Relationship between elastic and superconducting properties of high-T_c superconductors

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By incorporating the dependence of the elastic properties of the high-T_c superconductors on the order parameter, one can explain the deviations from the BCS theory which are observed in the high-T_c superconductors in terms of the jump in the specific heat, the isotope effect, and the ratio of the superconducting gap to the superconducting transition temperature.

Experiments on the temperature dependence of the bulk modulus below the superconducting transition temperature in $La_{1.85}Sr_{0.15}CuO_4$ (Ref. 1) and $YBa_2Cu_3O_7$ (Refs. 2–4) have revealed that the stiffness increases unusually rapidly with decreasing temperature. Bishop *et al.*[2] suggested that the temperature dependence observed for the sound velocity was proportional to Δ^2, the square of the superconducting gap width. We should point out that the same dependence had been suggested previously.[5] This dependence can also be derived from the ordinary BCS theory, although the quantitative agreement with experiment is not always perfect. Let us assume that the effect observed in Refs. 1–4 is an established fact. Let us also use the expression

$$k = k_0 + k'\Delta^2 \tag{1}$$

for the bulk modulus, where for LaSrCuO we have[1] $k' = (6\text{–}10)\times 10^{36}\ \text{erg}^{-1}\cdot\text{cm}^{-3}$, while for YBaCuO we have[2-4] $k' = (2\text{–}3)\times 10^{36}\ \text{erg}^{-1}\cdot\text{cm}^{-3}$, where k_0 is the bulk modulus in the normal state.

Below we will show how expression (1) is manifested as changes in the equation describing the temperature dependence of the superconducting gap, in the gap width at absolute zero, in the superconducting transition temperature, in the jump in the specific heat upon the superconducting transition, and, finally, in the isotope effect.

The basic idea of the present letter is that experimental dependence (1) makes the phonon component of the free energy, F_{ph}, dependent on the superconducting gap Δ. In the model of corresponding Grüneisen states, this component $F_{ph} = \theta(\Delta) f[T/\theta(\Delta)]$, turns out to depend on Δ by virtue of the functional dependence $\theta(\Delta) = \theta + \theta'\Delta^2$ for the Debye temperature. We can thus write the approximate equation

$$F_{ph} = \theta f(T/\theta) + \Delta^2 \theta' \varphi(T/\theta), \tag{2}$$

where $\varphi(x) = f(x) - xf'(x)$ and $f(0) > 0$.

The approach which we are taking here has an analog in the approach taken in the self-consistent fluctuation-phonon theory of the magnetism of metals, where the analog of (1) and (2) is a similar dependence of the elastic modulus and of the phonon free energy on the magnetic order parameter.[7]

For the electron component of the free energy of a superconductor we use the expression[8]

$$F_e = \nu V \int_0^{\kappa\theta} d\epsilon \{ \frac{\Delta^2}{2\epsilon} \tanh \frac{\epsilon}{2\kappa T_0} - \kappa T \ln \frac{1 + \cosh(\sqrt{\epsilon^2 + \Delta^2}/\kappa T)}{1 + \cosh(\epsilon/\kappa T)} \}, \tag{3}$$

where V is the volume, ν is the density of states at the Fermi level, κ is the Boltzmann constant, and T_0 would be the superconducting transition temperature if we were to ignore the phonon component. Expressions (2) and (3) lead to the following equation for the temperature dependence of the superconducting gap:

$$\int_0^{\kappa\theta} d\epsilon [\frac{\tanh(\sqrt{\epsilon^2 + \Delta^2}/2\kappa T}{\sqrt{\epsilon^2 + \Delta^2}} - \frac{\tanh(\epsilon/2\kappa T_0)}{\epsilon}] = \frac{2\theta'}{\nu V} \varphi(\frac{T}{\theta}). \tag{4}$$

This equation differs from the standard equation in that it has a right side, which is determined entirely by phonons and which is a consequence of dependence (1). At absolute zero we find from Eq. (4)

$$\Delta(T=0) \equiv \Delta_0 = \frac{\pi}{\gamma} \kappa T_0 \exp[- \frac{2\theta'}{\nu V} f(0)] = 1{,}76 \kappa T_0 \exp[- \frac{2\theta'}{\nu V} f(0)]. \tag{5}$$

The change in Δ_0 which arises here is a consequence of zero-point vibrations. For the superconducting transition temperature T_c, Eq. (4) correspondingly yields

$$\ln \frac{T_0}{T_c} = \frac{2\theta'}{\nu V} \varphi(\frac{T_c}{\theta}). \tag{6}$$

According to this equation, the hardening (or softening) of the elastic modulus which corresponds to $\theta' > 0$ (or $\theta' < 0$) leads to a decrease (or increase) in T_c and a decrease (or increase) in Δ_0. Equations (5) and (6), on the other hand, allow us to write the ratio

$$2\Delta_0/\kappa T_c = (2\pi/\gamma) \exp(\Lambda) = 3{,}52 \exp(\Lambda), \tag{7}$$

where $\Lambda = (2\theta'/\nu V)[\varphi(T_c/\theta) - f(0)]$ does not have a component corresponding to zero-point vibrations. The same parameter, Λ, determines the jump in the specific heat at the point of the phase transition:

$$\Delta C = \frac{\pi^2}{2A_3} \nu \kappa^2 T_c (1 + p\Lambda)^2 = \frac{\pi^2}{2A_3} \nu \kappa^2 T_c [1 + p \ln \frac{\gamma \Delta_0}{\pi \kappa T_c}]^2, \tag{8}$$

where $A_3 = 1.05$, and $p = d \ln[\varphi(T_c/\theta) - \varphi(0)]/d \ln(T_c/\theta)$. We can also write an expression for the effect of the changes in the moduli in (1) on the isotope effect:

$$\alpha = - \frac{d\ln T_c}{d\ln M_i} = \frac{1}{2}\{1-[\Lambda + \frac{2\theta'}{\nu V}f(0)](1+p\Lambda)^{-1}\}, \quad (9)$$

where M_i is the mass of the ion. According to (8) and (9), the jump in the specific heat becomes larger than that in the BCS theory, and the isotope effect smaller, as the elastic modulus hardens ($\Lambda > 0$). The magnitude of the effect is determined by the values of the parameters p, Λ, and $2\theta' f(0)/\nu V$. Let us estimate these parameters in the Debye model with $f(0) = \varphi(0) = (9/8)\kappa N_A$ and $\varphi(x) = \varphi(0) + 9\kappa N_A x^4 \int_0^{1/x} dz z^3 \times [\exp(z) - 1]^{-1}$, where N_A is the number of atoms. Using experimental data on the change in the sound velocity,[1-4] and taking into account the actual parameter values of the high-T_c superconductors,[9,10] we find $p = 4$, $\Lambda \sim (0.5\text{–}1) \times 10^{-2}$ and $2\theta' f(0)/\nu V \sim (0.4\text{–}0.6)$ for LaSrCuO and $p = 2.7$, $\Lambda \sim (0.1\text{–}0.4)$, and $2\theta' f(0)/\nu V \sim (0.6\text{–}2.4)$ for YBaCuO. Since the quantity Λ is small for LaSrCuO, the change in the elastic modulus which we discussed above does not lead to a significant deviation of $2\Delta_0/\kappa T_c$ in (7) or ΔC in (8) from their values in the BCS theory, because the thermal phonons become "frozen solid." In YBaCuO, in contrast, expressions (7)–(9) lead to $2\Delta_0/\kappa T_c = (4\text{–}6)$, $\Delta C/T_c \sim (20\text{–}60)$ mJ/(K^2·mole) when the level of thermal excitation of the phonons (at $T \sim T_c$) is comparatively high. This result is close to the experimental values $[2\Delta_0/\kappa T]_{\exp} \sim (4\text{–}8)$ mJ/(K^2·mole) (Ref. 10) and $[\Delta C/T_c]_{\exp} \sim (30\text{–}60)$ mJ/(K^2·mole) (Ref. 9). The change in elasticity accompanying the superconducting transition is manifested in a different way in the isotope effect. Since α in (9) depends strongly on the renormalization of the temperature-independent energy of the zero-point vibrations, a change in the isotope effect is possible both in YBaCuO, under the condition $\alpha < 0.2$, and in LaSrCuO, under the condition $\alpha \sim (0.3\text{–}0.1)$, in agreement with experiment.[11,12]

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