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Possible higher temperature superconductivity in the modulation-doped superlattice structure of cuprate superconductors

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ABSTRACT

We design a new structure for a cuprate superconductor indicating the possibility of higher temperature superconductivity using our recently proposed composite fermions theory. It is constructed with modulation-doped superlattice structures, which are often used in the design of semiconductor superlattice devices. The superconductive critical temperature (T_c) was calculated in the superlattice structures of the superconductor in which the optimal doped CuO_2 layer was sandwiched between two less-doped CuO_2 layers. We find that if these structures could be realized in a cuprate superconductor such as $Bi_2Sr_2Ca_2Cu_3O_{10}$ or $HgBa_2Ca_2Cu_3O_9$, the highest T_c could attain the level of 300 K at atmospheric pressure.

1. Introduction

After Bednorz and Müller [1] discovered the first cuprate superconductor in 1986, the maximum T_c of high-temperature superconductors was assumed to be 135 K of Hg-1223 [2]. In 2015, however, it was reported that the T_c value of H_2S was 203 K at 150 GPs [3]. To discover higher T_c superconductors, especially material indicating superconductivity at room temperature and atmospheric pressure, many trials and errors will be necessary. The theoretical approach will also be necessary to succeed. Recently, we proposed a theory of high-temperature superconductivity that emphasized that the electronic state of superconductors can be described by the composed fermions [4–6]. In this theory, *d-p* antiferromagnetic interaction and doping quantity in CuO_2 planes are primary factors for determining the T_c of superconductors. The highest T_c is determined by optimizing these factors, but its value has been limited due to the trade-off relations between factors. In this letter, modulation-doped superlattice structures, which are often used in semiconductor devices [7], are proposed in order to avoid these trade-off relations, and the approach to realizing a higher T_c is considered in a cuprate superconductor with modulation-doped superlattice structures.

2. Formulation

2.1. Effective Hamiltonian in a single CuO_2 layer

The starting Hamiltonian is an extended *d-p* model for a single layer of square planar in cuprate superconductors

$$H = \sum_{i\sigma} \varepsilon_d d^+_{i\sigma} d_{i\sigma} + \sum_{j\sigma} \varepsilon_p p^+_{j\sigma} p_{j\sigma} + \sum_{i\sigma} \sum_{j\in\{i\}} \left(\varepsilon_{ij} d^+_{i\sigma} p_{j\sigma} + \text{H.c.}\right) + \sum_i U d^+_{i\uparrow} d_{i\uparrow} d^+_{i\downarrow} d_{i\downarrow} + \sum_{ij\sigma\sigma'} V_{ij} d^+_{i\sigma} d_{i\sigma} p^+_{j\sigma'} p_{j\sigma'}, \quad (1)$$

where the operator $d^+_{i\sigma}$ creates Cu 3*d* holes at site *i*, $p^+_{j\sigma}$ creates O 2*p* holes at site *j*, $\varepsilon_d = 0$, and ε_{ij} is the nearest-neighbor hopping integral. *U* is the Coulomb repulsion at the Cu site, and V_{ij} is the interaction between neighboring Cu and O sites. In (1), the vacuum is defined as filled Cu d^{10} and Op^6 states. Considering the *d-p* covalency effect, the operator combining the O states around the Cu ion is defined as $\tilde{p}^+_{i\sigma} = 0.5 \sum_{j\in\{i\}} \varepsilon_{ij} |\varepsilon_{ij}|^{-1} p^+_{j\sigma}$ in which ε_{ij} is given by $\varepsilon_{ij} = -\varepsilon < 0$ $(j = 1, 2)$, $\varepsilon > 0$ $(j = 3, 4)$ [8]. Since the relation of $\sum_j p^+_{j\sigma} p_{j\sigma} = 2 \sum_i \tilde{p}^+_{i\sigma} \tilde{p}_{i\sigma}$ is satisfied in the Cu–O planes, Hamiltonian (1) is changed such that

$$H = 2 \sum_{i\sigma} \varepsilon_p \tilde{p}^+_{i\sigma} \tilde{p}_{i\sigma} + \sum_{i\sigma} \left(\varepsilon d^+_{i\sigma} \tilde{p}_{i\sigma} + \text{H.c.}\right) + \sum_i U d^+_{i\uparrow} d_{i\uparrow} d^+_{i\downarrow} d_{i\downarrow} + 2 \sum_{i\sigma\sigma'} V_i d^+_{i\sigma} d_{i\sigma} \tilde{p}^+_{i\sigma'} \tilde{p}_{i\sigma'}. \quad (2)$$

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Since the operator $\tilde{p}^+_{i\sigma}$ is not orthogonal between the neighboring Cu sites, it does not exactly satisfy anti-commutation relations. However, as approximated here, $\tilde{p}^+_{i\sigma}$ can be a well-defined fermion operator. To the second order in perturbation theory on the condition of $\varepsilon < U$, let us determine the effective Hamiltonian (2). First in the second term of (2), the terms acting on the interaction U as a perturbation can be selected as follows:

$$H' = \sum_{i\sigma}\left\{\varepsilon\left[n_{d\sigma'}d^+_{i\sigma}\tilde{p}_{i\sigma}(1-n_{p\sigma'})+(1-n_{d\sigma'})d^+_{i\sigma}\tilde{p}_{l\sigma}n_{p\sigma'}\right]+\text{H.c.}\right\}, \tag{3}$$

where H' indicates the terms in the presence of fermions with the opposite spin at either d or p sites, because the ground state is not assumed here to include double occupancy states. The Coulomb interaction U in the ground state can be effectively eliminated from the starting Hamiltonian because double occupancy states at d-sites are inhibited by Coulomb repulsion. Considering the second term except H' in (2), Hamiltonian (2) is modified by

$$\begin{aligned} H = {} & 2\sum_{i\sigma}\varepsilon\tilde{p}^+_{i\sigma}\tilde{p}_{l\sigma}+\sum_{i\sigma}\langle 1-n_{p\sigma'}\rangle\left(\varepsilon d^+_{i\sigma}\tilde{p}_{i\sigma}+\text{H.c.}\right) \\ & +2\sum_{i\sigma\sigma'}V_i d^+_{i\sigma}d_{i\sigma}\tilde{p}^+_{i\sigma'}\tilde{p}_{i\sigma'} \\ & +\sum_{i\sigma\neq\sigma'}\left[\left\langle n_{d\sigma'}(1-n_{p\sigma'})\right\rangle+\left\langle(1-n_{n\sigma'})n_{p\sigma'}\right\rangle\right]^2 \\ & \times\left(-J_1 d^+_{i\sigma}d_{i\sigma}\tilde{p}^+_{i\sigma'}\tilde{p}_{i\sigma'}-J_2 d^+_{i\sigma}\tilde{p}_{i\sigma}\tilde{p}^+_{i\sigma'}d_{i\sigma'}\right), \end{aligned} \tag{4}$$

where $J_1=\varepsilon^2(U-2\varepsilon_p-2V_i)^{-1}$, $J_2=\varepsilon^2(2\varepsilon_p-2V_i)^{-1}$, and occupancy factors such as $(1-n_{p\sigma'})$ are averaged using $\langle 1-n_{p\sigma'}\rangle$. Although the former part of the fourth term in (4) corresponds to the kinetic energy due to the hopping between sites, it is neglected here due to the second-order kinetic energy. The latter part corresponds to the effective anti-ferromagnetic interaction between d-p fermions. Thus, the effective Hamiltonian is finally obtained as

$$\begin{aligned} H_{eff} = {} & 2\sum_{i\sigma}\varepsilon\tilde{p}^+_{l\sigma}\tilde{p}_{i\sigma}+\sum_{i\sigma}\langle 1-n_{p\sigma'}\rangle\left(\varepsilon d^+_{i\sigma}\tilde{p}_{l\sigma}+\text{H.c.}\right) \\ & +2\sum_{l\sigma\sigma'}V d^+_{i\sigma}d_{i\sigma}\tilde{p}^+_{i\sigma'}\tilde{p}_{i\sigma'}, \end{aligned} \tag{5}$$

where $V = V_i + 0.5V_{\sigma\sigma'}$ (V_i: Coulomb interaction between the nearest neighboring sites in (1), $V_{\sigma\sigma'}$: anti-ferromagnetic interaction $V_{\sigma\sigma'} = -[\langle n_{d\sigma'}(1-n_{p\sigma'})\rangle+\langle(1-n_{n\sigma'})n_{p\sigma'}\rangle]^2 J_1 < 0 \sigma\neq\sigma'$).

Now the ground state of the effective Hamiltonian (5) will be generally considered in two states depending on the doping conditions. One of these is the state in the neighborhood of the insulator (so-called Mott insulator) and the other is the superconducting state based on the band picture.

2.2. Superconductive critical temperature T_c

Let us consider the case of the superconducting state based on the band picture. Since the representation in momentum space is appropriate in this region, the effective Hamiltonian of (5) is transformed into

$$\begin{aligned} H = {} & \sum_{\mathbf{k}\sigma}\varepsilon_p p^+_{\mathbf{k}\sigma}p_{\mathbf{k}\sigma}+\sum_{\mathbf{k}\sigma}\langle 1-n_{p\sigma'}\rangle\varepsilon s(\mathbf{k})\left(-id^+_{\mathbf{k}\sigma}p_{\mathbf{k}\sigma}+ip^+_{\mathbf{k}\sigma}d_{\mathbf{k}\sigma}\right) \\ & +\sum_{\mathbf{k}\mathbf{k}'\mathbf{k}''\sigma\sigma'}V\theta_{\mathbf{k}\mathbf{k}'}d^+_{\mathbf{k}\sigma}d_{\mathbf{k}'\sigma}p^+_{\mathbf{k}''\sigma'}p_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'',\sigma'}, \end{aligned} \tag{6}$$

where $s(\mathbf{k})=\sin k_x+\sin k_y$, $\theta_{\mathbf{k}\mathbf{k}'}=\cos(k_x-k'_x)+\cos(k_y-k'_y)$. The Cu–O distance is used as the length unit. The operators $p^+_{\mathbf{k}\sigma}, d^+_{\mathbf{k}\sigma}$, which are the Fourier transformation of $p^+_{i\sigma}, d^+_{i\sigma}$, construct new fermion operators defined by unitary transformation

$$\begin{aligned} & b^+_{\mathbf{k}\sigma}=\alpha_{\mathbf{k}}d^+_{\mathbf{k}\sigma}+i\beta_{\mathbf{k}}p^+_{\mathbf{k}\sigma}, \qquad c^+_{\mathbf{k}\sigma}=\beta_{\mathbf{k}}d^+_{\mathbf{k}\sigma}-i\alpha_{\mathbf{k}}p^+_{\mathbf{k}\sigma}, \\ & \alpha^2_{\mathbf{k}}+\beta^2_{\mathbf{k}}=1, \end{aligned} \tag{7}$$

where $b^+_{\mathbf{k}\sigma}$, $c^+_{\mathbf{k}\sigma}$ satisfy anti-commutation relations. Notice that the operators $p^+_{\mathbf{k}l\sigma}$ satisfy the anti-commutation relations exactly, but are the approximated operators of $\tilde{p}^+_{inl\sigma}$ in momentum space.

In this doping region the relation of $\langle n_{d\sigma'}\rangle\approx 1$, $\langle 1-n_{p\sigma'}\rangle\approx 1-0.5\delta$ will be generally reasonable. On the condition of $\alpha_{\mathbf{k}}\beta_{\mathbf{k}}\varepsilon_p = (1-0.5\delta)\varepsilon s(\mathbf{k})(\beta^2_{\mathbf{k}}-\alpha^2_{\mathbf{k}})$, the Hamiltonian (6) is represented by

$$\begin{aligned} H = {} & \sum_{\mathbf{k}\sigma}\varepsilon_p\left(\beta^2_{\mathbf{k}}-\alpha^2_{\mathbf{k}}\right)^{-1}\left(\beta^2_{\mathbf{k}}b^+_{\mathbf{k}\sigma}b_{\mathbf{k}\sigma}-\alpha^2_{\mathbf{k}}c^+_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\right) \\ & +N^{-1}\sum_{\mathbf{k}\mathbf{k}'\mathbf{k}''\sigma\sigma'}V\theta_{\mathbf{k}\mathbf{k}'}\left(\alpha_{\mathbf{k}}\alpha_{\mathbf{k}'}\beta_{\mathbf{k}''}\beta_{\mathbf{k}-\mathbf{k}'+\mathbf{k}''}b^+_{\mathbf{k}\sigma}b_{\mathbf{k}'\sigma}b^+_{\mathbf{k}''\sigma'}\right. \\ & \times b_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'',\sigma'}+\alpha_{\mathbf{k}}\alpha_{\mathbf{k}'}\alpha_{\mathbf{k}''}\alpha_{\mathbf{k}-\mathbf{k}'+\mathbf{k}''}b^+_{\mathbf{k}\sigma}b_{\mathbf{k}'\sigma}c^+_{\mathbf{k}''\sigma'}c_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'',\sigma'} \\ & +\beta_{\mathbf{k}''}\beta_{\mathbf{k}-\mathbf{k}'+\mathbf{k}''}\beta_{\mathbf{k}}\beta_{\mathbf{k}'}c^+_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma}b^+_{\mathbf{k}''\sigma'}b_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'',\sigma'} \\ & \left.+\beta_{\mathbf{k}}\beta_{\mathbf{k}'}\alpha_{\mathbf{k}''}\alpha_{\mathbf{k}-\mathbf{k}'+\mathbf{k}''}c^+_{\mathbf{k}\sigma}c_{\mathbf{k}'\sigma}c^+_{\mathbf{k}''\sigma'}c_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'',\sigma'}+\cdots\right). \end{aligned} \tag{8}$$

Note that $V=V_c+V_{\sigma\sigma'}\approx V_{\sigma\sigma'}<0$, because in this doping region the Coulomb interaction V_c can be neglected due to the screening effect of carriers. Since the energy level of the $b^+_{\mathbf{k}\sigma}$ band is higher than the $c^+_{\mathbf{k}\sigma}$ band, let us consider only the $b^+_{\mathbf{k}\sigma}$ band containing the Fermi surface. In this situation, the interactive contribution of $c^+_{\mathbf{k}\sigma}$ fermions will be almost negligible. It is only necessary to consider the kinetic energy of the $b^+_{\mathbf{k}\sigma}$ fermions, and the attractive interaction between them. This suggests that Eq. (8) is reduced to a BCS-like Hamiltonian. In BCS theory, the neighborhood of the Fermi surface in which there exists attractive interaction with the phonon is only considered to calculate the superconductive critical temperature. A similar treatment will be applied here, although the attractive anti-ferromagnetic interaction between $b^+_{\mathbf{k}\sigma}$ fermions is not necessarily limited to the neighborhood of the Fermi surface. In this treatment, $b^+_{\mathbf{k}\uparrow}, b^+_{-\mathbf{k}\downarrow}$ pairs will mainly contribute to the attractive interaction; then, it is possible to justify using a BCS-like approach to calculate the critical temperature. However, the present theory is different from the BCS theory in that Cooper pairs can be uniquely created by the composite fermions constructed with the specific ratio of $d^+_{\mathbf{k}\sigma}$ and $p^+_{\mathbf{k}\sigma}$ holes. Thus the BCS-like wave function will be adopted as the ground state of (8).

$$|\Psi_S\rangle=\prod_{\mathbf{k}\sigma}\left(u_{\mathbf{k}}+v_{\mathbf{k}}b^+_{\mathbf{k}\uparrow}b^+_{-\mathbf{k}\downarrow}\right)|0\rangle, \quad u^2_{\mathbf{k}}+v^2_{\mathbf{k}}=1. \tag{9}$$

The gap equation is then obtained as

$$\begin{aligned} & \Delta_{\mathbf{k}}=-0.5\sum_{\mathbf{k}'}\Delta_{\mathbf{k}'}V_{\mathbf{k}\mathbf{k}'}\left(\Delta^2_{\mathbf{k}}+\varepsilon^2_{\mathbf{k}}\right)^{-1/2}, \\ & V_{\mathbf{k}\mathbf{k}'}=N^{-1}V\alpha_{\mathbf{k}}\alpha_{\mathbf{k}'}\beta_{\mathbf{k}}\beta_{\mathbf{k}'}\theta_{\mathbf{k}\mathbf{k}'}, \end{aligned} \tag{10}$$

where $\varepsilon_{\mathbf{k}}=0.5(\varepsilon_p+\sqrt{4(1-0.5\delta)^2\varepsilon^2 s^2(\mathbf{k})+\varepsilon^2_p})-\varepsilon_F)$. Replacing the sum in the gap equation with an integral, the solution that is even in $\mathbf{k}$ is given by $\Delta_{\mathbf{k}}=\Delta_0\alpha_{\mathbf{k}}\beta_{\mathbf{k}}$ $(\cos k_x\pm\cos k_y)$. The solution decreasing Coulomb interaction is $\Delta_{\mathbf{k}}\propto(\cos k_x-\cos k_y)$, which agrees with the experimental fact of the anisotropic gap of high-temperature cuprate superconductors [9]. Therefore, Δ_0 is determined by the relation

$$\begin{aligned} 1 = {} & -0.5\pi^{-2}V\int\alpha^2_{\mathbf{k}}\beta^2_{\mathbf{k}}(\cos k_x-\cos k_y) \\ & \times\cos k_x\left[\Delta^2_0\alpha^2_{\mathbf{k}}\beta^2_{\mathbf{k}}(\cos k_x-\cos k_y)^2+\varepsilon^2_{\mathbf{k}}\right]^{-1/2}d\mathbf{k}. \end{aligned} \tag{11}$$

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