Nuclear relaxation rate and the Knight shift in layered *S/N* structures

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We calculate the rate of nuclear relaxation and the Knight shift in the model of a layered superconductor, which is a stack of alternating superconducting (S) and normal (N) layers (these may be, for instance, the Cu–O planes and Cu–O chains in a 1-2-3 compound). Superconductive pairing is present only in the S-layers, and superconductivity in the N-layers appears because of the proximity effect. We also show that within the framework of this model there is an explanation for the absence in high-T_c superconductors of a peak in the nuclear relaxation rate near T_c (this absence has been observed in experiments) and for the power dependence of the nuclear relaxation rate T_1^{-1} on temperature at low temperatures.

1. INTRODUCTION

The nuclear magnetic resonance (NMR) method serves as an important tool for extracting information about the electronic structure and the properties of high-T_c superconductors. Recent experiments[1-4] have confirmed that the temperature dependence of the nuclear relaxation rate in high-T_c superconductors cannot be described within the framework of the standard BCS theory.[5] A common feature of high-T_c superconductors is the absence of a jump in the nuclear relaxation rate T_1^{-1} immediately below T_c and the fact that the formulas of the ordinary BCS theory do not describe the shape of the T_1^{-1} vs T curve (e.g., a power-law curve) at lower temperatures. There have been several attempts to describe theoretically the special features of NMR in high-T_c superconductors (see, e.g., Refs. 6–8), where the ideas used to explain the anomalous behavior of the T_1^{-1} vs T curve range from antiferromagnetic correlations on copper atoms[6] to nontrivial superconductive pairing.[7,8]

In the present paper we show that nuclear relaxation in high-T_c superconductors can be explained without resorting to assumptions concerning nontrivial pairing or relaxation through additional degrees of freedom if one allows for the existence of different conducting layers in high-T_c superconductors. A large body of experimental data corroborates this assumption. The results of many experiments (see, e.g., Refs. 3, 4, and 9) show that in 1-2-3 and 1-2-4 compounds the pairing of carriers occurs in Cu–O planes and is absent in chains (although the conduction in chains is metallic).

Various types of conducting planes can also exist in the family of bismuth and thallium superconductors. For instance, the unit cell of 2-2-2-3 compounds has three successively arranged Cu–O layers. Since the middle Cu–O layer has a structure that differs from that of the side layers, its superconductive properties may also differ from those of the side layers.[10] This assumption is supported by the results of experiments reported in Ref. 11 which registered two different Knight shifts on copper, from the Cu atoms in the middle layer and from Cu atoms in the side layers. At the same time, Ref. 12 reports on the discovery of a sheet of the Fermi surface related to Bi–O layers in the $Bi_2Sr_2CaCu_2O_{8+\delta}$, which attests to the metallic nature of the Bi–O layers (although the carriers in these layers do not participate in superconductive pairing). This suggests that the role of Bi–O layers is to a certain degree similar to that of Cu–O chains in 1-2-3 compounds.

Thus, there is ample experimental evidence of the existence of alternating superconducting (S) and normal (N) layers in high-T_c superconductors. For this reason we present below the results of calculations of the nuclear relaxation rate and the Knight shift for a layered S/N structure. Models of this kind have been employed in Refs. 13–18. Although this model is considered within the framework of the ordinary weak coupling approximation, it successfully describes the results of tunneling measurements involving high-T_c superconductors[14-16] and of optical conductivity[17,19] and Raman spectra of high-T_c superconductors.[18]

Superlattices with layers whose thickness is that of atomic separation, such as $YBa_2Cu_3O_x/PrBa_2Cu_3O_y$ (Ref. 20) and $Y_xPr_{1-x}Ba_2Cu_3O_y/YBa_2Cu_3O_z$ (Ref. 21), also belong to superconducting systems with alternating layers of two different types. Because in the $Y_{0.8}Pr_{0.2}Ba_2Cu_3O_y/YBa_2Cu_3O_z$ structure both layers, $Y_xPr_{1-x}Ba_2Cu_3O_y$ and $YBa_2Cu_3O_z$, are superconductors with markedly different critical temperatures, such a structure constitutes a very convenient object for studying proximity effects.

A characteristic feature of the S/N model is the logarithmic nature of singularities in the density of states, in contrast to the common square-root behavior of singularities in BCS theory. As demonstrated below, this type of singularities can explain the absence of a jump in the nuclear relaxation rate near T_c. The density of states inside the gap in the S/N system may be nonzero because of the effect of proximity of the N- and S-layers even in the case of s-pairing, which leads to a deviation of the nuclear relaxation rate at low temperatures from the value predicted by the BCS theory (in this case $T_1^{-1}(T)$ is a power function of temperature). Such a temperature dependence is indeed observed for $T_1^{-1}(T)$ in the majority of cases (see, e.g., Refs. 1–4). In the present paper we also list the results of calculating the temperature dependence of the Knight shift in S- and N-layers. Within the framework of our model, the nuclear relaxation rates in S- and N-layers exhibit different temperature dependencies, which agrees with the experimental data of Refs. 3 and 4.

Since our main goal is to qualitatively describe NMR in high-T_c superconductors, we do not consider the exact structure of the hyperfine interaction Hamiltonian responsible for nuclear relaxation and the Knight shift. The similarity of the temperature behavior of the Knight shifts in copper, oxygen, and yttrium[22,23] shows that the characteristics features of NMR for a given conducting layer can be explained on the basis of the electron spin susceptibility com-

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mon to the layer. The differences between the values of the nuclear relaxation rate and the Knight shift in Cu and O nuclei are, apparently, due to different form factors for copper and oxygen. Thus, for our goals it is enough to calculate the dynamic and static spin susceptibilities of the conduction electrons in S- and N-layers.

2. FORMULATION OF THE MODEL

Let us start by discussing the characteristic features of the S/N model. We consider a set of equidistant metallic layers coupled by a weak bond, with superconductive pairing occurring only on S-layers. We also assume that the electronic spectra of all the layers are the same and that $\hbar = k_B = 1$.

To describe the electron motion from layer to layer (along the z axis) in the tight-binding approximation, we change to the Wannier representation[24] in the direction perpendicular to the layers. Since we are considering an S/N structure with two layers per unit cell, in the electronic spectrum there appear two bands corresponding to two different eigenfunctions $\psi_{q1}(z)$ and $\psi_{q2}(z)$, where q is the quasimomentum in the direction perpendicular to the layers. From these functions we go to the Wannier functions

$$\tilde{w}_1(z-2md) = N^{-1/2}\sum_q \psi_{q1}(z)e^{2iqmd},$$
$$\tilde{w}_2(z-2md) = N^{-1/2}\sum_q \psi_{q2}(z)e^{2iqmd}, \tag{1}$$

with d the distance between the layers, m the number of the unit cell, and N the total number of cells (periods) along the z axis. Using the functions $\tilde{w}_1$ and $\tilde{w}_2$, we can build two linear combinations, one of which vanishes at all N-layers and the other at all S-layers. We denote these new functions by w_1 and w_2, respectively.

In the second-quantization representation the electron operator in the S/N system can be written as

$$\psi_\sigma(\mathbf{r}, z) = \frac{1}{(\Omega N)^{1/2}}\sum_{\mathbf{k}qm}\{c_{\mathbf{k}q1\sigma}\exp(i\mathbf{kr}+2iqmd)w_1(z-2md)$$
$$+c_{\mathbf{k}q2\sigma}\exp[i\mathbf{kr}+iq(2m+1)d]w_2(z-(2m+1)d)\}, \tag{2}$$

where $c_{\mathbf{k}q\alpha\sigma}$ is the electron annihilation operator, $\mathbf{r}$ and $\mathbf{k}$ the two-dimensional position and momentum vectors in the layer plane, and Ω the normalization area in this plane.

The Hamiltonian of the S/N system in the mean-field approximation is

$$H = \sum_{\mathbf{k}q\alpha\sigma}\xi(\mathbf{k})\bar{c}_{\mathbf{k}q\alpha\sigma}c_{\mathbf{k}q\alpha\sigma} - \Delta\sum_{\mathbf{k}q}\bar{c}_{\mathbf{k}q1\downarrow}\bar{c}_{-\mathbf{k}-q1\uparrow} - \Delta^*\sum_{\mathbf{k}q}c_{\mathbf{k}q1\uparrow}c_{-\mathbf{k}-q1\downarrow}$$
$$+\sum_{\mathbf{k}q\sigma}t(q)(\bar{c}_{\mathbf{k}q2\sigma}c_{\mathbf{k}q1\sigma}+\bar{c}_{\mathbf{k}q1\sigma}c_{\mathbf{k}q2\sigma}), \qquad t(q)=2t\cos(qd), \tag{3}$$

where $\bar{c}_{\mathbf{k}q\alpha\sigma}$ is the electron creation operator and $\xi(\mathbf{k})$ the energy of quasiparticles in the normal state measured from the Fermi level, the subscript $\alpha = 1,2$ numbers the layers in a unit cell ($\alpha = 1$ for the S-layers and $\alpha = 2$ for the N-layers), and the constant t is specified by the overlap integral for the Wannier functions localized at neighboring layers,

$$t = E_F\int_{-\infty}^{\infty} w_1(z)w_2(z+d)dz, \tag{4}$$

with E_F the Fermi energy. The superconducting gap is determined by the self-consistency condition

$$\Delta = -\frac{\lambda}{\Omega N}\sum_{\mathbf{k}q}\langle c_{\mathbf{k}q1\uparrow}c_{-\mathbf{k}-q1\downarrow}\rangle, \tag{5}$$

where λ is the electron-electron coupling constant.

The temperature Green functions for the S/N system have the following form:[25]

$$G_{\alpha\alpha'\sigma\sigma'}(\mathbf{k}q, \tau-\tau') = -\frac{1}{(\Omega N)^{1/2}}\langle T_\tau c_{\mathbf{k}q\alpha\sigma}(\tau)\bar{c}_{\mathbf{k}q\alpha'\sigma'}(\tau')\rangle,$$
$$F_{\alpha\alpha'\sigma\sigma'}(\mathbf{k}q, \tau-\tau') = \frac{1}{(\Omega N)^{1/2}}\langle T_\tau c_{\mathbf{k}q\alpha\sigma}(\tau)c_{-\mathbf{k}-q\alpha'\sigma'}(\tau')\rangle, \tag{6}$$
$$\bar{F}_{\alpha\alpha'\sigma\sigma'}(\mathbf{k}q, \tau-\tau') = \frac{1}{(\Omega N)^{1/2}}\langle T_\tau \bar{c}_{\mathbf{k}q\alpha\sigma}(\tau)\bar{c}_{-\mathbf{k}-q\alpha'\sigma'}(\tau')\rangle.$$

The functions F and G satisfy the following Gor'kov equations (in Matsubara frequencies):

$$\begin{pmatrix} i\omega-\xi(\mathbf{k}) & -t(q) & \Delta & 0 \\ -t(q) & i\omega-\xi(\mathbf{k}) & 0 & 0 \\ \Delta^* & 0 & i\omega+\xi(\mathbf{k}) & t(q) \\ 0 & 0 & t(q) & i\omega+\xi(\mathbf{k}) \end{pmatrix}$$
$$\times\hat{G}_\alpha(\mathbf{k}, q, \omega) = \frac{1}{(N\Omega)^{1/2}}\begin{pmatrix} \delta_{\alpha 1} & 0 \\ \delta_{\alpha 2} & 0 \\ 0 & \delta_{\alpha 1} \\ 0 & \delta_{\alpha 2} \end{pmatrix},$$
$$\hat{G}_\alpha(\mathbf{k}, q, \omega) = \begin{pmatrix} G_{1\alpha}(k,q,\omega) & F_{1\alpha\uparrow\downarrow}(\mathbf{k},q,\omega) \\ G_{2\alpha}(k,q,\omega) & F_{2\alpha\uparrow\downarrow}(\mathbf{k},q,\omega) \\ F_{1\alpha\uparrow\uparrow}(\mathbf{k},q,\omega) & -G_{\alpha 1}(-k,-q,-\omega) \\ F_{2\alpha\uparrow\uparrow}(\mathbf{k},q,\omega) & -G_{\alpha 1}(-k,-q,-\omega) \end{pmatrix}, \tag{7}$$

Proceeding from these equations, we can easily determine the energy of the quasiparticle in the superconducting state:

$$\omega_{1,2}^2(\mathbf{k}, q) = \xi^2(\mathbf{k}) + t^2(q) + \Delta^2/2$$
$$\pm[4t^2(q)\xi^2(\mathbf{k}) + \Delta^4/4 + t^2(q)\Delta^2]^{1/2}. \tag{8}$$

The excitation spectrum (8) has a gapless branch $\omega_2(\mathbf{k},q)$ [$\omega_2 = 0$ at $\xi = t(q) = 0$] because of the presence of N-layers. The gapless nature of superconductivity manifests itself, for one thing, in the fact that the temperature dependence of such quantities as the nuclear relaxation rate in IR absorption for $T \ll T_c$ (in contrast to the ordinary behavior predicted by the BCS theory) is represented by a power function. The characteristic features of spectrum (8) also lead to an unusual (logarithmic) nature of the singularities in the density of states. The density of states in the S/N model has been studied in Ref. 16.

Bulaevskiĭ and Zyskin[14] noted that in the case of Josephson coupling of the layers ($t \ll T_c$) there are two distinct temperature regimes for the N-layers. Although Cooper pairing is absent in the N-layers, superconductivity is induced in these layers because of the proximity effect. For this reason the anomalous Green function of the N-layers is finite:

$$F_{22\uparrow\downarrow}(\mathbf{k}, q, \omega) = \frac{1}{(N\Omega)^{1/2}}\frac{\Delta t^2(q)}{[\omega^2+\omega_1^2(\mathbf{k}, q)][\omega^2+\omega_2^2(\mathbf{k}, q)]}. \tag{9}$$

At low temperatures ($T \ll T_c$) only small ξ and $t(q)$ are essential. Hence, $\omega_1 \approx \Delta$ and the expression for $\omega_2(\mathbf{k},q)$ can be written in the approximate form

$$\omega_2^2(\mathbf{k}, q)=\xi^2(\mathbf{k})+t^4(q)/\Delta^2. \quad (10)$$

As follows from Eqs. (9) and (10), at low temperatures the quantity $\Delta(q) = t^2(q)/\Delta$ acts as a gap for the N-layers. At temperatures higher than t^2/Δ superconductivity practically does not penetrate the N-layers, but when $T \ll t^2/\Delta N$, the N-layers become fully "superconductive." Hence, at $T \approx t^2/\Delta$ the nature of the temperature dependencies of all superconductive properties of the S/N system changes.

In the opposite limiting case, $t \gg T_c$, there is averaging of properties of separate layers and the S/N model loses its specific features. In this paper we give the results describing NMR for both the case of Josephson coupling of layers ($t \ll T_c$) and at intermediate values of the overlap integral ($t \approx T_c$). The latter case is the most interesting. The t-to-T_c ratio can be estimated, for instance, from measurements of the torque in an external field[26,27] and measurements of the upper critical field.[28,29] According to the data listed in Refs. 26 and 27, in bismuth superconductors the ratio of the correlation lengths along and across the Cu–O layers, ξ_{ab}^2/ξ_c^2, is approximately $\lambda_c^2/\lambda_{ab}^2 \approx 10^4$, with λ_{ab} and λ_c the respective London penetration depths, and the condition $t < T_c$ is sure to be met. At the same time in 1-2-3 compounds the electronic anisotropy is smaller. It can be hoped that in the vast family of high-T_c superconductors there are compounds both with $t \ll T_c$ and with $t \approx T_c$.

3. CALCULATING THE NUCLEAR RELAXATION RATE IN A LAYERED S/N SYSTEM

Since our main goal is to clarify the basic features of NMR in a layered S/N system with Josephson coupling of the layers, we choose a simplified model to describe the coupling of nuclear spin with the conduction-electron spins. The rate $T_{1(\alpha)}^{-1}$ of relaxation of a nucleus localized at the α ($\alpha = 1,2$) layer is[30]

$$T_{1(\alpha)}^{-1}=\frac{T}{2(g\mu_B)^2\omega_e}\Big[A^2\,\mathrm{Im}\,\chi_{+-}(\alpha,\omega_e) + \sum_{\beta=1,2} b_{\alpha\beta}^2\,\mathrm{Im}\,\chi_{+-}(\beta,\omega_e)\Big], \quad (11)$$

where μ_B is the Bohr magneton and A the hyperfine coupling constant, $\omega_e = \mu_B B$, with B the external field, g is the g-factor of electrons in the crystal, and $\chi_{+-}(\alpha,\omega_e)$ is the transverse spin susceptibility of conduction electrons at the α layer. The first term on the right-hand side of (11) describes the isotropic contact interaction of the conduction electrons and nucleus in the same layer. The second term allows for the anisotropic dipole-dipole interaction of the nuclear spin in layer α with electrons that can be in either the same layer ($\beta = \alpha$) or in neighboring layers ($\beta \neq \alpha$). Equation (11) does not allow for crystal field effects, which introduce nothing new into the calculations. Note that since the electron magnetic moment is much larger than the nuclear, Eq. (11) must contain just the electron frequency ω_e and not the nuclear frequency $\omega_N = \mu_N B$, with μ_N the nuclear magneton.[31] But since both frequencies, ω_e and ω_N, are low, it is unimportant which is used in (11).

It is convenient to write Eq. (11) in the form

$$T_{1(\alpha)}^{-1}=\frac{T}{2(g\mu_B)^2\omega_e}\sum_{\beta=1,2} A_{\alpha\beta}^2\,\mathrm{Im}\,\chi_{+-}(\beta,\omega_e), \quad (12)$$

where the parameters $A_{\alpha\alpha}^2$ describe the contact and anisotropic dipole-dipole interactions of electrons in layer α with a nucleus in the same layer, and the parameters $A_{\alpha\beta}^2$ ($\alpha \neq \beta$) describe the dipole-dipole interaction of a nucleus in layer α with electrons in layer β.

The transverse spin susceptibility $\chi_{+-}(\alpha,\omega_e)$ is given by the temporal Fourier transform of the retarded spin Green function

$$iG_{+-}^R(\alpha, t_1-t_2) = \begin{cases} \langle S_+(\alpha,t_1)S_-(\alpha,t_2)-S_-(\alpha,t_2)S_+(\alpha,t_1)\rangle, & t_1>t_2, \\ 0, & t_1<t_2, \end{cases} \quad (13)$$

where $S_+ = \psi_\uparrow^+\psi_\downarrow$ and $S_+ = \psi_\downarrow^+\psi_\uparrow$ are the ordinary electron spin operators in the second quantization representation.

Thus, $\chi_{+-}(\alpha,\omega_e)$ can be obtained as a result of an analytic continuation ($i\omega \to \omega_e + i\delta$) of the polarization operator

$$G_{+-}(\alpha,\omega) = -\frac{T}{N\Omega}|w_\alpha(0)|^4 \times \sum_{\mathbf{k}\mathbf{k}'qq'\omega'} [G_{\alpha\alpha}(\mathbf{k},q,\omega')G_{\alpha\alpha}(\mathbf{k}',q',\omega+\omega') + \bar{F}_{\alpha\alpha\downarrow\uparrow}(\mathbf{k},q,\omega')\bar{F}_{\alpha\alpha\uparrow\downarrow}(\mathbf{k}',q',\omega+\omega')], \quad (14)$$

where $w_\alpha(0)$ is the value of the electron wave function at the nucleus. Equations (11), (12), and (14) are valid provided that the binding energy t of the layers is much lower than the Fermi energy E_F an electron moving in a layer. It is the condition that $E_F \gg |t|$, which apparently must hold true in high-T_c superconductors, that makes it possible to ignore the off-diagonal (in layer indices α and β) Green functions in the polarization operator and retain in (14) only the diagonal functions $G_{\alpha\alpha}$ and $F_{\alpha\alpha}$ (see the Appendix).

To analytically continue the polarization operator (14), it is convenient to employ the spectral representation of the Green functions:[25]

$$G_{\alpha\alpha'\sigma\sigma'}(\mathbf{k},q,\omega)=\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\mathrm{Im}\,G^R_{\alpha\alpha'\sigma\sigma'}(\mathbf{k},q,x)\,dx}{x-i\omega},$$
$$F_{\alpha\alpha'\sigma\sigma'}(\mathbf{k},q,\omega)=\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\mathrm{Im}\,F^B_{\alpha\alpha'\sigma\sigma'}(\mathbf{k},q,x)\,dx}{x-i\omega}. \quad (15)$$

Using this representation, we can easily sum over ω in (14), with the result that the spin susceptibility can be written as

$$\chi_{+-}(\alpha,\omega_e) = -\frac{(g\mu_B)^2|w_\alpha(0)|^4}{\pi^2 N\Omega} + \sum^{\mathbf{k}\mathbf{k}'qq'}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}[\mathrm{Im}\,G_{\alpha\alpha}^R(\mathbf{k},q,x)\,\mathrm{Im}\,G_{\alpha\alpha}^R(\mathbf{k}',q',y) + \mathrm{Im}\,\bar{F}^R_{\alpha\alpha\downarrow\uparrow}(\mathbf{k},q,x)\,\mathrm{Im}\,F^R_{\alpha\alpha\uparrow\downarrow}(\mathbf{k}',q',y)]\frac{f(x)-f(y)}{x-y+\omega_e+i0}\,dx\,dy, \quad (16)$$

where $f(x) = [\exp(x/T)+1]^{-1}$ is the Fermi distribution function. Since ω_e is much lower than the temperature, we have

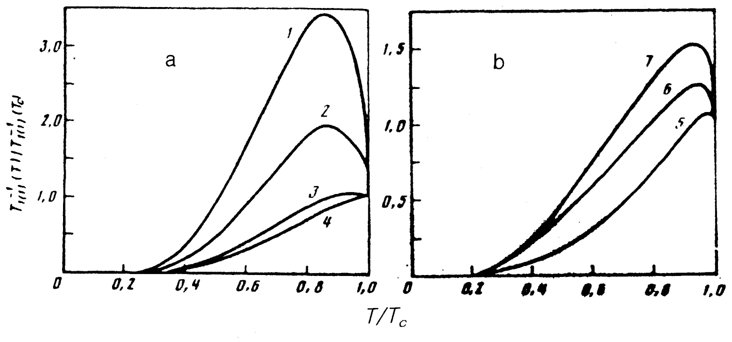

FIG. 1. (a) $T^{-1}_{1(1)}(T)/T^{-1}_{1(1)}(T_c)$ as a function of temperature at the superconducting layer at small (a) and large (b) values of the overlap integral t: (1) $t=0.01\ T_c$, (2) $t=0.15\ T_c$, (3) $t=0.36\ T_c$, (4) $t=0.5\ T_c$, (5) $t=0.75\ T_c$, (6) $t=2\ T_c$, and (7) $t=3\ T_c$. In this figure and in Fig. 2 we ignore the off-diagonal elements of tensor $A_{\alpha\beta}$ in Eq. (12) in view of their smallness.

$$\frac{\operatorname{Im}\chi_{+-}(\alpha,\omega_e)}{\omega_e} = \frac{(g\mu_B)^2|w_\alpha(0)|^4}{\pi N\Omega} \times\sum_{\mathbf{k}\mathbf{k}'qq'}\int_{-\infty}^{\infty}[\operatorname{Im}G_{\alpha\alpha}{}^R(\mathbf{k},q,x)\operatorname{Im}G_{\alpha\alpha}{}^R(\mathbf{k}',q',x+\omega_e) + \operatorname{Im}\bar{F}^R_{\alpha\alpha\downarrow\uparrow}(\mathbf{k},q,x)\operatorname{Im}F^R_{\alpha\alpha\uparrow\downarrow}(\mathbf{k}',q',x+\omega_e)]\left(-\frac{\partial f}{\partial x}\right)dx. \quad (17)$$

In contrast to the ordinary result of the BCS theory for an isotropic (three-dimensional) superconductor,[5] in our case $\operatorname{Im}\chi_{+-}(\alpha,\omega_e)$ and $T^{-1}_{1(\alpha)}$ do not diverge as $\omega_e\to 0$. This is due to the logarithmic nature of the singularities in the density of states of the S/N system (contrary to the usual square-root nature of the singularities in the BCS theory).

The temperature curves for the rate $T^{-1}_{1(1)}$ of nuclear relaxation on superconducting layers for different values of parameter t are depicted in Fig. 1. For these curves the temperature T has been normalized to the critical temperature T_c, which depends on t and is therefore different for different curves. Note that to obtain a finite value of $T^{-1}_{1(\alpha)}(T)$ there was no need to allow for the broadening of quasiparticle levels, in contrast to the ordinary situation.[32] At $t=0.01\ T_c$ the $T^{-1}_{1(1)}$ vs T curve has a sharp peak near T_c, since in the case of small t/T_c the effect of the N-layers on the S-layers is low. Here the temperature dependence of the rate of relaxation on N-layers, $T^{-1}_{1(2)}$, follows the Korringa relation almost exactly [see Fig. 2(a)]. As t increases, the peak on the $T^{-1}_{1(1)}$ vs T curve practically disappears. If, in addition, we take into account the energy-level broadening caused by the finite quasiparticle lifetimes, the peak in the nuclear relaxation rate near T_c characteristic of the BCS theory is absent (as observed, for instance, in experiments reported in Refs. 1–4). The low-temperature (for $T<t^2/\Delta$) behavior of the $T^{-1}_{1(2)}$ vs T curve at $t/T_c=0.36$ and 0.5 differs from linear (characteristic of normal metals), since superconductivity is induced in the N-layers because of the proximity effect [Fig. 2(a)].

As t grows, the system becomes ever more three-dimensional and the properties of the S- and N-layers undergo effective averaging [see the curves corresponding to $t>T_c$ in Fig. 1(b)]. For this reason there again appears a peak near T_c on the $T^{-1}_{1(1)}$ vs T curve. It must be noted that for sufficiently large t (i.e., at such values of the overlap integral at which the correlation length ξ_c in the direction perpendicular to the layers exceeds the distance between the levels), there also appears, because of the proximity effect, a peak near T_c on the temperature curve of the rate $T^{-1}_{1(2)}$ of nuclear relaxation on an N-layer. The S/N system in this case behaves practically like an anisotropic three-dimensional superconductor [the curve for $t=2T_c$ in Fig. 2(b)].

Thus, in two limiting cases, when the coupling of layers is very weak ($t\ll T_c$) and when it is strong ($t>T_c$), the behavior of the rate of nuclear relaxation on S-layers is ordinary. The values of t at which the peak in the $T^{-1}_{1(1)}$ vs T curve near T_c practically disappears lie within the $0.3T_c$ to $0.5T_c$ range. It is quite possible that this situation is realized in some high-T_c superconductors.

Because of the complexity of the excitation spectrum (8), the analytic temperature dependence of $T^{-1}_{1(\alpha)}$ can be obtained only for low temperatures ($T\ll T_c$). In this temperature range only the gapless branch $\omega_2(\mathbf{k},q)$ of the excitation spectrum (8) plays the leading role. Also, when $T\ll T_c$, the approximate expression (10) for ω_2 can be used. All this makes it possible to establish, when $T\ll T_c$, approximate expressions for $\operatorname{Im}\chi_{+-}(\alpha,\omega_e)$, which together with (12) determine the temperature dependence of $T^{-1}_{1(\alpha)}$:

$$T\frac{\operatorname{Im}\chi_{+-}(\alpha=1,\omega_e)}{(g\mu_B)^2\omega_e} = 7\frac{N^2(0)|w_1(0)|^4}{2\pi\Delta t^2}T^4 \quad \text{in the } S\text{-layer}, \quad (18)$$

$$T\frac{\operatorname{Im}\chi_{+-}(\alpha=2,\omega_e)}{(g\mu_B)^2\omega_e} = 16{,}9\frac{N^2(0)|w_2(0)|^4\Delta}{8\pi t^2}T^2 \quad \text{in the } N\text{-layer}, \quad (19)$$

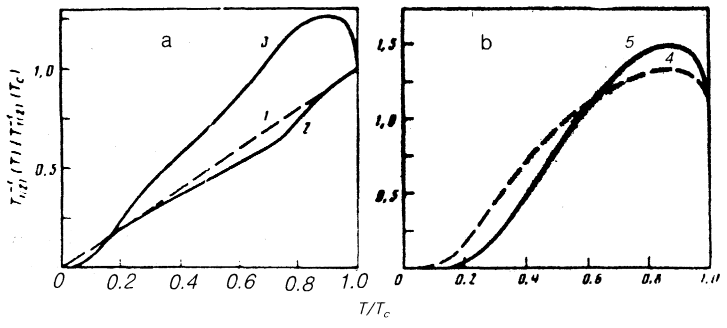

FIG. 2. $T^{-1}_{1(2)}(T)/T^{-1}_{1(2)}(T_c)$ as a function of temperature at the normal layer at small (a) and large (b) values of the overlap integral t: (1) $t=0.01\ T_c$, (2) $t=0.36\ T_c$, (3) $t=0.5\ T_c$, (4) $t=0.75\ T_c$, and (5) $t=2\ T_c$.

when $T \ll t^2/\Delta$ and

$$T\frac{\operatorname{Im}\chi_{+-}(\alpha=1,\omega_c)}{(g\mu_B)^2\omega_c}=\frac{2\pi N^2(0)\,|w_1(0)|^4 t^4}{\Delta^4}T \quad \text{in the } S\text{-layer}, \tag{20}$$

$$T\frac{\operatorname{Im}\chi_{+-}(\alpha=2,\omega_c)}{(g\mu_B)^2\omega_c}=\frac{\pi N^2(0)\,|w_2(0)|^4}{4}T \quad \text{in the } N\text{-layer}, \tag{21}$$

when $T_c \gg T \gg t^2/\Delta$. Here $N(0)$ is the density of states in the layer. As Eqs. (18)–(21) show, gapless excitations in an S/N system lead to a relaxation rate that depends on temperature for $T \ll T_c$ as a power function (in contrast to the standard result of the BCS theory). This behavior of T_1^{-1} as a function of T agrees with the experimental data (see Sec. 5).

4. THE KNIGHT SHIFT IN THE S/N SYSTEM

The hyperfine interaction of conduction electrons and a nucleus generates an additional magnetic field ΔH on the nucleus that is proportional to the static spin susceptibility χ_α of the conduction electrons in layer α (Ref. 31):

$$\frac{\Delta H}{H}=\frac{8\pi}{3}\chi_\alpha |w_\alpha(0)|^2 n^{-1}, \tag{22}$$

where n is the electron number density. Thus, the Knight shift is directly linked with the temperature average of the z-component of the electron spin operator on the nucleus. In layer α the average value of the z-component of the electron spin operator is given by the following expression:

$$\langle S_z(\mathbf{r}=0,\alpha)\rangle=\frac{|w_\alpha(0)|^2}{2(N\Omega)^{1/2}}T\sum_{\mathbf{k}q\omega}[G_{\alpha\alpha\uparrow\uparrow}(\mathbf{k}q\omega)-G_{\alpha\alpha\downarrow\downarrow}(\mathbf{k}q\omega)]. \tag{23}$$

Using Poisson's summation formula

$$T\sum_\omega G_{\alpha\alpha\uparrow\uparrow}(\mathbf{k},q,\omega)=-\frac{1}{2\pi}\lim_{u\to+0}\oint_C\frac{G_{\alpha\alpha\uparrow\uparrow}(\mathbf{k},q,z)e^{iuz}}{e^{iz/T}+1}dz, \tag{24}$$

where contour C encompasses the zeros of the denominator but not the poles of the function $G_{\alpha\alpha\uparrow\uparrow}(\mathbf{k},q,z)$ in the complex z plane, we can easily perform the summation over the Matsubara frequencies in (23).

As noted in Sec. 2, there is a gapless branch in the excitation spectrum of a layered S/N system with overlap integrals that are the same for all pairs of layers. This must lead to a discrepancy between the actual temperature dependence of the Knight shift and the one predicted by the BCS theory, which manifests itself, however, only at temperatures much lower than T_c. In our model the ratio of the Knight shift in the superconducting phase, K_S, to that in the normal phase, K_N, depends on the temperature (for $T \ll T_c$) as a power function. As does the ratio of the relaxation rates in the S- and N-states, the temperature dependence of K_S/K_N changes at temperatures of the order of t^2/Δ. Calculations show that for $T \ll t^2/\Delta$ and $t \ll T_c$,

$$\frac{K_S(\alpha=1)}{K_N}=1{,}72\frac{T^{3/2}}{\pi t(2\Delta)^{1/2}} \tag{25}$$

in the S-layer and

$$\frac{K_S(\alpha=2)}{K_N}=3{,}98\frac{(2T\Delta)^{1/2}}{4\pi t}. \tag{26}$$

in the N-layer; in the opposite limiting case where $T_c \gg T \gg t^2/\Delta$,

$$\frac{K_S(\alpha=1)}{K_N}=\frac{2t^2}{\Delta^2} \tag{27}$$

in the S-layer and

$$\frac{K_S(\alpha=2)}{K_N}=1. \tag{28}$$

in the N-layer.

At higher temperatures $[T > T_c/\ln(T_c/t)]$ the temperature dependence of K_S/K_N is close to the ordinary result of the BCS theory.[33] At sufficiently small values of parameter t/Δ the discrepancy between the value of K_S/K_N at the S-layer and the standard result manifests itself only when the contribution of conduction electrons to the Knight shift is practically nil.

At present there is no clarity concerning the experimentally determined values of K_S/K_N: some researchers (see, e.g., Ref. 34) report observations of power dependences of K_S/K_N on temperature for $T \ll T_c$, while other researchers[9] obtained K vs T dependences closer to those predicted by the BCS theory. It must be noted in this connection that in certain conditions the temperature dependences of K obtained within the framework of the S/N model may not obey a power law at low temperatures. As shown in Ref. 14, impurities, which are always present in samples, mix the trajectories of electrons moving in S- and N-layers and, therefore, restore the gap in the excitation spectrum. In this case, for $T \ll T_c$ there should be no power dependences in the Knight shift, but because of the proximity of N- and S-layers the peak in the nuclear relaxation rate near T_c is still suppressed.

5. DISCUSSION

In no experiment in high-T_c superconductors known to us has a peak on the T_1^{-1} vs T curve near T_c been observed. This allows us to conclude, at least in principle, that there is no true gap in the excitation spectrum, which may be the case in nontrivial (d) pairing (see, e.g., Refs. 7 and 8). At the same time, the gapless nature of the excitation spectrum can appear in the model with s-pairing, too. Such a possibility has been discussed in the present work. In our model the gapless branch of the excitation spectrum is related to the group of electrons moving along the normal layers. As shown above, in a layered S/N model the effect of proximity of the N- and S-layers effectively suppresses the peak in the T_1^{-1} vs T curve near T_c. Below we compare the main results obtained within the framework of the S/N model with the experimental NMR data on high-T_c superconductors.

In our model the rates of nuclear relaxation on N- and S-layers depend on temperature differently. If the coupling of neighboring layers is sufficiently weak, the T_1^{-1} vs T dependence for N-layers behaves in the usual Korringa manner near T_c. In 1-2-3 and 1-2-4 compounds the Cu–O planes act as S-layers, and the Cu–O chains possibly act as N-layers. This is corroborated, for one thing, by recent experiments[3,4] involving $YBa_2Cu_4O_{8.04}$ in which markedly different temperature dependencies of T_1^{-1} at copper sites Cu(1) (in chains) and Cu(2) (in planes) were registered. Moreover, in the T_1^{-1} vs T dependence for copper in chains the linear term is predominant, a property preserved down to the lowest temperatures possible. At the same time, the rate T_1^{-1} of relaxation on copper nuclei in Cu–O planes decreases with temperature much faster than in Cu–O chains, which suggests strong superconductivity in planes and much weaker superconductivity in chains. The same difference in the temperature dependences of T_1^{-1} at copper sites Cu(1) and Cu(2) in $YBa_2Cu_3O_7$ was registered in Refs. 35 and 36 and is related to the formation of two different superconducting gaps, on planes and on chains.

The gapless nature of the excitation spectrum leads to a power-law dependence of T_1^{-1} on temperature at low temperatures, instead of the activation-type dependence characteristic of the BCS theory. This agrees with the experimental results listed in Refs. 1–4. For instance, the authors of Ref. 2 discovered that the rate of nuclear relaxation at the copper sites Cu(2) in the $YBa_2Cu_3O_7$ in the entire temperature range from zero to T_c is described fairly well by the product $T\exp(T/T^*)$, where $T^*(H)$ is a characteristic temperature depending on the external field H. For $T \ll T_c$ the dependence transforms into a power law. In earlier papers (see, e.g., Ref. 37) temperature dependences of T_1^{-1} that did not agree with the formulas of the BCS theory at low temperatures were also reported.

At the same time, a number of experiments suggest (see, e.g., Ref. 38) that for the completely oxygen-saturated $YBa_2Cu_3O_7$ compound the T_1^{-1} vs T dependence follows the ordinary Korringa relation. This points to a metallic conduction in Cu–O planes and to the fact that the nuclear relaxation rate is basically determined by the ordinary contact interaction of a nucleus with s-electrons, which has been assumed in the present paper.

Thus, the crude model discussed here does, apparently, reflect some features of NMR in high-T_c superconductors, although it is based on simplified assumptions concerning the mechanisms of nuclear relaxation in high-T_c superconductors and is considered in the weak binding approximation.

The results of calculations of the nuclear relaxation rates in a model that in a certain sense is close to our model has briefly been discussed by Tachiki and Takahashi,[39] but they used, as they did in an earlier paper[19] on optical absorption, a far more cumbersome model in which the tight-binding approximation is employed to describe the motion not only along the z axis but between separate ions in the Cu–O planes. The drawback of their model is the large number of arbitrary parameters. Obtaining analytic results within the framework of the model would seem to be very difficult.

A somewhat different approach to describing NMR in high-T_c superconductors was developed in Refs. 6, 40, and 41, whose authors assume that antiferromagnetic fluctuations in Cu–O planes play the leading role in the relaxation of nuclear spins. The model[6,40,41] of an "almost antiferromagnetic Fermi liquid" provides a good description of nuclear relaxation in the oxygen-deficient $YBa_2Cu_3O_{6.63}$ compound,[22] in which the T_1^{-1} vs T dependence behaves in no special way near T_c not only at Cu(1) sites but also at Cu(2) sites in planes. At the same time, in completely oxygen-saturated 1-2-3 compounds the rate of nuclear relaxation at Cu(2) sites sharply drops directly below T_c, which unambiguously points to a transition to superconductivity. For this reason, nuclear relaxation in high-T_c can hardly be described using the one concept of an "almost antiferromagnetic Fermi liquid"; one must allow for the ordinary relaxation mechanism. As Monien and Pines have shown by their calculations,[40] the effect of antiferromagnetic correlations may considerably lower the peak in the T_1^{-1} vs T dependence near T_c, but allowing only for antiferromagnetic fluctuations cannot, apparently, explain the nature of the temperature dependence of T_1^{-1} at Cu(1) sites in chains (for a discussion of the model suggested in Ref. 6 for the case of $YBa_2Cu_3O_7$ see Ref. 2).

Thus, the question of the mechanisms of nuclear relaxation in high-T_c superconductors has still to be answered. Our paper is devoted to nuclear relaxation in the S/N model with weak coupling of the layers. We argue that such a model can indeed provide a good description of NMR experiments involving high-T_c superconductors.

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APPENDIX

Let us write the expression for S_+ explicitly, allowing for the small overlap of the wave functions of electrons localized at neighboring layers. Since the action of operator S_+ leads to no electron transitions between neighboring layers, the spin density on layer $\alpha = 1$ in the mth unit cell can be written as

$$S_+(\mathbf{r}, m, \alpha=1, t) = \frac{1}{\Omega N} \sum_{\mathbf{k},q,\mathbf{p},Q} [\bar{c}_{\mathbf{k}+\mathbf{p},q+Q,1\uparrow}(t) c_{\mathbf{k}q1\downarrow}(t) |w_1(0)|^2$$

$$+\bar{c}_{\mathbf{k}+\mathbf{p},q+Q,2\uparrow}(t) c_{\mathbf{k}q2\downarrow}(t) |w_2(d)|^2 2\cos(Qd)] \exp(-i\mathbf{p}\mathbf{r} - 2im\,dQ). \tag{29}$$

The second term on the right-hand side is connected with electrons localized at neighboring layers and is $(|w_2(d)|^2/|w_1(0)|^2)^{-1}$-fold smaller than the first term. Since the characteristic energy for the electron movement in a layer is the Fermi energy E_F, the following order-of-magnitude estimate holds true: $|w_2(d)|^2/|w_1(0)|^2 \approx t/E_F$. The characteristic energies in our problem are T, T_c, and the overlap integral t, which is much smaller than E_F. For this reason the second term in (29) can be discarded: this is possible because the contact interaction is actually determined by the electron wave function at the nucleus.

Since the retarded Green function (13) is given by the temperature average of two spin operators taken at the same layers, all the electron Green functions in the polarization operator (14) are diagonal in the layer indices α and β, and we arrive at Eqs. (16) and (17).

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