentally investigated in detail by a direct measurement of the polarization of the nucleus which initiated this process (i.e. in the initial state only the β-nucleus ^{8}Li was polarized, its polarization in course of time mixes between ^{8}Li and the nearest ^{8}Li nuclei, and the information about this is obtained from the kinetics of depolarization of the β-nucleus). The process was discovered for the first time in Ref. 9 (see also Ref. 4) and then in Ref. 16. It is the main relaxation channel for the ^{8}Li β-nuclei in LiF over a wide range of temperatures (including room temperature) and magnetic fields $\mathscr{H}_0$. This, in particular, is determined by a coincidence of g-factors of ^{8}Li and ^{6}Li nuclei with an accuracy of 0.6%, owing to which the field $\mathscr{H}_0 = 150$–200 G, which practically suppresses cross relaxation for the remaining spins, almost does

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not weaken flip-flop transitions between ^{8}Li and ^{6}Li. The basic results of investigations of polarization transfer in the spatially-disordered spin system ^{8}Li-^{6}Li are given in Ref. 5 (experiment) and Refs. 6, 7 (theory). Below we present a brief summary of three types of processes of this class.

4.1. Delocalization of polarization is described by the kinetic equation

$$\dot{p}_{i0} = -\sum_j (\nu_{ji}p_{i0} - \nu_{ij}p_{j0}), \quad p_{i0}(t=0) = \delta_{i0}, \tag{3}$$

where $p_{i0}(t)$ is the polarization of the ith spin from the ^{8}Li-^{6}Li system ($i=0$ corresponds to ^{8}Li and $i \neq 0$, to ^{6}Li) provided that only a ^{8}Li spin was polarized at first, and ν_{ji} is the transfer rate of polarization from the ith spin to the jth spin. With a sufficient accuracy it can be assumed that

$$\nu_{ij} = \xi_i \nu_0 r_0^6 r_{ij}^{-6}(1 - 3\cos^2\vartheta_{ij})^2, \quad \xi_0 = \xi = 3, \quad \xi_{i\neq 0} = 1; \tag{4}$$

here ϑ_{ij} is the angle between the external field $\vec{\mathscr{H}}_0$ and the vector r_{ij}, which connects the spins, r_0 is the distance between the nearest spins, and ξ_i accounts for the difference between ^{8}Li ($I_0 = 2$) and ^{6}Li ($I_{k\neq 0} = 1$) spins. The field of applicability of Eqs. (3) and (4) and possible deviations from them are considered in Refs. 5, 6, and 18.

From the theoretical point of view, the problem is to obtain a solution of Eqs. (3) averaged over a random distribution of impurities in a crystal. This is one of the tasks of the problem of random walks in disordered systems, one of the most complex and interesting problems of modern theoretical physics.[6,19] This, in particular, follows from a comparison of the representation of the solutions of such problems by functional integrals[20] with similar representations for other well-known problems.

A general idea of the kinetics of delocalization of excitations in the case of a dipole transfer of type (3), (4) is given by the approximate formula

$$P_{00}(t) = \langle p_{00}(t)\rangle = Q(t) + (1 - Q(t))\frac{\xi}{[\mu\beta(t+\tau)]^{3/2}}\left[1 + \frac{\varphi}{[\mu\beta(t+\tau)]^{1/2}}\right], \tag{5}$$

where

$$Q(t) = \langle \exp(-\sum_j \nu_{ji}t)\rangle = \exp[-(\beta t)^{1/2}]; \tag{6}$$

here P_{00} is the probability to observe excitation (polarization) at a point where it began its motion, angle brackets denote averaging over impurity configurations, the Förster constant β is proportional to the transfer rate at an average distance, and numerical parameters μ, $\beta\tau$, and φ are calculated in Ref. 6. In Refs. 5 and 21 the $P_{00}(t)$ dependence was studied experimentally in the domain $P_{00}(t) > 0.1$ and it was shown that Eq. (5) and a number of its modifications are in good agreement with experiment. At present the long-time asymptotic behavior of the process is of particular interest. Preasymptotic behavior, predicted by Eq. (5), was confirmed during optical investigations of localized exciton transfer.[22]

4.2. When a variable field with the frequency $\omega = \omega_L(^8\text{Li}) + \omega_L(^6\text{Li}) \approx 2\omega_L(^8\text{Li})$, which is equal to the sum of Larmor frequencies of ^{8}Li and ^{6}Li nuclei, is superimposed on the ^{8}Li-^{6}Li system, double-spin flip-flip and flop-flop transitions are initiated, whose rate is $\sim r_{ij}^{-6}$, as well as ν_{ij}, but they do not conserve the total polarization of the system. A completely microscopic description of this process for $P_{00}(t) > 0.1$ can be obtained by using the first three terms of the expansion of P_{00} in terms of the impurity concentration $c \ll 1$ (in fact, in terms of $(\beta t)^{1/2}$), which is supported by experiment.[5,23] An important qualitative effect here consists of the fact that the dependence of the effective relaxation rate of the β-nuclei on the relative intensity of weak resonance double-spin transitions is nonanalytic. This is determined by the above-mentioned breakdown of the integral of the motion and by the disordered nature of the system.

4.3. Spatial diffusion of the ^{8}Li-^{6}Li nuclei becomes significant as the temperature increases, and, moreover, the kinetics of depolarization of the ^{8}Li nuclei of the form $P_{00} \approx \exp[-(\beta t/(\xi+1))]^{1/2})$, where $\beta \sim c^2\nu_0$, which practically coincides with (5) for $\beta t \lesssim 1$, is transformed into $P_{00} = \exp(-Wt)$ with $W \sim c\nu_0$. This transition is studied in Refs. 5 and 24. It is also well explained quantitatively within the framework of concentration expansions and can be the basis for studying rare jumps of lithium nuclei with characteristic frequencies of about 1 s^{-1}.

5. Investigations by the β-NMR method of random walks in disordered systems with dipole transfer are the verifications of quite rigid predictions of the microscopic theory. At present experiment and theory concerning the given problems are in good agreement.

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