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ON THE THEORY OF SUPERCONDUCTIVITY IN HIGH-TEMPERATURE SUPERCONDUCTORS

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Experimental approaches to estimating the parameter of resonance coupling between spin fluctuations and longitudinal phonons in superconducting copper oxides have been considered. Coupling parameter estimates were obtained based on bulk modulus λ measurements. The result allows us to assert that the critical temperature of high-temperature superconductors can be increased to room temperature.

In our recent works [1, 2], we demonstrated the possibility, in principle, of synthesizing new high-temperature superconductors with critical temperature T_c of the order of room temperature. However, this possibility still remains unrealized because of limitations inherent in the preparation of high-temperature systems. This, in the first place, concerns the exchange correlation length r [1, 2] involved in the expression for parameter ζ of spin-phonon coupling in a high-temperature superconducting phase [1, 2],

$$\zeta = \frac{g\hbar k_c}{\sqrt{J_0 s M_i}}, \tag{1}$$

where $g = U_{i-e}/J_0$, U_{i-e} is the electron-ion potential, J_0 is the exchange interaction potential in the system of electric current carriers in the high-temperature superconducting phase, $k_c = 2\pi/r_c$ is the reciprocal correlation length, M is the reduced mass of ions in the unit cell, and $s = 1/2$ is the spin of the electron. A comparison of the calculation and the experimental data [3] shows that the exchange correlation length r_e in $La_{2-x}Sr_xCuO_4$- and $YBa_2Cu_3O_{6+\delta}$-type systems, where $\delta = 0.98$, is limited to $r_e \cong 10$ Å by the period of the antiferromagnetic unit cell $l_s = 2\pi/k_s$, where k_s is the length of the antiferromagnetic structure vector in a dielectric (antiferromagnetic) phase. Another important parameter which determines the effect of resonant amplification of electron-phonon coupling (λ_{e-ph} [2, 3]) is the interelectronic exchange interaction potential J_0.

Unfortunately, there exist no model that can be used for reliably calculating J_0 from first principles because of the extreme complexity of high-temperature superconducting compounds. Neither can the results of experimental estimates of J_0 based on magnetic correlation length measurements in the system of low-energy spin fluctuations by neutron diffraction techniques [4] be considered convincing, because single crystals of the required dimensions ($V = 1$ cm^3) have not been synthesized as yet. In this work, we therefore suggest a fairly simple procedure for estimating the exchange coupling parameter from the results of bulk modulus λ measurements both in the high-temperature superconducting and in nonsuperconducting antiferromagnetic phases. For this purpose, the dependence of J_0 on λ should be determined.

Let us consider the effective magnetoelastic Hamiltonian of a high-temperature superconducting phase [1–3]

$$\mathcal{H}^{\text{eff}}_{m-u} = \int dx \left\{ \frac{1}{2k_c^2} J_0 s (A_{i\nu})^2 - \frac{1}{2} J_0 s \left(1 - \frac{k_s^2}{k_c^2}\delta_{2i}\right)\Omega_i + \frac{1}{2}(\lambda_0 u_{ll}^2 + 2\varkappa_0 u_{lm}^2) \right\}, \tag{2}$$

where $A_{i\nu} = \dfrac{\partial \Omega_i}{\partial x_\nu}$, Ω_i is the quasiequilibrium (slowly varying with time) magnetization of both paramagnetic ($i = 1$) and antiferromagnetic ($i = 2$) phases; λ_0 and $\varkappa_0$ are the bulk and shear moduli, respectively, of the antiferromagnetic phase; and u_{lm} are the components of the elastic strain tensor.

The total bulk modulus in the high-temperature superconducting phase is found from the condition

$$\lambda = \frac{\delta^2 \mathcal{H}^{\text{eff}}_{m-u}}{\delta u_{ll}^2}. \tag{3}$$

To determine λ from (3), (2) should be expanded in terms of diagonal components u_{ll} of the strain tensor. Actually, we will have to expand the components of magnetization gradient tensor $A_{i\nu}(x)$. Indeed,

$$A_{i\nu}(x) = A_{i\nu}(x_0) + \frac{\partial^2 \Omega_i}{\partial x_{\nu 0} \partial x_{\nu' 0}} u_{\nu'} + A_{i\nu'}(x_0) u_{\nu'\nu}. \tag{4}$$

Substituting (4) into (2) and calculating variational derivative (3), we obtain the bulk modulus of the superconducting phase in the form

$$\lambda = \lambda_0 + \frac{1}{k_c^2} J_0 s (A_{i\nu})^2, \tag{5}$$

whence

$$J_0 s = \lim_{\substack{x_0 \to r_c \\ k_c \to k_s + 0}} \frac{\lambda - \lambda_0}{(A_{i\nu})^2 / k_c^2}. \tag{6}$$

The final expression for the exchange coupling parameter can be obtained with the use of the expressions for $\Omega_1(x)$ and $\Omega_2(x)$ which describe magnetization changes in the space of slow (low-energy) spin fluctuations

$$\begin{aligned} \Omega_1 &= \Omega_{10}^{(1)} \cos(k_c x) + \Omega_{10}^{(2)} \sin(k_c x), \\ \Omega_2 &= \Omega_{20}^{(1)} \cos(\widetilde{k}_c x) + \Omega_{20}^{(2)} \sin(\widetilde{k}_c x), \end{aligned} \tag{7}$$

where $\widetilde{k}_c = \sqrt{1 - k_s^2/k_c^2}$. This yields

$$J_0 s = \frac{\lambda - \lambda_0}{(\Omega_{10}^{(2)})^2}. \tag{8}$$

Equation (8) can therefore be used to estimate the exchange coupling parameter in the electronic system when a substance undergoes the transition from the antiferromagnetic to the superconducting phase, i.e., when the antiferromagnetic long-range order is fully suppressed. In (8), $|\Omega_{10}^{(2)}| \cong 1/v_0$, where v_0 is the minimum volume per one site of the magnetic unit cell [1]. The bulk modulus value determined experimentally in [5] is $\lambda = 1.21 \times 10^{12}$ erg/cm^3.

It is a much more difficult task to determine the bulk modulus of the antiferromagnetic phase (λ_0). At present, the required experimental data are lacking, which made us use the classical "jelly" model to estimate λ_0 [6]. According to this model, the expression for the bulk modulus can be written as

$$\lambda_0 = \frac{3e^2}{40\pi r_0^4}, \tag{9}$$

where r_0 is the mean ionic radius in the covalently bound Cu–O system responsible for the origination of the antiferromagnetic long-range order. With r_0 from [4], $r_0 = 0.84$ Å, we obtain $\lambda_0 = 1.12 \times 10^{12}$ erg/cm^3. Using $v_0 \lesssim 10^{-23}$ cm^3 in (8) yields $J_0 s \cong 10^{-13}$ erg for the parameter of interelectronic exchange coupling.

We can now estimate the spin-phonon coupling parameter ζ which determines the exchange amplification of the effective electron-phonon coupling in high-temperature superconducting phase. Using the tables given in [4], we find that $\zeta = 2$. According to [2], this initial ζ value is sufficient for increasing T_c to a near-room temperature through increasing ζ by several units. The key problem is to decrease the exchange correlation length r_c. This can be done by decreasing the volume of the magnetic unit cell. It would, therefore, make sense to synthesize compounds with cubic or tetragonal (orthorhombic) symmetry containing a minimal number of magnetic planes. The Neel temperature T_N of the antiferromagnetic phase should be as high as possible which provides for, after doping in order to destroy the antiferromagnetic long-range order, the maximum density of electric current carriers and the minimum possible exchange correlation length in the electronic system.

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