Pressure Dependence of Exchange Parameters and Neel Temperature in La_2CuO_4

ANATOLII YA. FISHMAN* AND VALENTIN YA. MITROFANOV
Institute of Metallurgy, Ural Division, Russian Academy of Sciences, 101 Amundsen Street, Ekaterinburg 620016, Russia

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Abstract. Microscopic mechanisms responsible for the observed pressure dependencies of the Neel temperature T_N and parameters of isotropic and anisotropic exchange interaction in the orthorhombic antiferromagnet La_2CuO_4 are investigated. Within the framework of the Anderson microscopic theory of superexchange interaction, the expressions establishing interrelation between parameters of isotropic and anisotropic (both symmetric and antisymmetric) exchange interactions and by the structural parameters describing the Cu–O–Cu bonding angle and the Cu–O bond length in La_2CuO_4 are obtained. Experimentally determined pressure dependencies of structural parameters by H. Takahashi et al., allow one to present pressure dependencies of exchange parameters and T_N in an apparent form.

INTRODUCTION

The measurements of superconducting and normal state magnetic, spectral properties of cuprates under hydrostatic and uniaxial pressure can give sufficient information about a possible pairing interaction for high-T_c-superconductivity.[1] In particular, these studies allow testing the viability of spin-fluctuation theories. High-pressure spectroscopic studies on antiferromagnetic La_2CuO_4 [2,3] are essential for understanding the mechanisms responsible for the remarkable pressure dependence of the Neel temperature as well as for explaining the qualitative details and trends of the magnetic interactions among different Cu–O materials.

La_2CuO_4 exhibits an antiferromagnetic ordering bellow the Neel temperature $T_N = 320$ K, which is low with respect to the intralayer exchange parameter J and is determined by magnetic anisotropy and/or interlayer exchange coupling. The orthorhombic antiferromagnet $La_2CuO_{4+\delta}$ is one of the most suitable objects for understanding the relationship between magnetic and structural features. It is connected to a strong dependence of intra- and interlayer exchange interactions on structural parameters in La_2CuO_4: the Cu–O–Cu bond angle (θ), the Cu–O bond length (r), octahedral tilt angle (ψ), and rhombic distortion (σ). It is known[4] that hydrostatic pressure has a strong influence on the structural properties of La_2CuO_4. Convenient structure features that correlate with pressure are the CuO_6 octahedral tilt angle and the Cu–O bond length, which decrease with increasing pressure in the orthorhombic phase. As a result the

*Author to whom correspondence should be addressed.
E-mail: fishman@uran.ru

application of pressure also alters the Neel temperature T_N [3] and exchange parameters, in particular, the intraplane exchange parameter J [2] in La_2CuO_4.

In this study, the microscopic mechanisms responsible for the observable pressure dependencies of T_N and the intralayer exchange parameters in La_2CuO_4 are investigated. Within the framework of Anderson theory of the superexchange[5] and the advanced theory of anisotropic exchange interactions,[6] the expressions describing obvious dependence of the intralayer exchange parameters and T_N on the structural parameters are obtained. The proposed theoretical dependencies and existing experimental data on pressure dependencies of structural parameters in La_2CuO_4 [4] explain, qualitatively and quantitatively, pressure dependencies of magnetic parameters and the T_N observed experimentally.

THEORETICAL MODEL

Generally the temperature of magnetic ordering T_N is a function of six parameters[3] describing the intralayer and interlayer isotropic and anisotropic exchange interactions. In the present report a baric dependence of T_N will be analyzed within the framework of the simple model in which T_N is determined by the intraplane magnetic anisotropy.[7] In this case explicit dependencies of the intralayer exchange parameters on structural features can be obtained. The corresponding Hamiltonian describing the intralayer exchange interactions in La_2CuO_4 has the following form:

$$H = \sum_{\langle i,k\rangle} \left(J\left(S_i S_k\right) + J_a S_{iz} S_{kz} + D\left[S_i S_k\right]_x \right) \qquad (1)$$

where $<i,k>$ stands for pairs of nearest-neighbors counted once, and the parameters J_a and D describe symmetric and antisymmetric anisotropic exchange interactions, respectively.

If the bond angle θ is reduced from 180° by φ and only the σ-bonding overlap is employed, the corresponding dependence of the intralayer exchange J on the structural parameters r and θ in La_2CuO_4 becomes[8–10]

$$J = J_0 r^{-n} \cos^2\theta \qquad (2)$$

where J_0 is the constant, $\theta = 180° - 2\varphi$, and φ is the angle between the directions Cu–O and Cu–Cu in a basic layer. A variety of experiments in insulating compounds, conventional metal-oxide and metal-halide magnets,[10] have shown that the exchange parameter J depends on the metal–ligand bond length r, varying as $J \cong 1/r^2$ with $10 \le n \le 12$.

Further, the microscopic expressions for exchange parameters J_a and D will be deduced in the framework of Anderson theory of the superexchange interaction[5] and advanced theory of anisotropic exchange,[6] and then their obvious dependencies on the structural parameters in La_2CuO_4 are determined. Anisotropic exchange J_a is responsible for the "easy-plane" anisotropy, which confines the Cu moments in the CuO_2 layer. The magnitude of J_a for La_2CuO_4 has been estimated experimentally to be –0.23 K.[11] In insulating magnets the magnitude of the anisotropic exchange

$$J_a = J_{md} + J_{pd}$$

is determined by a superposition of the magnetic dipolar interaction (J_{md}) and pseudodipolar exchange (J_{pd}).[12] The pseudodipolar exchange J_{pd} arises from the combined effect of the isotropic exchange H_{ex} and the spin-orbit coupling $V_{so} = \lambda(\mathbf{LS})$. If the two copper ions have the ground o_i, o_k and excited e_i, e_k states, the interaction J_{pd} comes from the third-order perturbation process with terms that are linear in the exchange interaction of ions i and k and quadratic in the spin-orbit coupling of ions i and k[6,12]

$$\frac{\left\langle o_i o_k \right| \lambda\left(\mathbf{L}_i\mathbf{S}_i\right) \left| e_i o_k \right\rangle \left\langle e_i o_k \right| H_{ex} \left| e_i o_k \right\rangle \left\langle e_i o_k \right| \lambda\left(\mathbf{L}_i\mathbf{S}_i\right) \left| o_i o_k \right\rangle}{\left(E_{e_i} - E_{o_i}\right)^2}$$

$$\frac{\left\langle o_i o_k \right| \lambda\left(\mathbf{L}_i\mathbf{S}_i\right) \left| e_i o_k \right\rangle \left\langle e_i o_k \right| \lambda\left(\mathbf{L}_k\mathbf{S}_k\right) \left| e_i e_k \right\rangle \left\langle e_i e_k \right| H_{ex} \left| o_i o_k \right\rangle}{\left(E_{e_i} - E_{o_i}\right)\left(E_{e_i} + E_{e_k} - E_{o_i} - E_{o_k}\right)} \qquad (3)$$

plus terms that are Hermitian conjugate to the above terms and in which ion i is interchanged with ion k. Generally the numerical values of anisotropy parameters J_a depend on four distinctly different perturbation theory contributions I–IV.[6] Historically a situation emerged[12] in which type-I contribution, corresponding to the first term in eq 3, was used without rigorous substantiation for any ions and spin values. At the same time the spin-independent exchange interaction H_{ex} is not considered in standard approaches to the analysis of J_a (see, e.g., refs 13, 14). Our consideration has shown that for the La_2CuO_4, only type-I and type-II processes, presented in eq 3, are active.

The term in H_{ex}, which describes the isotropic exchange interaction between the ground- and excited-states of a pair, can be written as[15]

$$H_{ex} = \sum_{\alpha,\alpha'} \sum_{\beta,\beta'} \left[(1/4) n_i(\alpha\alpha') n_k(\beta\beta') + \left(\mathbf{s}_i(\alpha\alpha')\mathbf{s}_k(\beta\beta')\right) \right] j_{\alpha\alpha',\beta\beta'} \qquad (4)$$

using the operators and notations introduced in ref 15. Here α, α', β, β' are the symbols of summation over the d-orbitals. The expression for $j_{\alpha\alpha',\beta\beta'}$ contains two main competing contributions—antiferromagnetic "kinetic" exchange and ferromagnetic "potential" or "direct" exchange.[4] We can easily obtain the following expres-

$$J_{pd} = \frac{1}{4}\left\{\left(\frac{\Delta g_z}{g}\right)^2\left[j_{\nu\zeta} - j_{\nu\nu,\zeta\zeta}\right] - 2\left(\frac{\Delta g_x}{g}\right)^2\left[j_{\nu\xi} - j_{\nu\nu,\xi\xi}\right] - 2\left(\frac{\Delta g_y}{g}\right)^2\left[j_{\nu\eta} - j_{\nu\nu,\eta\eta}\right]\right\}$$

$$\frac{\Delta g_i}{g} = -\lambda\sum_e \left|\langle e|L_i|o\rangle\right|^2 (E_e - E_o)^{-1} \qquad (5)$$

sion for the exchange-relativistic contribution to the parameter J_{pd}

Here $j_{\alpha\beta} \equiv j_{\alpha\beta,\alpha\beta}$, Δg_i ($i = x, y, z$) is the spin-orbit correction to the g-factor ($g = 2$). If we discard the small rotations of $[CuO]_6$ octahedron, then $\nu \propto x^2 - y^2$, $\xi \propto yz$, $\eta \propto xz$, $\zeta \propto xy$. It is easy to show that in the considered case ($\theta \cong 174^o$ and $J = 1490$ K)[16] the contribution of the "kinetic" exchange to $j_{\alpha\alpha',\beta\beta'}$ in eq 5 is proportional to $J(\lambda_\pi/\lambda_\sigma)^2\sin^2\theta$ where λ_π and λ_σ are the covalence parameters appropriate to the π and σ bonding, respectively. The spin-orbit corrections to the "direct" exchange, in disagreement with ref 13 as well as to the above-mentioned "kinetic" exchange, do not contribute to J_{pd} in La_2CuO_4 since $j_{\alpha\beta} \approx j_{\alpha\alpha,\beta\beta}$ in eq 5. In order to clarify the origin of anisotropy J_{pd} in La_2CuO_4, we consider the contribution to the isotropic exchange, $j_{\alpha\beta}$, which comes from a third-order perturbation process and takes into account the transfer of an electron from the closed orbital of one copper ion into a half-filled orbital of the neighboring copper ion.[5] If we consider a pair of Cu ions along the y direction in the CuO_2 layer, then the magnitude of the effect is equal to

$$j^{(III)}_{\nu\zeta} = j^{(III)}_{\nu\xi} = -2I\left(b^2_\sigma + b^2_\pi\right)U^{-2}$$
$$j^{(III)}_{\nu\eta} = -2b^2_\sigma IU^{-2} \qquad (6)$$

where I is the intra-atomic exchange integral, b_σ and b_π are the hopping integrals via p_σ and p_π ligand orbitals,[5] and U is the energy required to put two electrons on the same ion (the Hubbard energy). Assuming the following relations $b^2_\sigma = \chi b^2_\pi$, $\Delta g_x = \Delta g_y$, we obtained

$$j_{pd} = \frac{JI}{8U}\left\{-\left(\Delta g_z/g\right)^2\left(1 + 1/\chi\right) + 2\left(\Delta g_z/g\right)^2\left(2 + 1/\chi\right)\right\} \qquad (7)$$

Using $\Delta g_z \cong 0.3$, $\Delta g_x \cong 0.1$, $J = 1500$ K, $I/U \cong 0.1$, $\chi = 3$, we obtain $J_{pd} \cong -0.34$ K.

In the simplest case, when the g-factors g_i and g_k are isotropic and equal in magnitude, the expression for J_{md} reduces to $J_{md} = 3g\beta^2/2R^2$, where β is the Bohr magneton and $R = 2r\cos\varphi$ is the Cu–Cu path length. The magnetic dipolar interaction contributes to the anisotropy by 0.07 K. Thus we obtain $J_a \cong -0.27$ K. This value is compatible with the corresponding data for La_2CuO_4.[11]

The antisymmetric exchange interaction D causes not only an output of Cu moments from a basic layer on an angle $\sim D/2J \cong 0.17^o$, but also the presence of a weak orthorhombic anisotropy $\sim D^2/J < J_a$. The dominant contribution to D arises from a second-order perturbation process[6b,17] with terms that are linear in the exchange interaction (H_{ex}) and the spin-orbit coupling (V_{so}) for ions i and k. The corresponding microscopic expression for parameter D can be written as

$$|D| = \sqrt{2}J\sin(2\varphi)(\Delta g_x/g)(\lambda_\pi/\lambda_\sigma) \qquad (8)$$

Taking $\lambda_\pi/\lambda_\sigma = 0.7$, $\varphi \cong 3°$, $J \cong 1500$ K, we can obtain $|D| \cong 7.7$ K, and this value is in agreement with the experimental data $|D| = (6.4 \pm 0.7)$ K.[18] Thus, the proposed microscopic theory of anisotropic exchange interactions in the orthorhombic antiferromagnet La_2CuO_4 adequately describes the experimental results.

Now we can obtain expressions for the exchange parameters J, J_a, D, which are obviously dependent on the structural parameters r and φ. We shall preliminarily make the following approximation concerning the magnitudes Δg_i. The anisotropy of g-factors results from the fact that the energy intervals between the ground state and the excited states xy, xz, yz of copper ion in La_2CuO_4 differ due to the tetragonal and orthorhombic components of the crystal field. We shall turn to the cubic symmetry and remove the deviations due to the tetragonal crystal field and orthorhombicity. Thus we can write $\Delta g_i \propto 1/\Delta E$, where $\Delta E = 10\,Dq$ is the splitting of d state in the cubic crystal field. Further, we shall take into account the Anderson approximation for ΔE: $\Delta E \propto t$,[5] where $t \propto r^{-n/2}$ is the hopping integral in the theory of superexchange. Thus, the following ratios can be written for the Δg_i-factors

$$\Delta g_z/4g = \Delta g_x/g = \Delta g_y/g = Ar^{n/2} \qquad (9)$$

where A is a constant.

The expressions for the exchange parameters in eq 1 as a function of structural parameters r and φ ($\varphi << \pi/2$) have the following form:

$$J = J_0(1 - 4\varphi^2)r^{-n}$$
$$J_a = (3\beta^2/4)r^{-3}(1 + 6\varphi^2) - (J_0IA^2/4U)(1 - 4\varphi^2)(6+7/\chi)$$
$$|D| = d\varphi\, r^{-n/2},\ d = 2\sqrt{2}J_0A\lambda_\pi/\lambda_\sigma \qquad (10)$$

where we have omitted the term proportional to φ^3 in the expression for D.

DISCUSSION

The most accurate experimental data on pressure dependence of structural parameters in La_2CuO_4 at $T \sim T_N$ are described by the following expressions[4]

$$\varphi = \varphi_o(1 - P/P_{crit})^{1/2},\ r = r_o + \rho P \qquad (11)$$

where $\varphi_o = 3.13°$, $r_o = 1.905$Å, $\rho = 0.0065$Å/GPa, and P_{crit} is the critical pressure of orthorhombic–tetragonal phase transition at $T \sim 300$ K ($P_{crit} = 4.365$ GPa). The value of critical pressure P_{crit} has been determined from the data on pressure dependence of the orthorhombic distortion $\sigma = \sigma(P)$.[4]

The correlation between the exchange and structural parameters in La_2CuO_4 obtained above allows one to present the pressure dependence of exchange parameters ($P < P_{crit}$) in the following form:

$$\begin{aligned} &J(P) = J^0\left\{1 + (P/P_{crit})(4\varphi_0^2) - nP_{crit}/P_0\right\},\quad P_0 = r_0/\rho \\ &J_a(P) = J^0_{md}\left\{1 - 3(P/P_{crit})\left[2\varphi_0^2\left(1 - (2/3)J^0_{pd}/J^0_{md}\right) - P_{crit}/P_0\right]\right\} \\ &|D(P)| = |D^0|\left\{1 - 0.5(P/P_{crit})(1 - nP_{crit}/P_0)\right\} \end{aligned} \qquad (12)$$

where the upper index 0 in eq 12 means the magnitude of exchange parameters at the normal atmospheric pressure. It is easy to see that the increase of the intralayer exchange J with increase in pressure is connected, mainly, with the reduction of the Cu–O bond length r with pressure. Pressure dependence of J in La_2CuO_4 has been directly measured using high-pressure Raman scattering measurements.[2] A fit to the data for pressures $P < 6$ GPa gives $J(P) = 1390 + 19.3P$ (K).

In addition, it has been shown that at $P > 2$ GPa the intralayer exchange J varies as $J \propto r^{-n}$ with $n = 6.4 \pm 0.8$ and r, taken from the high-pressure X-ray measurements.[19] The theory predicts strong pressure dependence of exchange parameter J at $n = 7$ ($dJ/dP \cong 36$ K/GPa), which contradicts the data in ref 2. One of the apparent reasons of a discrepancy between the theory (eq 12) and experiment[2] for the baric coefficient dJ/dP is that the coefficient ρ in ref 6 was determined at an essentially lower pressure than in ref 19. The reduced sensitivity of the superexchange interaction J to P in ref 2 at the highest pressures may arise from transformations of the crystal structure at room temperature as the pressure-dependent orthorhombic–tetragonal phase transition occurs at $P_{crit} = 4.3$ GPa.

The reason for a weak dependence of anisotropic exchange J_a on P is that the basic structural element of a layer represents a rigid enough square lattice from the Cu–O links.

Increasing pressure causes the tilt angle ψ of CuO_6 octahedra and correspondingly φ to decrease, resulting in an essential pressure dependence of antisymmetric exchange D, as follows from eq 12.

Meaning an establishment of qualitative dependence of the Neel temperature T_N on pressure, we shall assume similarly[7] that the stability of the long-range antiferromagnetic ordering in La_2CuO_4 is determined by the intralayer anisotropy. Then expressions for T_N [7] and $T_N(P)$ at $P < P_{crit}$ can be written as

$$\begin{aligned} &T_N = 2J[\ln(J/D)]^{-1} \\ &T_N(P) = T^0_N\left\{1 - (P/P_{crit})\left[nP_{crit}/P_0 + 0.25(T^0_N/J)(1 - nP_{crit/P})\right]\right\} \end{aligned} \qquad (13)$$

As one would expect, estimated value $T_N = 533$ K appreciably exceeds experimental value $T_N = 325$ K. Assuming $|D| = 6$ K, $J = 1490$ K, $T^0_N = 533$ K, we obtained the positive baric coefficient of magnetic ordering temperature dT_N/dP at $n > 7$. As follows from eq 13, we can expect a rather weak increase of T_N with increase of pressure. A satisfactory coincidence with the experimental data for La_2CuO_4 [3] can be obtained at sufficiently large values of n ($n > 10$).

CONCLUSION

In summary, we have established interrelation between the intraplane exchange interactions and structural features in La_2CuO_4. We have shown that available experimental pressure dependencies of structural parameters[4] allow one to predict a strong pressure dependence of the superexchange interaction J and antisymmetric exchange D in La_2CuO_4. It is shown that change of the magnitude of the intralayer isotropic exchange J on pressure allows one, not only to compensate reduction of a Neel temperature due to reduction of crystal orthorhombicity, but also to lead to the observable resulting growth of the Neel temperature. The research carried out does not support a conclusion made in ref 20 about an unexpectedly large influence of the interlayer symmetric anisotropic exchange interaction on T_N.

Systematic inelastic neutron scattering measurements of the superexchange interaction J in undoped monolayer cuprates R_2CuO_4 (R = La, Nd, Pr)[21] show that J does not exhibit a monotonic dependence versus the Cu–O bond length r, in contrast to what could be expected from eq 2. A reasonable theoretical model of the superexchange interaction should take into account the change in crystal structure and the values of the effective magnetic parameters in eq 1 under pressure, based on the microscopic models of the long-range exchange interactions. In particular, a general form for the exchange interaction[8–10a] can be adopted for the interpretation of pressure-induced effects,

$$J(r,\theta) = f(r) \cdot h(\theta)$$
$$f(r) = Q(r) \cdot \exp(-ar + b/r)$$
$$h(\theta) = u + \nu \cdot \cos^2\theta \quad (14)$$

where $Q(r)$ is a polynomial in r.

In a wide enough class of magnets the exchange of the higher orders on spins can be essential. Use of the new high-resolution neutron scattering technique to study magnetic excitations has allowed discovery that interactions beyond those coupling nearest-neighbor Cu^{2+} ions are needed to account for the magnetism of $LaCuO_4$.[22] The exchange constants describing cyclic or ring exchange are proportional to $b^0_\sigma/U^3 \propto r^{-2n}$. Thus, the account of these interactions and random field treatment of the Dzyaloshinskii–Moriya interaction in $LaCuO_4$ [23] can essentially facilitate interpretation of the baric dependence of the Neel temperature.

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