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DYNAMIC CORRELATION OF LOCAL MAGNETIC FIELDS.CROSS-RELAXATION FORM FUNCTIONS OF ^{8}Li AND ^{6}Li NUCLEI IN LiF: Preprint ITEP 29-94/

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Cross-relaxation form functions (FFCR) $g^{-}_{xy}(\omega)$, considered herein, are the Fourier transforms of two-spin correlators $\langle I^{+}_{x}(t)I^{-}_{y}(t)I^{+}_{y}I^{-}_{x}\rangle_{0}/\langle I^{+}_{x}I^{-}_{y}I^{+}_{y}I^{-}_{x}\rangle_{0}$, where $I^{\pm}_{x}$ is a spin operator of impuritive nucleus located at the site x of the crystal lattice, $\langle\ldots\rangle_{0}=\mathrm{Tr}(\ldots)/\mathrm{Tr}1$. Functions $g^{-}_{xy}(\omega)$ are needed for the description of depolarization of impuritive ^{8}Li β-active nuclei in LiF crystals, contained several percents of ^{6}Li nuclei, at room temperatures and magnetic fields 150÷2500 G [1]. In this case depolarization of ^{8}Li is caused only by cross-relaxation (flip-flop process) with ^{6}Li nuclei, because g-factors of these nuclei are practically the same. An attempt to approximate FFCR even near their tops by a Gaussian with a variable second moment lead to a double discrepancy with theoretical values, while NMR form function $g(\omega)$ is nearly Gaussian at $g(\omega) > 0.01\cdot g(0)$. This discrepancy still held when took into account both three-particle clusters from impuritive nuclei (^{8}Li, ^{6}Li) and the static correlation of local fields [2]. The last one appears in its pure form when there are no flip-flop transitions of the host spins (^{7}Li, ^{19}F). The static correlation results only in a slight narrowing of the FFCR, while the observable narrowing is essentially larger. It implies the existence of

the dynamic correlation of the local fields [3], which is related to the influence of flip-flop processes of host spins. These processes influence also on another two-spin correlator $\langle I_x^+(t)I_y^+(t)I_y^-I_x^-\rangle_0$, which represens two-spin resonance [1,3] with the corresponding form function $g_{xy}^+(\omega)$.

Anderson-Weiss-Kubo (AWK) theory together with proper calculation of local field correlator allows to get an agreement between calculated and experimentally measured NMR form function $g(\omega)$ of impurity nuclei within the fifth orders of magnitude under its variation [4]. In this work we develop AWK-theory further for calculation of $g_{0r}^{\pm}(\omega)$, which depend on the vector r joining the cross-relaxation spins. If the motion of the local fields is approximated by a random normal process, $g_{0r}^{\pm}(\omega)$ could be presented in the form [1,3]

$$g_{0r}^{\pm}(\omega) = \int_{-\infty}^{+\infty}\frac{dt}{2\pi}\cdot e^{i\omega t}\langle T\exp(i\int_0^t d\tau(\hat{\omega}_{loc}(\tau,0)\pm\hat{\omega}_{loc}(\tau,r))\rangle_0 \approx \qquad (1)$$

$$\approx \int_{-\infty}^{+\infty}\frac{dt}{2\pi}\cdot e^{i\omega t}\cdot\exp[-2\int_0^t d\tau(t-\tau)(K_{00}(\tau)\pm K_{0r}(\tau))] .$$

$K_{0r}(\tau) = \langle\hat{\omega}_{loc}(\tau,r)\cdot\hat{\omega}_{loc}(0,0)\rangle_0$ is the correlator of the local fields created by the z-components of the host spins at a given pair of impuritive nuclei. In calculation of $K(\tau)$, the effect of impuritive spins on the host spins is ignored. Assuming that impurity nuclei is located at r, the local field operator can be written in frequency units as follows:

$$\hat{\omega}_{loc}(r) = \sum_{A=F,L}\hat{\omega}_{loc}^{(A)}(r), \qquad \hat{\omega}_{loc}^{(A)}(r) = \sum_{x\in A} d_{xr}^{(A)}A_x^z,$$

$$d_{xr}^{(A)} = \frac{g_I g_A \beta_n^2(1-3\cos^2\theta_{x-r})}{h|x-r|^3} . \qquad (2)$$

The coordinate summation is carried out over all sites in sublattice A except x=r. A takes on the values F and L. The spins of ^{19}F and ^{7}Li (with z-components F_x^z and L_x^z) are F=1/2 and L=3/2, respectively. $d_{xr}^{(A)}$ is the usual coefficient of the dipole-dipole interaction. Substituting eq.(2) into (1), we obtain

$$K_{0r}(t) = \sum_{A=F,L} K_{0r}^{(A)}(t),$$

$$K_{0r}^{(A)}(t) = \langle \hat{\omega}_{loc}^{(A)}(t,r)\cdot\hat{\omega}_{loc}^{(A)}(r)\rangle_0 =$$

$$= \frac{A(A+1)}{3} \sum_{x,y\in A} d_{0x}^{(A)} G_{xy}^{(A)}(t) d_{yr}^{(A)} . \qquad (3)$$

Here we have introduced the spin-diffusion propagator $G_{xy}^{(A)}(t) = \langle A_x^z(t)A_y^z\rangle_0 / \langle (A_x^z)^2\rangle_0$, which satisfies the following equations [4]

$$\partial G_{xy}^{(A)}/\partial t_{eff}^{(A)} = -\sum_{z\in A} \mathcal{D}_{xz}^{(A)} G_{zy}^{(A)}, \qquad \mathcal{D}_{xy}^{(A)} = -\nu_{xy}^{(A)} + \delta_{xy}\sum_{z\in A}\nu_{zx}^{(A)},$$

$$G_{xy}^{(A)}(t=0) = \delta_{xy}, \qquad (4)$$

where $\nu_{0r}^{(A)} = \frac{\pi A(A+1)}{\hbar}\cdot(d_{0r}^{(A)})^2\cdot T_{2A}$ is the polarization transfer probability, $T_{2A} = \int_0 g_{cA}(\tau)d\tau$ and $t_{eff}^{(A)} = \int_0^t (t-\tau)g_{cA}(\tau)\frac{d\tau}{T_{2A}}$. In was shown in [4] that the choice of $g_{cA}(\tau)$ as $\exp(-M_{2A}\tau^2)$, $ch^{-2}\sqrt{M_{2A}}\tau$ or $(1+\frac{2}{3}\cdot M_{2A}\tau^2)^{-3/2}$ (M_{2A} is one-spin second moment of the host nuclei) has very small influence on $g(\omega)$. Eqs.3,4 allow to obtain the final representation for $K_{0r}^{(A)}(t)$, which has to be used in numerical calculations:

$$K_{0r}^{(A)}(t) = \frac{A(A+1)}{3}\int_{B_1} \frac{\Omega\cdot d^3p}{(2\pi)^3}\,[d^{(A)}(p)]^2\cdot\exp[-ipr-\mathcal{D}^{(A)}(p)t_{eff}],$$

$$\mathcal{D}^{(A)}(p) = \sum_{r\in A} e^{ipr}\mathcal{D}_{0r}^{(A)}, \qquad d^{(A)}(p) = \sum_{r\in A} e^{ipr} d_{0r}^{(A)}. \qquad (5)$$

Here B_1 is the Brilluen zone, Ω stands for the volume of elementary

cell. The expression for $K_{00}(t)$ used in [4] was obtained as an approximation of eq.5.

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