Changes in the electronic spectrum of $YBa_2Cu_3O_{6.9}$ under radiative disordering: the ^{89}Y and ^{63}Cu NMR data

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We measured the components of the tensor of the ^{89}Y and ^{63}Cu NMR shifts and the spin-lattice relaxation rates of the ^{89}Y nuclei in the $YBa_2Cu_3O_{6.9}$ compound radiatively disordered by fast-neutron fluences $\Phi=(0–5)\times10^{19}$ cm^{-2}. This enabled us to estimate the variation of the spin contribution $\chi_s(q=0)$ to the magnetic susceptibility in the course of buildup of structural disorder. According to the data gathered, the density of electronic states near the Fermi energy decreases markedly in the process and terminates for nonsuperconducting samples with the formation of a Coulomb gap at the Fermi level. The ^{89}Y NMR data indicate the appearance, at low temperatures, of antiferromagnetic ordering among localized magnetic moments that appear in CuO_2 planes upon irradiation. In this paper we discuss the distinguishing features of spin-lattice relaxation in the ^{89}Y nuclei in the metallic-conduction region, which attest to the presence of an Anderson metal–insulator transition in the system considered and support the theoretical study.

1. INTRODUCTION

In experimental and theoretical work dealing with HTSC considerable efforts have been made to establish the distinguishing features of copper-based superconducting oxides. Special attention has been paid to an analysis of the effect of strong antiferromagnetic ($Q_{AF}\simeq\{\pi/a,\pi/a\}$) fluctuations of the spins of copper atoms in the perovskite CuO_2 layer on the energy spectrum of "current" oxygen states.[1] In the last two years NMR studies of $YBa_2Cu_3O_{7-\delta}$ compounds ($\delta=0.00;0.37$) (see Refs. 2–5) have provided ample proof of the existence of strong correlations between these two types of electron excitations. Since HTSC in cuprites is realized near the transition from the metallic to the semiconducting state, the behavior of spin susceptibility when structural disorder sets in is of particular interest. Apparently, the "purest" method of studying the effect of disorder on the physical properties of high-temperature superconductors is the radiative disordering by fast neutrons at low temperatures.[6] In this case the chemical composition of the compound remains practically unchanged, $\Delta\delta<0.1$. As for the properties of the initial $YBa_2Cu_3O_7$ compound, the buildup of the radiatively created structural disorder leads not only to a rapid drop of T_c but also to an increase of the abrupt variations in the kinetic properties, which points to the onset of localization effects in the energy spectrum of the carriers.[7,8] The behavior of the resistivity at fairly low degrees of the introduced disorder points to the existence of a continuous metal–semiconductor transition. At medium degrees of the disorder created by neutron radiation, hopping conduction has been found to coexist with superconductivity, accompanied by an anomalous increase in the absolute value of resistivity with the fluence. A Curie-like contribution $C/T+\vartheta$, attesting to formation of localized magnetic moments, appears in the temperature dependence of the magnetic susceptibility under radiative disordering. The concentration of the moments increases in proportion to the fast-neutron fluence Φ. When fluences corresponding to the semiconducting state are reached, ϑ becomes positive, which suggests antiferromagnetic interaction of the moments and the possibility of their becoming ordered. The temperature-independent contribution to the magnetic susceptibility χ_0 also increases as we go over to disordered samples with lower values of T_c.

It might be interesting in this connection to study by locally sensitive methods the variations of the electronic states in the conduction band in the metal-semiconductor transition caused by radiative disordering. As is known (see Refs. 2–5), the values of NMR shifts on ^{89}Y and ^{63}Cu nuclei are related to a homogeneous contribution to the spin susceptibility $\chi_s(q=0)$. At the same time the behavior of the spin-lattice relaxation rate for the nuclei of copper atoms in perovskite CuO_2 planes, $T_1^{-1}(^{63}Cu)\equiv{}^{63}R$, is determined in the main by the low-frequency part of the spectrum of the antiferromagnetic spin fluctuations near $q\simeq Q_{AF}=\{\pi/a,\pi/a\}$. Of considerable interest are studies of the features of the spin-lattice relaxation rate in yttrium, $T_1^{-1}(^{89}Y)\equiv{}^{89}R$. In view of the inversion symmetry in the positions of the yttrium atoms in relation to the nearest-neighbor copper atoms, the fluctuations of the hyperfine fields generated by the spins of the copper atoms are offset at the yttrium nucleus. As a result $^{89}R\sim T\chi_s(q=0)\tau_c$, where for the metallic state τ_c is the time that an electron with the Fermi energy stays near a resonant nucleus. For a free electron gas, $\tau_c\simeq a/v_F$. When localization effects manifest themselves in the conduction band, electrons with the Fermi energy stay ever longer near certain positions, which leads to a change in the strength, at NMR frequencies, of fluctuations of the hyperfine fields generated at the point where the test nucleus resides. This enables using the NMR method to study localization effects.

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This paper presents the results of measuring the temperature dependences of the NMR ^{89}Y and ^{63}Cu line shifts and the spin-lattice relaxation rate of ^{89}Y nuclei in order to extract information about the behavior of the spin contribution to the magnetic susceptibility in the $YBa_2Cu_3O_{6.9}$ compound radiatively disordered by fast neutrons with fluences up to $\Phi=5\times10^{19}$ cm^{-2} which lead to a semiconducting state.

2. SAMPLES AND THE EXPERIMENTAL METHOD

The measurements were conducted using ceramic $YBa_2Cu_3O_{6.9}$ samples. The transition temperature and the width ΔT_c of the transition to the superconducting state were determined from the diamagnetic response in measurements of the *ac* magnetic susceptibility. Irradiation by fast neutrons ($E>1$ MeV) was conducted at liquid-nitrogen temperatures. A detailed description of the results of neutron-diffraction and x-ray studies of these samples can be found in Ref. 9. Low-temperature irradiation had practically no effect on the oxygen content in the samples—$\Delta\delta<0.1$ even for nonsuperconducting samples—causing, basically, a redistribution of oxygen atoms in the O4 and O5 crystallographic positions in the Cu1–O plane. Superconductivity vanishes at $\Phi>1.2\times10^{19}$ cm^{-2} in the orthorhombic phase.

The NMR studies in the 2.2–300 K range were conducted using the ceramic $YBa_2Cu_3O_{6.9}$ samples oriented in a magnetic field $B=8$ T and subjected to fluences $\Phi=0$ at $T_c^{ons}=94.5$ K and $\Delta T_c=3$ K, $\Phi=5\times10^{18}$ cm^{-2} at $T_c^{ons}=70$ K and $\Delta T_c=8$ K, $\Phi=1.2\times10^{19}$ cm^{-2} at $T_c^{ons}=25$ K and $\Delta T_c=10$ K, $\Phi=2\times10^{19}$ cm^{-2} for $T_c^{ons}<4$ K, and $\Phi=5\times10^{19}$ cm^{-2}.

The nuclear quadrupole resonance (NQR) spectra in ^{63}Cu was recorded using a SXP 4–100 NMR spectrometer via phase-sensitive detection of the peak of the spin-echo signal under discrete variation of the transceiver-channel frequency.[10] The spin-lattice relaxation rate in ^{63}Cu was measured in the absence of a magnetic field at NQR frequencies using the method of a saturated spin-echo signal. The spin echo was created by a two-pulse sequence τ–t_{12}–2τ, with $\tau=2.5$ μs and $t_{12}<30$ μs.

The spin-lattice relaxation rate for ^{89}Y nuclei was measured in a magnetic field $B_0=8.1$ T by restoring the spin-echo signal through varying the repetition frequency of the sequence of rf pulses forming the echo.

The ^{89}Y NMR spectra were obtained for the normal-state region by introducing the Fourier transformation of the free induction signal. The values of the NMR line shifts, ^{89}K, were determined in relation to the position of the resonance line of YCl_3 dissolved in nitric acid, with allowance for the corrections discussed in Ref. 5. The ^{63}Cu NMR spectra of the $m=\frac{1}{2}\leftrightarrow-\frac{1}{2}$ transition were obtained for two orientations of the magnetic field with respect to the *c* axis of the crystals. We registered the peak of the spin-echo signal under discrete variations of the transceiver-channel frequency. In the course of measurements the least possible time lag between the pulses forming the echo was selected, $t_{12}\leqslant20$ μs. The components of the tensor of the Cu2-position NMR line shifts were determined from the position of the resonance lines of the $m=\frac{1}{2}\leftrightarrow-\frac{1}{2}$ transition with allowance for the measured values of NQR frequencies ν_Q (see Ref. 10). For the Cu2 positions the analysis was carried out on the assumption that the tensors of the electric-field gradients and NMR shifts are axisymmetric, and only line-shift corrections up to the second order of the perturbation theory for nuclear quadrupole interaction were taken into account:

$$\nu_{\parallel}=\nu_0(1+K_{\parallel}), \tag{1}$$

$$\nu_{\perp}=\nu_0(1+K_{\perp})+\frac{3}{16}\frac{\nu_Q^2}{\nu_0}. \tag{2}$$

Here ν_0 is the value of the NMR frequency of ^{63}Cu in a diamagnetic solution. The values of $\Delta K_{\perp}$ and $\Delta\nu_Q$ increase under disordering, which leads to an increase in the error of determining the quantities. Allowing for diamagnetic corrections in the superconducting state that are related to the vortex structure of the magnetic field in the sample leads to a shift in the resonance frequency $\nu_{\perp}$ (Cu2). At $B_0=8.1$ T the shift $\Delta\nu_{\perp}<50$ kHz lies within the error margins in determining the line's center.

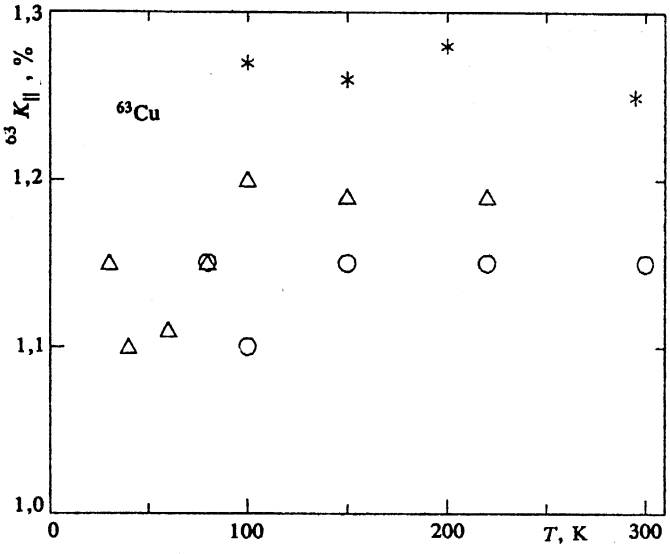

FIG. 1. Temperature dependence of the NMR ^{63}Cu line shift $K_{\parallel}$ (c$\parallel$ H_0) in the $YBa_2Cu_3O_{6.9}$ compound irradiated by fast neutrons with the following fluences: *—$\Phi=0$; ○—$\Phi=5\times10^{18}$ cm^{-2}; Δ—$\Phi=1.2\times10^{19}$ cm^{-2}.

3. EXPERIMENTAL RESULTS AND DISCUSSION

3.1. The ^{63}Cu NMR line shift

Figures 1 and 2 depict the temperature dependence of the NMR ^{63}Cu line shifts in the Cu2 positions for the cases where the *c* axis of the crystallites is oriented parallel ($^{63}K_{\parallel}$) and perpendicular ($^{63}K_{\perp}$) to the constant magnetic field. For the initial sample of $YBa_2Cu_3O_{6.9}$ ($\Phi=0$) the obtained values are close to those given in Refs. 12, 13,

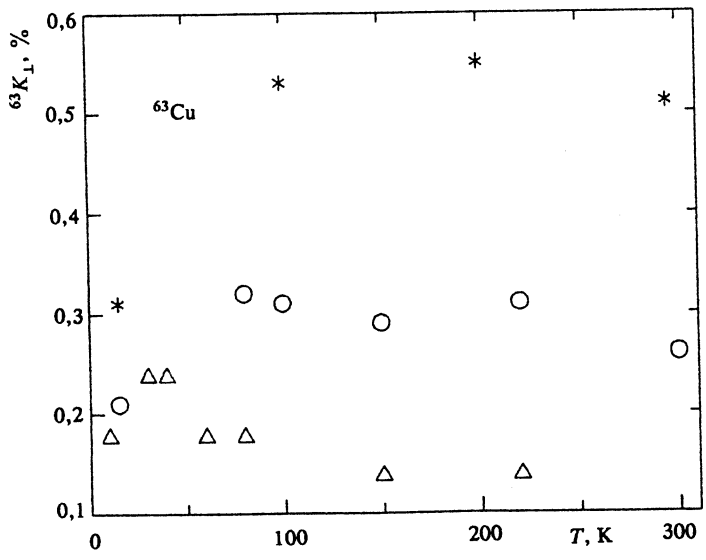

FIG. 2. Temperature dependence of the NMR ^{63}Cu line shift $K_\perp$ ($\mathbf{c}\perp H_0$) in the $YBa_2Cu_3O_{6.9}$ compound irradiated by fast neutrons with the following fluences: *—$\Phi=0$; ○—$\Phi=5\times10^{18}$ cm^{-2}; Δ—$\Phi=1.2\times10^{19}$ cm^{-2}.

and 4 and reflect the temperature-independent behavior of the NMR shift components in the normal state.

As disordering proceeds, there is an essential decrease even at low fluences in both components of the NMR shift on Cu nuclei. Moreover, in the sample irradiated with $\Phi=1.2\times10^{19}$ cm^{-2} and situated at the threshold of the transition to the region of nonsuperconducting semiconductors $^{63}K_\perp$, acquires a temperature dependence, namely, $^{63}K_\perp$ grows as the temperature drops.

The total NMR ^{63}Cu line shift consists of two main contributions, the spin contribution K_s and the contribution K^L associated with Van Vleck paramagnetism χ^{VV} of the $3d$ copper atoms:

$$^{63}K_{\parallel\,(\perp)}=K^L_{\parallel\,(\perp)}+K_{s\parallel\,(\perp)}, \tag{3}$$

$$K^L_{\alpha\alpha}=4\mu_B^2\left\langle\frac{1}{r^3_{3d}}\right\rangle\sum_n\frac{|\langle 0|\hat L_\alpha|n\rangle|^2}{E_n-E_0}=2\mu_B^2\left\langle\frac{1}{r^3_{3d}}\right\rangle\chi^{VV}_{\alpha\alpha}, \tag{4}$$

$$^{63}K_{s\parallel\,(\perp)}=\frac{1}{\mu_B}(A_{\parallel\,(\perp)}+4B)\chi_s. \tag{5}$$

The spin contribution K_s is proportional to the product of the homogeneous spin susceptibility, $\chi_s(q=0)$, which is assumed isotopic, following the ideas of Mila and Rice,[13] and to the sum of the hyperfine coupling constants $A_{\parallel\,(\perp)}$ and B. The hyperfine constants $A_{\alpha\alpha}$ and B correspond, respectively, to the direct hyperfine interaction with the ^{63}Cu nucleus and the interaction induced by the neighboring copper atoms, in the hyperfine interaction Hamiltonian suggested in Ref. 13 in order to describe NMR on Cu(2) copper atoms in CuO_2 planes:

$$\hat H=\sum_i \mathbf{I}_i\cdot A\mathbf{S}_i+\sum_{\substack{i,j\\ i\neq j}} B\mathbf{I}_i\cdot\mathbf{S}_j. \tag{6}$$

The susceptibility $\chi^{VV}_{\alpha\alpha}$ is determined by the mutual position of the energy levels of the $3d$ orbitals of the free states, d_{xy} (d_{xz} and d_{yz}), in relation to the almost full $d_{x^2-y^2}$ state near the Fermi energy.

To separate these contributions we used the results of measurements of the NMR line shift ^{63}K in the superconducting state. Several researchers[14] have shown that in the initial $YBa_2Cu_3O_7$ compound $^{63}K_\parallel$ remains practically unchanged under a transition to the superconducting state, while $^{63}K_\perp$ drops considerably. The explanation is that the spin contribution $^{63}K_{s\parallel}$ is exceptionally small in view of the assumed balance between the hyperfine constants ($A_\parallel\simeq -4B$). As the results of measurements of $^{63}K_\parallel$ (Cu2) in the superconducting state show, this situation remains valid for irradiated samples. Hence, we may conclude that the decrease in $^{63}K_\parallel$ with increasing fluence is associated with a decrease in χ^{VV}. On the basis of calculations of the position of the energy levels $3d^9$ of the copper ion in $YBa_2Cu_3O_7$, Penington, Durand, and Slichter[12] found a value of roughly 4 for the ratio $^{63}K^L_\parallel/^{63}K^L_\perp$ for the shift in the orbitals of excited states E_{xy} amounting to 2 eV (and to 2.2 eV for E_{xz} and E_{yz}) with respect to the orbitals of the ground state $E_{x^2-y^2}$.

Note that at a fluence of $\Phi=5\times10^{18}$ cm^{-2} corresponding to a fairly high value of T_c, at which the metallic nature of the sample conduction is retained, this ratio of the orbital shifts remains practically unchanged. However, for a sample with $\Phi=1.2\times10^{19}$ cm^{-2}, where hopping conductivity manifests itself at $T<100$ K, there is a sharp decrease in $^{63}K^L_\perp$, which leads to a more than twofold increase in the $^{63}K^L_\parallel/^{63}K^L_\perp$ ratio. This may indicate an increase in the energy (with respect to that of the ground state) of the E_{xy} and E_{yz} states, the virtual transitions from which contribute nothing to $^{63}K^L_\parallel$.

Let us now turn to an analysis of variations in the spin contribution in the event of radiative disordering. For the initial $YBa_2Cu_3O_{6.9}$ compound the decrease in the shift of $K_\perp$ in the superconducting state, $^{63}K_\perp$ (100 K) $-$ $^{63}K_\perp$ (15

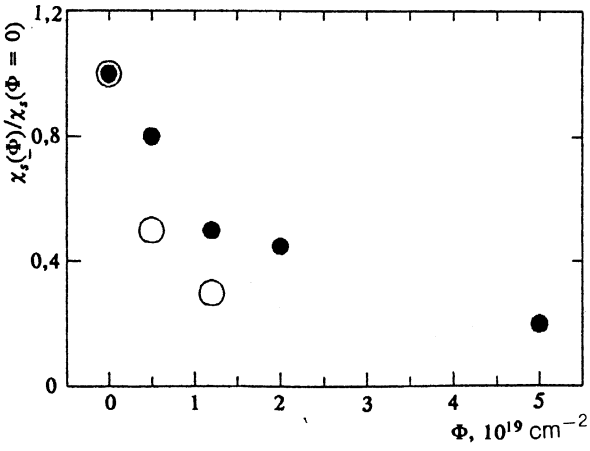

FIG. 3. Spin susceptibility $\chi_s(q=0)$ as a function of the fast-neutron fluence in $YBa_2Cu_3O_{6.9}$: ●—NMR data on ^{63}Cu ($T=300$ K), and ○—NMR data on ^{89}Y ($T=300$ K).

K)$=^{63}K_s=0.26\%$, is close to the data from the literature. Using the values of the hyperfine coupling constants $A_\perp=32$ kOe/μ_B and $B=40.3$ kOe/μ_B (Ref. 14), we arrive at the following estimate for the spin contribution to the magnetic susceptibility for the initial $YBa_2Cu_3O_{6.9}$ sample: $\chi_s/2\mu_B^2=2.3$ (eV at.Cu)$^{-1}$. As the fluence increases, the spin contribution K_s drops. This reflects the fact that the homogeneous part of the spin susceptibility in irradiated samples decreases. Figure 3 depicts the results of estimating the fractional variation of the homogeneous spin susceptibility $\chi_s(q=0)$ for different samples by using the $\Delta^{63}K_\perp$ measurements in the transition to the superconducting state. Since the main contribution to $\chi_s(q=0)$ is related to the Pauli paramagnetism of electronic states near the Fermi energy,[6] we can say that when disorder sets in in $YBa_2Cu_3O_{6.9}$, the decrease in transition temperature is accompanied by a sharp drop in the density of states at the Fermi level. It is still difficult to point to the crucial factor determining the behavior of the density of states near the Fermi energy in structural disordering of $YBa_2Cu_3O_{6.9}$. This may be the smearing of a Van Hove singularity whose presence near E_F in ordered compounds has been discussed in a number of papers. However, the temperature-independent behavior of χ in the normal-state region makes this assumption unlikely. We are probably dealing here with a correlation "pseudogap" at the Fermi level, related to the manifestation of disorder effects in a correlated electron gas.[15] On the insulator side this pseudogap is transformed into a Coulomb gap resulting from the interaction of electrons in localized states.[16]

When the fluence increases to $\Phi=2\times10^{19}$ cm^{-2} and nonsuperconducting samples are used there appears in the NMR ^{63}Cu spectrum of the $m=\frac{1}{2}\leftrightarrow-\frac{1}{2}$ transition (Fig. 4) a single line described by a set of parameters of NMR line shifts, $K_b=K_c=0.25\pm5\%$ and $K_a=1.0\pm1\%$, and of quadrupole coupling constants, $\nu_Q=20\pm1$ MHz and $\eta=0.85\pm5$, corresponding to the case of a nonaxisymmetric tensor of the gradients of the electric field on a nucleus. Such a change is also observed in NQR spectra:[10] there is a sharp drop in the strength of the lines in the $\nu=28$–32 MHz frequency range corresponding to the position of the NQR lines of the Cu2 positions of superconducting disordered $YBa_2Cu_3O_{6.9}$ samples. We may therefore assume that the observed NMR spectrum is determined by copper atoms in the Cu1 positions. Apparently, the sharp drop in strength of the lines of the Cu2 positions is caused by the formation of localized magnetic moments μ in CuO_2 planes. The dipole fields generated by a localized electron spin lead to a sharp decrease in the relaxation times of the neighboring nuclei.[17] Putting $\mu\simeq0.6\mu_B$ and using the Curie constant $C=5\cdot10$ K mol^{-1} for the given fluence, we easily conclude that the mean separation of localized moments does not exceed 2–3a.

As noted earlier in Ref. 10 regarding the sample with $\Phi=2\times10^{19}$ cm^{-2}, lowering the temperature leads to an observable deviation from the $C/(T+\vartheta)$ dependence in the behavior of magnetic susceptibility below 20 K, which suggests the emergence of ordering among localized moments. Indirect indications of this tendency to ordering are the additional growth in the width of anomalies in the NMR spectrum of Cu1 positions and a small increase in the NMR line shifts in this temperature range. At $T=5$ K (Fig. 4), $K_b=K_c=0.30\pm5\%$. For the sample with the highest fluence of $\Phi=5\times10^{19}$ cm^{-2}, the additional broadening of the anomalies in the spectrum occurs already at temperatures below 100 K. The shift of the low-frequency part of the spectrum toward lower frequencies is mainly caused by the growth in the electron density in Cu1 positions. Indeed, the NQR spectrum of copper for this fluence constitutes a broad inhomogeneously broadened line in the 18–24 MHz frequency range for the copper isotopes ^{63}Cu and ^{65}Cu. We made several attempts to observe the NMR signal of copper in a local field at low temperatures in the 90–100 MHz frequency range. At $T=2.2$ K we observed in the entire frequency range a weak spin-echo signal with a spin-spin relaxation time T_2 less than 5 μs. So rapid a relaxation of nuclear spin did not allow reliable reproduction of the spectrum in full. For this, apparently, the experiment must be carried out at a lower temperature. Below we will return to the problem of the possible ordering of localized magnetic moments in CuO_2 by considering the ^{89}Y NMR data ($I=1/2$). The absence of quadrupole effects of broadening of the yttrium NMR line makes it possible in this case to draw more definite conclusions about the presence of magnetic ordering[18] among localized moments in CuO_2 planes for a highly disordered state of the $YBa_2Cu_3O_{6.9}$ compound.

3.2. The ^{89}Y NMR line shift and spin-lattice relaxation rate in the normal state

The data on the behavior of the NMR line shift ^{89}K for $YBa_2Cu_3O_{6.9}$ samples in the normal state is shown in Fig. 5. For the initial compound our results are in good agreement with the data of Alloul, Ohno, and Mendels,[5] thus demonstrating the temperature-independent behavior of $^{89}K=-70\pm20$ ppm. As disorder sets in, a decrease in the absolute value of ^{89}K is observed (just as it is for ^{63}K) and at $\Phi=1.2\times10^{19}$ cm^{-2} ^{89}K becomes positive.

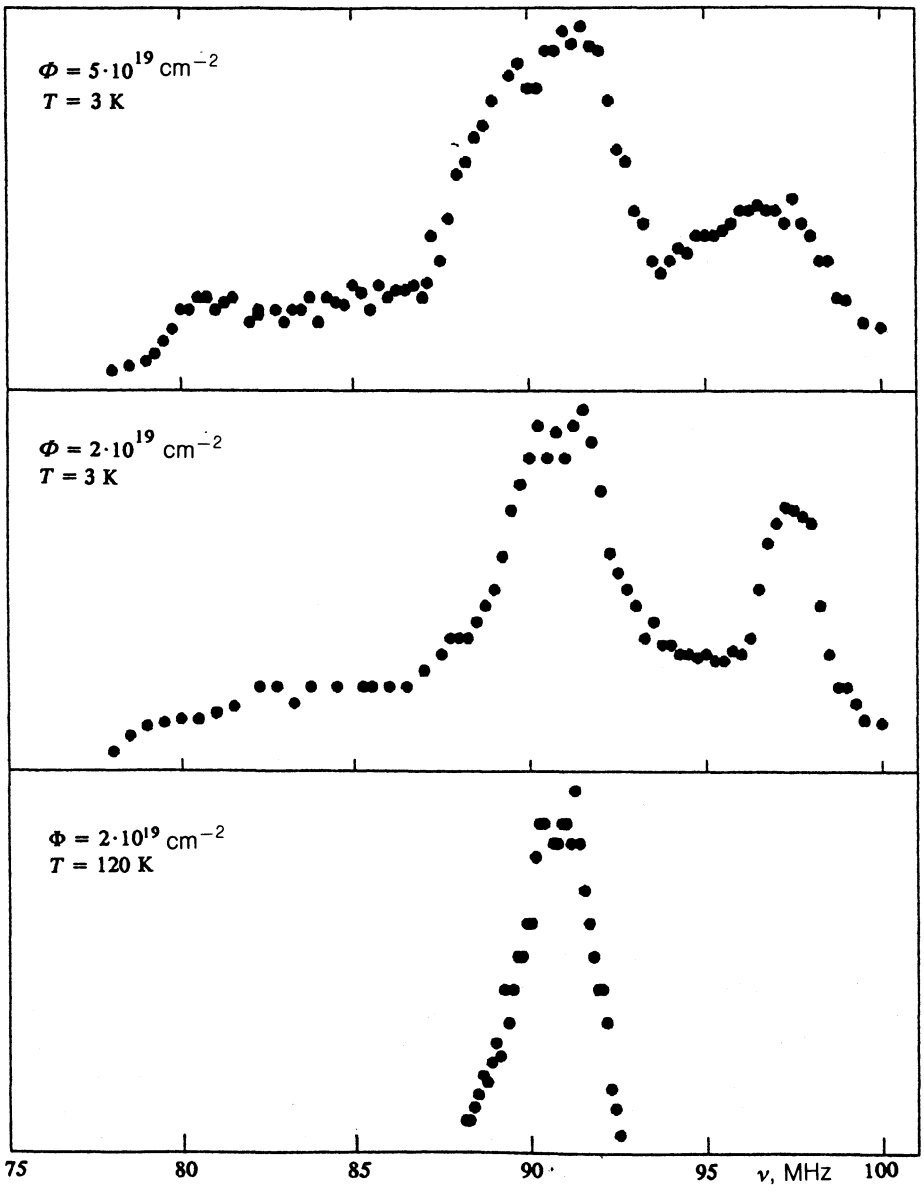

FIG. 4. NMR ^{63}Cu spectra in disoriented $YBa_2Cu_3O_{6.9}$ samples irradiated by fluences of fast neutrons corresponding to the nonsuperconducting state.

As disorder increases, the shift acquires a temperature dependence: the absolute value of the shift is seen to decrease as the temperature drops. The growth in the error of determining ^{89}K arises mainly from the increase in the inhomogeneous ^{89}Y NMR linewidth in irradiated samples. The temperature behavior of ^{89}K is in many respects similar to that of $YBa_2Cu_3O_{7-\delta}$ with close values of T_c. The reader will find a detailed discussion of the nature and behavior of the NMR ^{89}Y line shift for $YBa_2Cu_3O_{7-\delta}$ in Ref. 5. The total NMR ^{89}Y line shift can be explained by two contributions, the chemical shift $^{89}K_{\text{ch.sh}}$ of the filled electron shells (which does not depend on temperature and oxygen content) and the Knight shift $^{89}K_s$:

$$^{89}K = {}^{89}K_{\text{ch.sh}} + {}^{89}K_s. \quad (7)$$

The second term on the right-hand side is proportional to the homogeneous spin susceptibility χ_s and is negative because of the effects of exchange polarization of the filled shells by the electrons of the Cu($3d$)–O($2p\sigma$) molecular orbital, which has a nonzero spin density on the yttrium atom. As is known, the presence of such a Cu–O coupling is the starting point in discussing various models of the electronic structure of high-temperature superconductors with perovskite CuO_2 layers. In this case the behavior of ^{89}K reflects that of the spin contribution of the states of the oxygen atoms.

Studies of crystalline fields of the rare-earth ions Ho^{3+} and Er^{3+} in radiatively disordered samples of $HoBa_2Cu_3O_7$ and $ErBa_2Cu_3O_7$ (Ref. 19) have shown that the structural disorder introduced has no effect on the immediate charge environment, retaining even the scale of hyperfine magnetic splitting in the rare-earth ion. It may be assumed that the absence of a shift in the valence levels is also retained for the Y^{3+} ion in the $YBa_2Cu_3O_{6.9}$ compound subjected to radiative disordering. In this case the size of the chemical shift $^{89}K_{\text{ch.sh}}$ can be expected to remain unchanged under irradiation. This assumption is confirmed by the data on NMR line shifts in yttrium, depicted in Fig. 5 for nonsuperconducting disordered samples. As the temperature

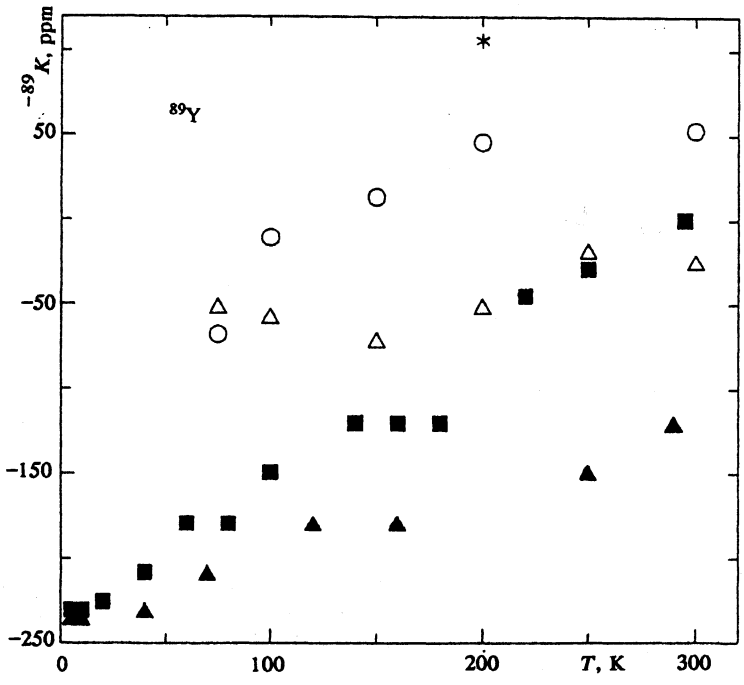

FIG. 5. The behavior of the NMR ^{89}Y line shift for the normal-state region in the $YBa_2Cu_3O_{6.9}$ compound irradiated by fast neutrons with the following fluences: *—$\Phi=0$; ○—$\Phi=5\times10^{18}$ cm^{-2}; Δ—$\Phi=1.2\times10^{19}$ cm^{-2}; ■—2×10^{19} cm^{-2}; ▲—5×10^{19} cm^{-2}.

drops, ^{89}K assumes a value equal to 220 ppm, which is close to the value of the orbital (chemical) shift $K_{ch.sh}=200$ ppm in the ordered $YBa_2Cu_3O_{6.9}$ compound (Ref. 20) and to $K_{ch.sh}=155$ ppm in $YBa_2Cu_3O_{6.85}$ and $YBa_2Cu_3O_{6.63}$ (Ref. 21). Thus, it can be said that in nonsuperconducting disordered samples the spin contribution $^{89}K_s$ tends to a value close to zero as the temperature lowers. At $\Phi=2\times10^{19}$ cm^{-2} the "freezing" of the spin contribution occurs for temperatures below 20 K, and at the maximum fluence of $\Phi=5\times10^{19}$ cm^{-2} we have $^{89}K_s\simeq0$ at temperatures below 80 K. We see that the NMR ^{89}Y data supports the conclusion drawn from the analysis of NMR ^{63}Cu line shifts for superconducting samples that the density of electronic states at the Fermi level decreases with disordering and that a gap forms near the Fermi energy for nonsuperconducting samples. Note that according to the ^{89}Y NMR data, as the fluence increases the rate at which $\chi_s(q=0)$ decreases lowers (Fig. 3).

The increase of ^{89}K with temperature can be attributed to the temperature dependence of the spin contribution to the magnetic susceptibility:

$$\chi_s(T)=2\mu_B^2\int N(E)f'(E)dE, \tag{8}$$

with

$$f(E)=1/\left(\exp\left\{-\frac{E-\mu}{kT}\right\}+1\right)$$

the Fermi distribution function. Here one must also assume that the value of the chemical potential μ lands in the energy range inside the gap forming in the electronic spectrum.[15]

Note that ^{89}K and $^{63}K_\perp$ considered as functions of temperature have opposite signs in the sample with the greatest disorder. This behavior is difficult to interpret if the value of the hyperfine field induced on the yttrium atom is assumed constant. Nor is it possible to exclude the possibility that an additional redistribution of the spin density appears in the region of small values of q when disorder sets in. This statement can be justified by the experimental ^{17}O NMR data on the O2 and O3 positions. We believe that the results of measurements of the rate of spin-lattice relaxation on ^{89}Y nuclei depicted in Fig. 5 favor the assumption that the spin density of the current carriers acquires a spatial inhomogeneity. For the superconducting samples studied in the metallic-conduction region the temperature behavior of the rate ^{89}R of spin-lattice relaxation in the normal state is described fairly well by a linear dependence with a slope that increases with the fluence. Such a temperature behavior is indicative of a Korringa mechanism of relaxation in metals:[22]

$$^{89}R_K=2\gamma^2hk_BTH_{st}^2\left(\frac{\chi_s}{2\mu_B^2}\right)^2=2\gamma^2hk_BTH_{st}^2N^2(E_F). \tag{9}$$

Since the spin susceptibility decreases as the fluence grows, the above formula does not explain why the rate of spin-lattice relaxation of ^{89}Y grows in disordered samples. Formula (9), obtained for the limit of short correlation times of electron motion in the conduction band $\omega_N\tau_c=2\pi\nu_0\tau_c\ll1$, assumes that the correlation time τ_c is roughly equal to the time that an electron moving with the Fermi velocity v_F needs to travel the distance between the closest yttrium atoms:

$$\tau_c\simeq\frac{a}{v_F}\simeq hN(E_F). \tag{10}$$

Warren[23] appears to have encountered a similar situation in analyzing the anomalous increase in the rate of spin-lattice relaxation in In_2Te_3 for a region where the manifestation of localization effects in the conduction band is substantial. A more thorough theoretical analysis is

TABLE I.

	$YBa_2Cu_3O_{6.9}$					
	σ,Ω^{-1} cm^{-1} (Ref. 8)		$^{89}\eta_N$	η(calc. (12), $T=300$ K)		η_N
Φ, 10^{18} cm^{-2}	$T=100$ K	$T=300$ K	$T=300$ K	$\sigma_c=10^3\ \Omega^{-1}$ cm^{-1}	$\sigma_c=450\ \Omega^{-1}$ cm^{-1}	$\sigma_c=450\ \Omega^{-1}$ cm^{-1}
0	2500	1000	1.0	1.2	1.10	1.00
5	500	330	1.5	2.3	1.80	1.60
12	170	180	4.0	6.0	3.00	2.80
20	10	33	3.3	30.0	13.00	

given in the Appendix. According to Ref. 22, Eq. (9) can be modified in the following manner for the case where τ_c deviates from the value (10) for free electrons:

$$^{89}R=\frac{^{89}\gamma^2 hk_B}{2\mu_B^2}\,^{89}K_s^2T\,\frac{\tau_c}{hN(E_F)}=\frac{^{89}\gamma^2 hk_B}{2\mu_B^2}\,^{89}K_s^2T\nu, \quad (11)$$

where $\eta=R/R_K$ is the gain due to the increase in the time that an electron stays near the nucleus involved in NMR, the increase being caused by the approach to the localized metal-insulator transition. With this factor we relate the increase in ^{89}R. For instance, for the sample with $\Phi=1.2\times10^{19}$ cm^{-2} the increase becomes as large as $\tau_c(\Phi=1.2\times10^{19}\ \text{cm}^{-2})(\tau_c(\Phi=0))^{-1}\approx5(1)$, which roughly agrees with a fivefold increase in the effective time of interaction of the electron spin with the nucleus. According to Eq. (A12), in the metallic-conduction region the enhancement factor η can be expressed in terms of the sample's conductivity as follows:

$$\eta=\frac{T_1^K}{T_1}\simeq\frac{\tau_c}{hN(E_F)}\simeq1+\frac{\pi}{3}\frac{\sigma_c^2}{\sigma(\sigma+\sigma_c)}, \quad (12)$$

where σ_c is the so-called minimum metallic conductivity,[23] whose values lie in the 100–1000 mΩ^{-1} cm^{-1} range. When analyzing ^{89}Y NMR experiments the frequency dependence of σ can be ignored, setting it at the dc value. To compare the results with (12), we use the conductivity data gathered for the same samples. As demonstrated in Ref. 8, for fluences $(5–10)\times10^{18}$ cm^{-2} the curves representing the temperature dependence of the resistivity ρ exhibit in the low-temperature range a section with $d\rho/dT<0$ fairly well described by the dependence $\rho(T)\propto\exp(QT^{-1/4})$ with $Q=2.1(N(E_F)R_{loc}^3)^{-1/3}$, a dependence is characteristic of localized-state conduction; this complicates somewhat the further analysis. In the high-temperature range ($T>100$ K) the metallic nature of conduction with $d\rho/dT>0$ was found to be predominant in all the investigated samples. In what follows we use these values of conductivity. Table I lists the values of dc conductivity σ for the limits of the investigated metallic-conduction region of the irradiated $YBa_2Cu_3O_{6.9}$ samples. It also lists the values of the relative variation in the gain, $\eta_N=[^{89}R(\Phi)/^{89}R(\Phi=0)][\chi_s(\Phi=0)/\chi_s(\Phi)]^2$, due to the onset of structural disorder. The values are obtained from the data on ^{89}Y NMR and dc conductivity combined with Eq. (12) and with allowance for the decrease in χ_s under disordering. Best agreement is achieved for a minimum metallic conductivity $\sigma_c=450\ \Omega^{-1}$ cm^{-1}. This value agrees fully with the σ_c estimates usually given in the literature on Anderson localization (see Ref. 24).[1)]

Figure 7 depicts the dependence on the fluence of the normalized gain η_N, which characterizes the relative enhancement of spin-lattice relaxation due to localization effects with allowance for variations in the density of states at the Fermi level in the $YBa_2Cu_3O_{6.9}$ compound under disordering. For $\Phi=1.2\times10^{19}$ cm^{-2} an increase in η accompanying a decrease in σ is observed.[7] The decrease in η_N for large fluences corresponding to nonsuperconducting $YBa_2Cu_3O_{6.9}$ samples, however, ceases to be described by Eq. (12): A decrease in σ is accompanied by a decrease in η. Such behavior of the gain with increasing disorder would seem to reflect a situation described theoretically in the Appendix and associated with the passage of the system through an Anderson transition. For the sample with $\Phi=2\times10^{19}$ cm^{-2} the degree of disorder is so high that, according to the conductivity data of Ref. 7, the sample is on the insulator side of the metal-insulator transition. In the Appendix we show that at the boundary of the metal–insulator transition the gain η must assume a maximum value. On the insulator side of the transition the gain is proportional to the product of the Fermi momentum p_F and the localization radius R_{loc}:

$$\eta\simeq p_F R_{loc}. \quad (13)$$

As we go deeper into the insulator phase, the value of η must decrease, owing to the decrease in R_{loc}, and result in a less effective Cu–O–Y interaction. Considering the data on ^{89}R at room temperature (Fig. 6), we notice that the rate of spin-lattice relaxation of yttrium nuclei ceases to increase at $\Phi=2\times10^{19}$ cm^{-2}. According to the results of the analysis in the Appendix, we can state that as the fluence grows the transition from the metallic state to the Anderson-insulator state occurs in the $(1–2)\times10^{19}$ cm^{-2} range, where η is at its maximum. Note once more that the discussion of the data refers to the high-temperature range $T>100$ K. At low temperatures, as Fig. 6 shows, $^{89}R(\Phi=2\times10^{19}\ \text{cm}^{-2}, T=20\ \text{K})=0.020$ cm^{-2} exceeds the respective value $R(\Phi=1.2\times10^{19}\ \text{cm}^{-2})=0.01$ cm^{-2}. The most likely reason for the increase in $^{89}R(\Phi=2\times10^{19}$ cm^{-2}) in the low-temperature range would seem to be the appearance of an additional fluctuational dipole contribution to the spin-lattice relaxation process, due to the magnetic ordering localized moments ensuing from the disordering in CuO_2 planes. This effect manifested itself most strikingly in the sample with the greatest fluence, where an

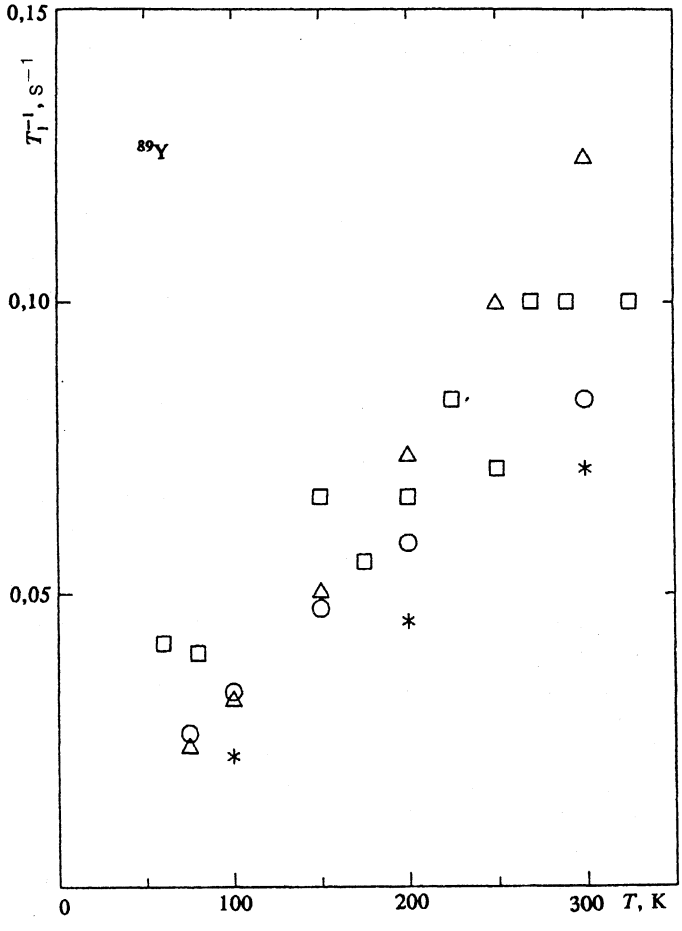

FIG. 6. Temperature dependence of the spin-lattice relaxation rate $T_1^{-1}(^{89}Y)$ in the $YBa_2Cu_3O_{6.9}$ compound irradiated by fast neutrons with the following fluences: *—$\Phi=0$; ○—$\Phi=5\times10^{18}$ cm^{-2}; Δ—$\Phi=1.2\times10^{19}$ cm^{-2}, and □—$\Phi=2\times10^{19}$ cm^{-2}.

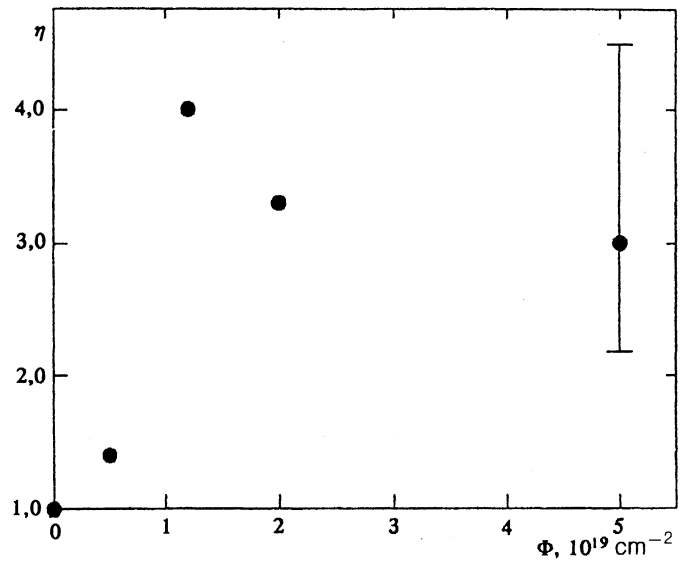

FIG. 7. $\eta_N=(^{89}R(\Phi)/^{89}R(\Phi=0))(\chi_s(\Phi=0)/\chi_s(\Phi))^2$ as a function of the fast-neutron fluence at $T=300$ K in $YBa_2Cu_3O_{6.9}$.

essentially nonexponential spin-lattice process takes place in the temperature range extending to room temperatures and complicates the analysis.

4. ANTIFERROMAGNETIC ORDERING OF LOCALIZED MAGNETIC MOMENTS IN CuO_2 PLANES

As was widely discussed in Ref. 26, the anomalous growth in the ^{89}Y NMR linewidth is one of the most sensitive tests for the presence of antiferromagnetic ordering in CuO_2 planes. The increase in the yttrium NMR linewidth is due to the static dipole fields $\mathbf{h}_{dip}=\Sigma_i\mathbf{m}/r_i^3$ generated by the magnetic moment of the environment at the point where the resonant nucleus is located. These fields may reach hundreds of oersteds. Figure 8 depicts the temperature dependence of the ^{89}Y NMR linewidth in the heavily irradiated $YBa_2Cu_3O_{6.9}$ samples with $\Phi\geqslant2\times10^{19}$ cm^{-2}. The reader can see that the temperature at which ordering begins increases with the fluence. Note that the magnetic-transition region is highly elongated, apparently owing to the created structural disorder. The transition can be assumed to be completed only in the sample with the maximum fluence at temperatures below 40 K, where the yttrium NMR linewidth has a constant value $\delta\nu\simeq85(5)$ kHz. The data may be interpreted as the first direct indication of the presence of antiferromagnetic short-range order of the localized magnetic moments produced in the CuO_2 planes as a result of radiative disorder in $YBa_2Cu_3O_{6.9}$. Naturally, our investigation does not permit judging the nature of ordering in the sense of the presence or absence of long-range order. The ordering in this case may be of the spin glass type.

5. CONCLUSION

From the analysis of the data on ^{63}Cu and ^{89}Y NMR line shifts we conclude that radiative disordering of the $YBa_2Cu_3O_{6.9}$ compound results in a decrease in the homogeneous spin susceptibility, which ends with the formation of a gap near the Fermi energy for nonsuperconducting samples with fast-neutron fluences Φ higher than 2×10^{19} cm^{-2}. Possibly we are observing the formation of a so-called Coulomb gap.[15,16]

The growth in the rate of spin-lattice relaxation in ^{89}Y under irradiation seems to suggest the onset of localization effects in the radiatively disordered $YBa_2Cu_3O_{6.9}$ compound. Experimental observation of the maximum of the normalized gain proves directly the existence of a localized transition in the system.

For fast-neutron fluences $\Phi>2\times10^{19}$ cm^{-2}, the localized magnetic moments formed by radiative disordering experience at low temperatures an antiferromagnetic short-range order; the temperature at which this order sets in increases with the fluence.

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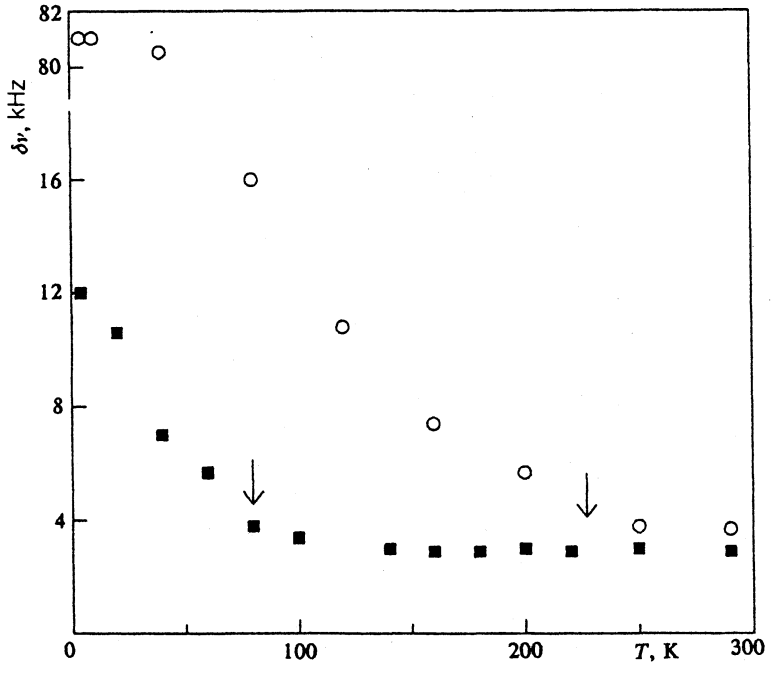

FIG. 8. Temperature dependence of the ^{89}Y NMR linewidth in the $YBa_2Cu_3O_{6.9}$ compound irradiated by fast neutrons with the following fluences: ■—$\Phi=2\times10^{19}$ cm^{-2} and ○—$\Phi=5\times10^{19}$ cm^{-2}. The arrows indicate the temperatures at which magnetic ordering begins.

APPENDIX: NMR RELAXATION AND LOCALIZATION

Measuring the NMR relaxation time T_1 is one of the experiments in which clear evidence can be obtained about electron localization in disordered systems (the Anderson transition). Actually, this fact was noted long ago by Warren,[23] who used this method to study metal–insulator transitions in semiconductor melts. Warren's qualitative treatment was confirmed by Gotze and Ketterlie,[27] whose ideas were based on a self-consistent localization theory. The main conclusion drawn in Refs. 23 and 27 was a growth of the reciprocal relaxation time T_1^{-1} in the metallic range as the system approaches the Anderson transition (compared to the behavior of the ordinary Korringa relaxation rate in metals[22]). Here, in addition to the results of Refs. 22, 23, and 27, we show that on the insulator side of the Anderson transition T_1^{-1} decreases with the electron localization radius (with increasing disorder). Thus, the Anderson transition is accompanied by a peak in T_1^{-1}, which can serve as experimental proof that a localized metal-insulator transition is realized. The reasoning that follows is based on the previously unpublished results of one of the authors (M.B.S.) obtained together with L. N. Bulaevskiĭ.[35] We set $\hbar=1$ in the majority of formulas below.

In systems with free electrons the main mechanism responsible for the coupling between the electrons and nuclear spins is the Fermi contact interaction, which leads to the following expression for T_1^{-1} (Ref. 22):

$$\frac{1}{T_1}=2A^2\frac{T}{g_e^2\mu_B^2\omega_N}\int\frac{d^3q}{(2\pi)^3}\,\mathrm{Im}\,\chi(\mathbf{q},\omega_N), \tag{A1}$$

where

$$\chi(\mathbf{q},\omega_N)=g_e^2\mu_B^2\left\langle\sum_{pp'}\sum_{\nu\nu'}\varphi_{\nu'\uparrow}(\mathbf{p}_+)\varphi^*_{\nu'\uparrow}(\mathbf{p}'_+)\varphi_{\nu\downarrow}(\mathbf{p}'_-)\right.$$
$$\left.\times\varphi^*_{\nu\downarrow}(\mathbf{p}'_-)\frac{f_{\nu'\uparrow}-f_{\nu\downarrow}}{\varepsilon_{\nu\downarrow}-\varepsilon_{\nu'\uparrow}+\omega_N+i\delta}\right\rangle \tag{A2}$$

is the electron susceptibility at the wave vector $\mathbf{q}$ and the NMR frequency ω_N. Here A is the usual hyperfine coupling constant, g_e the electron gyromagnetic ratio, μ_B the Bohr magneton, T the temperature, and $\mathbf{p}_\pm=\mathbf{p}\pm\frac{1}{2}\mathbf{q}$. Equation (A2) is written in the representation of the exact wave functions $\varphi_\nu(\mathbf{r})$ of an electron in the random field of a disordered system, and the ε_ν are the respective energy eigenvalues. The angle brackets stand for averaging over random configurations, and the arrows denote the direction of electron spin.

Using the inequality $\omega_N\ll\omega_e\ll T$, where ω_e is the electron Zeeman frequency, we get by direct calculation

$$\frac{1}{T_1}=2A^2TN(E_F)\pi\int\frac{d^3\mathbf{q}}{(2\pi)^3}\langle\langle\rho_{E_F}\rho_{E_F+\omega_e}\rangle\rangle_{\mathbf{q}}$$
$$=2A^2T\int\frac{d^3q}{(2\pi)^3}\,\mathrm{Im}\,\Phi^{RA}_{E_F}(\mathbf{q},\omega_e), \tag{A3}$$

where $N(E_F)$ is the density of electronic states at the Fermi level, and we have introduced the Fourier transform of the Berezinskiĭ–Gor'kov spectral density:[29]

$$\langle\langle\rho_E(\mathbf{r})\rho_{E+\omega}(\mathbf{r}')\rangle\rangle$$
$$=\frac{1}{N(E)}\left\langle\sum_{\nu\nu'}\varphi^*_\nu(\mathbf{r})\varphi_{\nu'}(\mathbf{r}')\varphi^*_{\nu'}(\mathbf{r}')\varphi_\nu(\mathbf{r}')\right.$$
$$\left.\times\delta(E-\varepsilon_\nu)\delta(E+\omega-\varepsilon_{\nu'})\right\rangle. \tag{A4}$$

In deriving the second expression in (A3) we used the relation[30] between the spectral density and the averaged two-particle Green function $\Phi^{RA}_{E_F}(\mathbf{q},\omega)$ of an electron in a disordered system.[31,32] Further calculations require a specific model for the Anderson transition, which we take to be the self-consistent localization theory in the form suggested by Wolfle and Vollhardt.[31,32] Then

$$\Phi^{RA}_{E_F}(\mathbf{q},\omega)=-\frac{N(E_F)}{\omega+iD_{E_F}(\omega)q^2}, \tag{A5}$$

where $D_{E_F}(\omega)$ is the generalized diffusion coefficient,

$$D_{E_F}(\omega)=i\frac{2E_F}{3}\frac{1}{M_{E_F}(\omega)}, \tag{A6}$$

with the "relaxation kernel" $M_{E_F}(\omega)$ determined by the well-known self-consistency equation,[31,32] whose solution has the form

$$M_{E_F}(\omega)=\begin{cases}\dfrac{i}{\tau_{E_F}} & \text{if } E_F\geqslant E_c \text{ (metal)},\\ \dfrac{i}{\tau_{E_F}}-\dfrac{\omega_0^2(E_F)}{\omega} & \text{if } E_F<E_c \text{ (insulator)}.\end{cases} \tag{A7}$$

Here τ_{E_F} acts as the generalized mean-free-path time, and the characteristic frequency $\omega_0(E_F)$ is related to the localization radius in an Anderson insulator as follows:

$$R_{loc}(E_F)=\frac{v_F}{\sqrt{3}\omega_0(E_F)}, \tag{A8}$$

where v_F is the Fermi velocity, and E_c the mobility threshold separating the localized and delocalized states on the energy axis. From this we can easily obtain[32,33]

$$\langle\langle\rho_{E_F}\rho_{E_F+\omega_e}\rangle\rangle_{\mathbf{q}}$$

$$=\begin{cases}\dfrac{1}{\pi}\dfrac{D_{E_F}q^2}{\omega^2+(D_{E_F}q^2)^2} & \text{if } E_F\geqslant E_c,\\ A_{E_F}(\mathbf{q})\delta(\omega)+\dfrac{1}{\pi}\dfrac{D_{E_F}q^2}{\omega^2+\omega_0^2(E_F)\tau_{E_F}+D_{E_F}q^2} & \text{if } E_F<E_c,\end{cases} \tag{A9}$$

where $A_{E_F}(\mathbf{q})=(1+R_{loc}(E_F)q^2)^{-1}$, and $D_{E_F}=\frac{1}{3}v_F^2\tau_E$ is the renormalized diffusion coefficient.

Equations (A7) and (A9) are valid for $\omega\ll\omega_c\simeq\gamma(p_F\xi_{loc}(E_F))^{-3}$, with γ the Drude rate of electron scattering by a disorder, $\xi_{loc}(E_F)$ the localization correlation length[29,30] coinciding with $R_{loc}(E_F)$ for $E_F<E_c$ (an Anderson insulator), and p_F the Fermi momentum. At the Anderson transition point ($E_F=E_c$) $\xi_{loc}(E_F)$ and $R_{loc}(E_F)$ diverge, thus demonstrating a critical behavior.[31,32] For $\omega_c\leqslant\omega\leqslant\gamma$ (including the mobility threshold, at which $\omega_c=0$) the generalized diffusion coefficient is determined by the well-known $\omega^{1/3}$-law of Gotze:[31,34]

$$D_{E_F}(\omega)=D_0^{E_F}\left(-\frac{i\omega}{2\gamma}\right)^{1/3}, \tag{A10}$$

where $D_0^{E_F}$ is the Drude diffusion coefficient. The characteristic frequency ω_c is determined by the condition $D_{E_F}(\omega_c)\sim D_{E_F}$. In this frequency range we have instead of (A9)

$$\langle\langle\rho_{E_F}\rho_{E_F+\omega_e}\rangle\rangle_{\mathbf{q}}=\frac{\sqrt{3}}{2\pi}\frac{\alpha^{2/3}\omega^{1/3}q^2}{\omega^2+\alpha^{2/3}\omega^{4/3}q^2+\alpha^{4/3}\omega^{2/3}q^4}, \tag{A11}$$

where $\alpha=D_0^{E_F}v_F/2\gamma$.

Using (A9) and (A3), we can easily calculate T_1^{-1}. This requires introducing additional cutoff of the integral over $\mathbf{q}$ at momenta of the order of the reciprocal mean free path $l^{-1}\sim\gamma/v_F$, since the above "diffusion" expressions are valid only in this region of momentum space. Near the mobility threshold (the Anderson transition) we have $l^{-1}\sim p_F$. Direct calculations for the metallic region ($E_F>E_c$) yield

$$\frac{1}{T_1}\simeq T_1^K\begin{cases}1+\dfrac{1}{p_Fl}\dfrac{\sigma_F}{\sigma}-\sqrt{\dfrac{\pi}{2}}\left(\dfrac{\omega_e}{E_F}\right)^{1/2}\left(\dfrac{\sigma_c}{\sigma}\right)^{3/2}\\ \quad\text{if } \sigma>\sigma_c\left(\dfrac{\omega_e}{\gamma}\right)^{1/3},\\ \dfrac{1}{(p_Fl)^2}\left(\dfrac{\omega_e}{2\gamma}\right)^{-1/3} \quad \text{if } \sigma\leqslant\sigma_c\left(\dfrac{\omega_e}{\gamma}\right)^{1/3},\end{cases}$$

$$\simeq\frac{1}{T_1^K}\begin{cases}1+\dfrac{\pi}{3}\dfrac{\sigma_c^2}{\sigma(\sigma+\sigma_c)} & \text{if } \sigma>\sigma_0\left(\dfrac{\omega_e}{E_F}\right)^{1/3},\\ \left(\dfrac{E_F}{\omega_e}\right)^{1/3} & \text{if } \sigma\leqslant\sigma_c\left(\dfrac{\omega_e}{E_F}\right)^{1/3},\end{cases} \tag{A12}$$

where T_1^K is the Korringa relaxation time,[22] which determines the relaxation of nuclear spins in a "good" metal:

$$\frac{1}{T_1^K}=2A^2T\pi[N(E_F)]^2. \tag{A13}$$

The characteristic conductivity $\sigma_c=e^2p_F/\pi^3/h^2$ coincides, in order of magnitude, with Mott's estimate of the minimum metallic conductivity.[24] In going over to the second expression in (A12) we used the equation $p_Fl=3(\sigma+\sigma_c)/\pi\sigma_c$ of Ref. 35 and expressed the result in terms of the measurable conductivity σ. Moreover, in the last expression we ignored terms of the order of $(\omega_e/E_F)^{1/2}$, which are small in almost any real situation. The unity on the right-hand side of (A12) is written explicitly so that the expression agrees with the ordinary results in the "pure" limit, where $\sigma\gg\sigma_c(p_Fl\gg1)$. Direct transition to the "pure" limit in the integral over $\mathbf{q}$ in Eq. (A3) is impossible if we use Eqs. (A9) and (A11), which are valid only for the "impure" case. Accordingly, (A12) should be considered an interpolation formula. The first expression in (12) practically coincides with the respective expression in Ref. 27, but here we have reduced it to a form more convenient for comparison with the experimental data.

Equation (A12) shows that in an Anderson transition ($\sigma\leqslant\sigma_c$) the NMR relaxation rate T_1^{-1} will grow consider-

ably in comparison with the Korringa relaxation rate. Moreover, in the narrow range near the transition point T_1 begins to depend on ω_e, that is, on the external magnetic field. Unfortunately, the dependence emerges only for $\sigma \leqslant \sigma_c (E_F/\omega_e)^{-1/3} \ll \sigma_c$, that is, in an extremely narrow neighborhood of the transition, which means that observing the $\omega_e^{-1/3}$-dependence of the NMR relaxation rate is extremely difficult experimentally, even for systems with low values of the Fermi energy, of the doped-semiconductor type. In this range the conductivity's temperature dependence, which was previously ignored, begins to play an essential role (everywhere above σ is the residual conductivity, obtained through extrapolation to $T=0$). On the other hand, the increase in the relaxation rate T_1^{-1} as the conductivity decreases (the degree of disorder grows) should be observed in a fairly broad region, starting with the well-known Ioffe–Regel limit $\sigma \sim 10^3 \Omega^{-1}$ cm^{-1} (Ref. 24). This behavior was observed in Warren's experiments[22] involving liquid semiconductors, and, above, it revealed itself in connection with ^{89}Y NMR experiments in the radiatively disordered $YBa_2Cu_3O_{6.9}$ compound.

In the localization region ($E_F < E_c$), calculations similar to those that led to (A12) yield

$$\frac{1}{T_1} \simeq \frac{1}{T_1^K} \times \begin{cases} \dfrac{1}{(p_F l)^2} \left(\dfrac{\omega_e}{\gamma}\right)^{-1/3} \simeq \left(\dfrac{E_F}{\omega_e}\right)^{1/3} \\ \quad \text{if } R_{loc}(E_F) \geqslant (N(E_F)\omega_e)^{-1/3}, \\ p_F R_{loc}(E_F) \\ \quad \text{if } R_{loc}(E_F) \leqslant (N(E_F)\omega_e)^{-1/3}. \end{cases} \quad \text{(A14)}$$

Obviously, here too the $\omega_e^{-1/3}$-dependence operates only within a very narrow region near the transition, where the localization radius $R_{loc}(E_F)$ is extremely large. As the Fermi level E_F moves deeper into the localization region (or as the degree of disorder increases), $R_{loc}(E_F)$ decreases, so that the relaxation rate T_1^{-1} diminishes together with the parameter $p_F R_{loc}$. The second expression in (A14) is valid at $p_F R_{loc} \sim 1$, when T_1^{-1} returns to values of the order of the Korringa rate. For smaller values of R_{loc} the approximation based on the self-consistent localization theory cannot be used, since in this theory R_{loc} cannot be smaller than roughly p_F^{-1}. Thus, T_1^K/T_1 passes through a maximum when the Fermi level crosses the mobility threshold. Experimental observation of such a maximum might serve as an important independent indication that an Anderson transition is realized in such a system. This behavior was, apparently, observed in the experiments on NMR relaxation of ^{89}Y in disordered $YBa_2Cu_3O_{6.9}$ described above. Naturally, similar measurements will need to be carried out on a more "dense" (in the degree of disorder) set of samples. This would enable studying in greater detail the neighborhood of the maximum and determining its position more exactly.

The physical meaning of the results is quite simple. NMR relaxation is via a flip of the nuclear spin by an electron flying past the nucleus and flipping its own spin. As the system approaches the Anderson transition, the conduction electrons in the vicinity of the given nuclear spin diffuse ever more slowly and, hence, interact with the spin over an ever increasing time interval, which is the reason why the relaxation rate T_1^{-1} grows.[23] The effect is most pronounced at the transition point, but subsequently, as the electrons remain localized in a region with dimensions of the order of R_{loc} surrounding the given nucleus, the localization radius decreases as the degree of disorder grows and an electron "carries away" less and less information about the nuclear spin, which leads to the decrease in T_1^{-1}.

In the above reasoning we ignored the temperature dependence of conductivity. In interpreting the experiment in the metallic region we used for the conductivity of the system at fairly high temperatures the parameter σ, which in our theoretical model has the meaning of conductivity at $T=0$. The zero value of σ corresponds to the Anderson transition point at $T=0$, while in the experiments (at finite values of T) a finite value of conductivity was observed, naturally. For this reason and also because of the effects of a negative thermal coefficient of resistance in the metallic region it usually is extremely difficult to determine the transition point from conductivity measurements. Measurements of NMR relaxation offer many more advantages. Moreover, we completely ignored electron-electron interaction, which would complicate the entire relaxation pattern, especially in view of the formation (due to disorder) of localized magnetic moments.[7] It is also worth noting that we ignored the effect of the external magnetic field, in which the NMR experiment was conducted, on the localization (the Anderson transition). This effect, in principle, is not small and shifts the Anderson transition to the region of large disorder degrees. For this reason, strictly speaking, the experiments discussed determine the position of the point of an Anderson transition in an external magnetic field.

[1)]The smaller value $\sigma_c = 250(30)\Omega^{-1}$ cm^{-1} given in Ref. 25 was obtained with the gain η normalized to the ratio $\chi_s(\Phi)/\chi_s(\Phi=0)$ rather than to the square of this ratio, as was done in the present paper. The difference stems from the fact that here we link the variation in χ_s with the decrease in the density of states at the Fermi level due to the formation of a pseudogap rather than with the variation of the correlation corrections to χ_s, as is done in Ref. 25.

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