JJAP Series 1
Superconducting Materials (1988) pp. 240–241

Possibility of High-T_c Superconductivity in Dense Magnetic Polarons

Yasutami TAKADA

Institute for Solid State Physics, University of Tokyo
7-22-1, Roppongi, Minato-ku, Tokyo 106, Japan

銅酸化物超伝導体を高密度磁気ポーラロン系と見なし，その超伝導機構を考えた。多磁気ポーラロン系での裸の電子間相互作用は，クーロン・ポテンシャル($\propto q^{-2}$)と局在スピン系のスピン揺動を媒介としたポテンシャル$C\chi(q)$との和である。(χは，スピン系の帯磁率，Cは電子とスピンとの結合定数を含む正の数である。)この系に対して，電子ガス($C=O$に対応する)に用いた方法で，第一原理から超伝導のT_cを計算した。Cの変化に伴うT_cの変化の様子はχの形に強く依存する。もし，$\chi(q)$の山が，$2k_F$付近(k_Fはフェルミ波数)にあると，T_cは，Cとともに著しく増大する。特に，電子密度径数r_sが6付近の場合には，T_cは容易に100 Kを越す。これは，クーロンによる長距離の電荷揺動からの引力と，局在スピン系の反強磁性的なスピン揺動からの短距離の引力とが協調して作りだした高温超伝導状態である。

When we combine the long-range charge fluctuations induced by the Coulomb interaction with the short-range interaction mediated by the exchange of anti-ferromagnetic spin fluctuations of localized spins as is realized in magnetic-polaron systems, superconductivity with T_c of the order of 100 K is expected to occur, when the r_s parameter of the system is around 6.

A salient feature of the high-T_c copper-oxide superconductors is that superconductivity appears in the close neighborhood of a magnetically ordered phase. This has led Anderson to the study of a model which contains only a short-range Coulomb repulsion.[1] At present, most people proceed along the direction. However, there are another feature of the system. The carrier density is low. If one considers this point to be more important, one should study a model which includes a long-range Coulomb repulsion.[2] In this paper, we report the calculated results of T_c obtained along this direction.

The present author has made quantitative studies of superconductivity in low-carrier-density systems such as doped $SrTiO_3$[3] and graphite-alkali metal intercalation compounds.[4] Through these studies, we have found that the long-range Coulomb interaction does not destroy but help superconductivity when the carrier density is low. In particular, it is predicted that superconductivity should appear even in an electron gas with the aid of the long-range charge fluctuations induced by the Coulomb interaction when the electronic density parameter, r_s, is larger than 3.9.[5] Since the systems treated so far do not have a mechanism which becomes effective at short-range distances, their T_c's are at most 1 K. But if we can introduce some mechanism to enhance short-range correlations and combine it with the long-range charge-fluctuation mechanism, we may be able to produce a high-T_c superconductor. A hint on the additional mechanism can be obtained, when we view the copper-oxides in the following way: The mobile carriers are the p-like holes at the oxide sites. If we regard the d-like holes at each copper site as localized spins which interact with the carriers through the d-p exchange interaction, a picture of a dense-magnetic-polaron system appears.

In magnetic-polaron systems, electrons with anti-parallel spins interact through both the long-range Coulomb repulsion and the exchange of spin fluctuations of localized spins, $C\chi(q)$, where $\chi(q)$ is the spin susceptibility of localized spins and a positive constant C contains the coupling constants between electrons and spins. An approximate form for $\chi(q)$ is usually given by

$$\chi(q)=B/[(q-Q)^2+D], \tag{1}$$

with some vector Q and constants B and D. When we take an angular average of Eq. (1), we may describe the Hamiltonian of the system as

$$H=\sum_{k\sigma}\varepsilon_k C^+_{k\sigma}C_{k\sigma}+\frac{1}{2}\sum_q\sum_{k\sigma}\sum_{k'\sigma'}V(q)\times C^+_{k+q\sigma}C^+_{k'-q\sigma'}C_{k'\sigma'}C_{k\sigma}, \tag{2}$$

with the bare interaction $V(q)$, given by

$$V(q)=\frac{4\pi e^2}{\kappa}\left[\frac{1}{q^2}+\frac{\varepsilon}{(q-q_0)^2+q_1^2}\right], \tag{3}$$

where κ is the dielectric constant. For the bare single-particle energy ε_k, we will take the parabolic form $k^2/2m^*$ with an effective mass m^*. When $q_0\approx 0$, the spin system has a tendency to order ferromagnetically, while for q_0 of the order of the Fermi wave number k_F, the second term in Eq. (3) represents the effect of anti-ferromagnetic spin fluctuations.

Once we know the Hamiltonian of the type of Eq. (2) , we can make a first-principles calculation of T_c for s-wave pairings by the method described in ref. 5. In Fig. 1 , we have plotted T_c in units of K* [$\equiv(m^*/m_e\kappa^2)$ degrees Kelvin] by solid curves as a function of q_0, where m_e is the mass of a free electron We have considered the case in which the width $q_1=0.2k_F$ and r_s [$\equiv m^*e^2/(0.521\kappa k_F)$] $=8$. For $q_0<1.8k_F$, T_c with the strength $\varepsilon=0.01$ is lower than that without the second term in Eq. (3) (i.e., $\varepsilon=0$). However, for q_0 larger than that , T_c is enhanced very much. (Dashed curves represent T_c with the use of the bare single-particle energy ε_k in the gap equation instead of the renormalized single-particle energy $\tilde{\varepsilon}_k$. These results give a useful guideline to estimate the magnitude

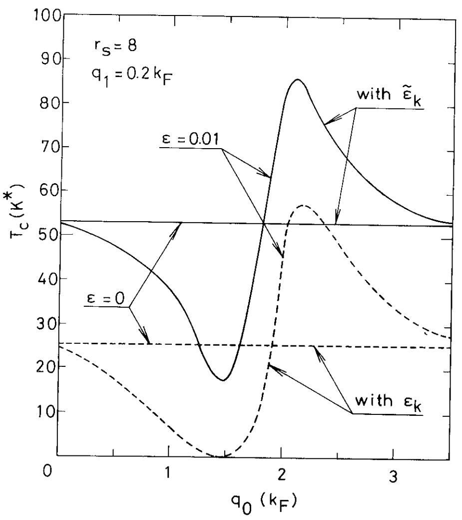
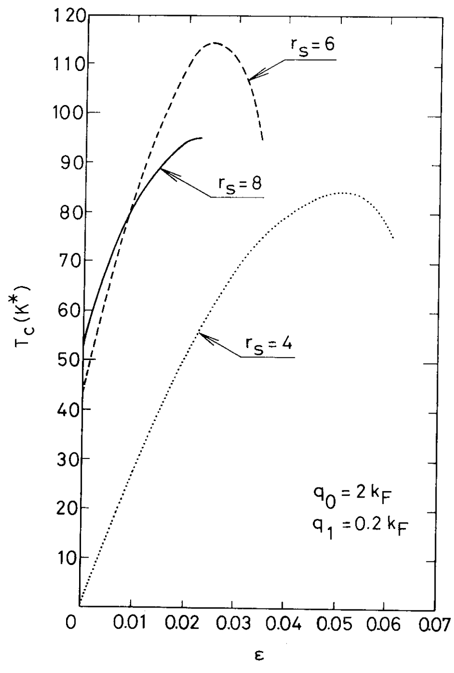


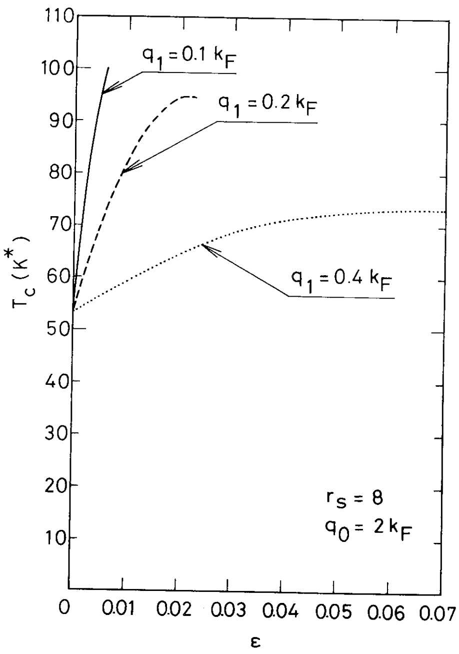
Fig. 1. Calculated T_c as a function of the peak position q_0 in Eq. (3). Solid and dashed curves represent, respectively, the results with the use of the fully renormalized and bare single-particle energies in the gap equation.

of errors involved in the calculation.) Qualitatively, this behavior of T_c agrees with the argument that ferromagnetic spin fluctuations suppress superconductivity with spin-singlet pairs, while anti-ferromagnetic ones enhance it.[6] In Figs. 2(a) and 2(b), we have given the results of T_c as a function of ε by changing r_s and q_1. We have fixed q_0 to $2k_F$. In these figures, we have shown the results only for the case in which $z_{k_F}^{-1}$, the renormalization factor at the Fermi surface, is positive, because negative $z_{k_F}^{-1}$ indicates that a metal-insulator transition occurs in the system. In general, T_c increases as q_1 becomes smaller. An optimum T_c over 100 K* is obtained for $r_s \approx 6$.

We have to make a few comments: Firstly, although T_c is enhanced very much by the second term in Eq. (3), the long-range nature of the first term is very important . If we replace $1/q^2$ with $1/(q^2+q_2^2)$, T_c decreases quite rapidly with the increase of q_2. For $q_2 > 0.4k_F$, superconductivity disappears. Secondly, we have to take account of lattice structures, when we treat short-range properties. In the present case, an angular-dependent interaction as indicated in Eq. (1) should be considered. Such an interaction will favor anisotropic pairs in general, but the present author believes from the experience in ref. 4 that the magnitude of T_c itself does not change so much from the value which we have obtained in this paper, even if the real shape of the gap is very different from an isotropic one. Thirdly, $V(q)$ should be spin-dependent in the magnetic-polaron system, while Eq. (3) is spin-independent. Thus, in order to make a more serious discussion on a possibility of high-T_c superconductivity in dense magnetic polarons, we have to extend our method to a spin-dependent formalism. In fact, our present method is implicitly spin-dependent and a small change in the bare potential between electrons with parallel spins does not give a large effect on T_c for anti-parallel-spin pairs.



(a)



(b)

Fig. 2. Calculated results of T_c as a function of ε for various values of r_s [case (a)] and q_1 [case (b)]. q_0 is fixed to $2k_F$. Only the cases for $z_{k_F}^{-1} > 0$ are shown in the figure.

References

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