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Evaluation of the effective holon–holon interaction by the slave-fermion method

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Abstract. The effective holon–holon interaction by exchanging the spinons in the resonating-valence bond model is derived by the slave-fermion method. We found that the interaction is attractive for the holon Cooper pair. Complexity due to Bose condensation of the spinons at $T = 0$ has been discussed.

Since the discovery [1] of high-T_c oxide superconductivity, a number of theoretical ideas have been proposed to explain the origin of this intriguing phenomenon. Anderson [2] first suggested that it could be described by the two-dimensional (2D) Hubbard model with a large on-site Coulomb repulsion U. He considered that the resonating-valence-bond (RVB) state is the ground state of this system and causes the superconductivity [3, 4]. Although experiments and much work show that the ground state is an antiferromagnetic order state at half-filling ($\delta = 0$) [5, 6], it is still an open question whether or not the RVB state can become the ground state and lead to superconductivity away from half-filling. So, it is still important to investigate the RVB model analytically.

The Hamiltonian for the square lattice Hubbard model is given by

$$H = -t \sum_{\langle ij \rangle} \sum_{\sigma} c_{i\sigma}^{+} c_{j\sigma} + U \sum n_{i\uparrow} n_{i\downarrow} \tag{1}$$

where $c_{i\sigma}^{+}$ and $c_{i\sigma}$ represent the electron creation and annihilation operators, respectively, at lattice site i with spin σ ($\equiv \uparrow$ or $\downarrow$), and $n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma}$. When $U \gg t$, this Hamiltonian can be expanded in a series of t/U [7, 8] and in the lowest order, the $t - J$ model can be obtained. Usually, the slave-boson technique has been widely used to treat the model [9, 10]. In this method, four auxiliary operators $e_i, s_{i\uparrow}, s_{i\downarrow}$ and d_i are introduced with the local constraint of

$$e_i^{+} e_i + d_i^{+} d_i + \sum_{\sigma} s_{i\sigma}^{+} s_{i\sigma} = 1. \tag{2}$$

Here e_i^{+} and d_i^{+} are interpreted as creation operators for empty and doubly occupied sites, respectively, and $s_{i\sigma}^{+}$ as creating a singly occupied i site with spin σ. The electron operator $c_{i\sigma}$ is expressed as

$$c_{i\uparrow} = e_i^{+} s_{i\uparrow} + d_i s_{i\downarrow}^{+} \qquad c_{i\downarrow} = e_i^{+} s_{i\downarrow} - d_i s_{i\uparrow}^{+}. \tag{3}$$

In the slave-boson formalism, e_i and d_i are considered as boson operators, but $s_{i\sigma}$ as fermions. If so, it is easy to show that electron operators $c_{i\sigma}^{+}$ and $c_{i\sigma}$ satisfy the anticommutation relations. In the large-U limit, the doubly occupied state can be neglected and d_i will be dropped from all expressions. The Hamiltonian can be written by only e_i, e_i^{+}, $s_{i\sigma}$ and $s_{i\sigma}^{+}$.

In the RVB model, e_i can be considered as a holon operator and $s_{i\sigma}$ as a spinon operator. Then the mean-field approximation with RVB order parameter is used to solve the Hamiltonian. However, as pointed out by Yoshioka [11] and Fiensberg *et al* [12], this method has several shortcomings. For example, at half-filling, the ground state obtained by the slave-boson method cannot show the expected antiferromagnetic order. Recently, Read and Chakraborty [13] suggested reversing the statistics assigned to e_i and $s_{i\sigma}$, i.e. the charge carriers e_i in the RVB model are fermions and the spin carriers $s_{i\sigma}$ are bosons. It is easy to demonstrate that electron operators $c_{i\sigma}^{+}$ and $c_{i\sigma}$ still satisfy the anticommutations relations in this case. We can also make the mean-field calculation using this formalism and call it slave-fermion formalism. Using this method, investigations of the normal-state properties of the system have been performed, and the results are encouraging [14, 15]. For example, it gives a ground state with a lower energy than that in the slave-boson formalism, and the ground state obtained by this new method shows long-range Néel order. At a finite temperature, the obtained specific heat and the magnetic susceptibility are consistent with the Monte Carlo calculation [16]. Moreover, away from the half-filling, the ground state by the slave-fermion method shows an incommensurate antiferromagnetic long-range order, which is qualitatively in agreement with recent experiment on the oxide superconductor.

From the above discussion, we believe that the slave-fermion formalism is probably more reasonable and better than the slave-boson formalism, and it is a good starting point to investigate the superconductivity of the high-T_c oxide superconductor. In this paper, we have used this slave-fermion method to treat the 2D single-band Hubbard model in the large-U limit and found that the effective interaction between two holons (now are fermions) can become attractive owing to exchange of the spinons, which supports the proposal of the BCS-like pairing of charged fermions for superconductivity in the oxide superconductor.

In the slave-fermion scheme, the Hubbard Hamiltonian in the large-U limit can be written in the following form:

$$H = -t\sum_{\langle ij\rangle}\sum_{\sigma} e_i e_j^{+} s_{i\sigma}^{+} s_{j\sigma} - J\sum_{\langle ij\rangle}(s_{i\uparrow}^{+} s_{j\downarrow}^{+} s_{j\downarrow} s_{i\uparrow} - s_{i\uparrow}^{+} s_{j\uparrow} s_{j\downarrow}^{+} s_{i\downarrow}) \qquad (4)$$

where $J = 4t^2/U$. The local constraint (2) can be removed by the Lagrange multiplier λ_i, which is replaced by a site-independent variable λ in the mean-field method.

Making the conventional Hartree–Fock factorization, the total Hamiltonian (4) can be written as

$$H = H_{01} + H_{02} + H_{12} \qquad (5)$$

where

$$H_{01} = tQ\sum_{\langle ij\rangle}\sum_{\sigma} s_{i\sigma}^{+} s_{j\sigma} - J\sum_{\langle ij\rangle}(s_{i\uparrow}^{+} s_{j\downarrow}^{+} s_{j\downarrow} s_{i\uparrow} - s_{i\uparrow}^{+} s_{j\uparrow} s_{j\downarrow}^{+} s_{i\downarrow}) + \lambda\sum_{i}\sum_{\sigma} s_{i\sigma}^{+} s_{i\sigma} \qquad (6)$$

$$H_{02} = 2tP\sum_{\langle ij\rangle} e_j^{+} e_i + \mu\sum_{i} e_i^{+} e_i - 8NPQt \qquad (7)$$

and

$$H_{12} = t\sum_{(ij)}\sum_{\sigma}(e_j^+e_i - Q)(s_{i\sigma}^+s_{j\sigma} - P). \tag{8}$$

Here the order parameters P and Q are defined as $P = \langle s_{i\sigma}^+s_{j\sigma}\rangle$ and $Q = \langle e_j^+e_i\rangle$, and N is the number of lattice points. μ is the chemical potential for holons, and λ the chemical potential for spinons, which are introduced to enforce the constraint $\langle e_i^+e_i\rangle = \delta$ and $\langle s_{i\sigma}^+s_{i\sigma}\rangle = \frac{1}{2}(1-\delta)$, where δ is the hole concentration. Let us introduce the RVB order parameter

$$\Delta_\tau = \tfrac{1}{2}\langle s_{i\uparrow}s_{i+\tau\downarrow} - s_{i\downarrow}s_{i+\tau\uparrow}\rangle \tag{9}$$

where $\tau = x$ or y, and $i+x$ and $i+y$ indicate a site next to the site i in the x and y directions, respectively. The boson (spinon) part H_{01} of the mean-field Hamiltonian (5) can be diagonalized by the following Bogoliubov transformation in momentum space:

$$\begin{aligned} s_{-k\uparrow} &= \exp(\mathrm{i}\tfrac{1}{2}\theta_k)(u_k\alpha_{-k} - v_k\beta_k^+)\\ s_{k\downarrow} &= \exp(\mathrm{i}\tfrac{1}{2}\theta_k)(u_k\beta_k - v_k\alpha_{-k}^+) \end{aligned} \tag{10}$$

where $u_k^2 = \frac{1}{2}(\varepsilon_k^s/E_k + 1)$ and $v_k^2 = \frac{1}{2}(\varepsilon_k^s/E_k - 1)$. ε_k^s is the kinetic energy of the spinons:

$$\varepsilon_k^s = \lambda - 2Jn_s + 2(tQ + \tfrac{1}{2}JP)(\cos k_x + \cos k_y) \tag{11}$$

here $n_s = \langle s_{i\sigma}^+s_{i\sigma}\rangle$. θ_k is the phase of λ_k: $\lambda_k = |\lambda_k|\exp(\mathrm{i}\theta_k)$, where λ_k is defined as

$$\lambda_k = 2J\mathrm{i}(\Delta_x\sin k_x + \Delta_y\sin k_y). \tag{12}$$

$E_k = [(\varepsilon_k^s)^2 - |\lambda_k|^2]^{1/2}$ is the quasi-particle excitation energy. Finally, we obtain

$$H_{01} = \sum_k E_k(\alpha_{-k}^+\alpha_{-k} + \beta_k^+\beta_k) + 2JN(|\Delta_x|^2 + |\Delta_y|^2) + 2NJ(n_s^2 + P^2) + \sum_k(E_k - \varepsilon_k^s). \tag{13}$$

Since E_k must be real, therefore $\varepsilon_k^s \geqslant |\lambda_k|$ but, when the temperature $T = 0$, at some $k = \{\kappa\}$, $\varepsilon_\kappa^s = |\lambda_\kappa|$, and E_κ can become zero. In this case, the transformation (10) is not defined, and the spinons can undergo Bose condensation at such κ. As discussed by Yoshioka [14], we should perform a special transformation:

$$\begin{aligned} s_{-\kappa\uparrow} &= (\tfrac{1}{2})^{1/2}\exp(\mathrm{i}\tfrac{1}{2}\theta_\kappa)(\xi_{-\kappa} + \eta_{-\kappa})\\ s_{\kappa\downarrow} &= (\tfrac{1}{2})^{1/2}\exp(\mathrm{i}\tfrac{1}{2}\theta_\kappa)(\xi_{-\kappa}^+ - \eta_{-\kappa}^+). \end{aligned} \tag{14}$$

So, the total Hamiltonian of spinons is

$$H_{01} = \sum_k{}' E_k(\alpha_{-k}^+\alpha_{-k} + \beta_k^+\beta_k) + \sum_\kappa 2\varepsilon_\kappa^s\xi_{-\kappa}^+\xi_{-\kappa} + 2JN(|\Delta_x|^2 + |\Delta_y|^2) + 2NJ(n_s^2 + P^2) + \sum_k{}'(E_k - \varepsilon_k^s) - \sum_\kappa\varepsilon_\kappa^s \tag{15}$$

where Σ' sums over such k that $k \neq \kappa$.

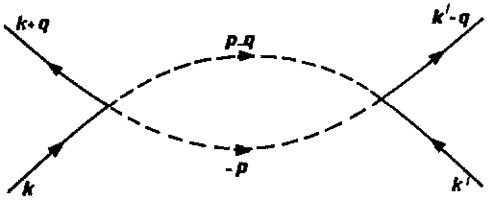

Figure 1. Only the 'anomalous' holon–holon scattering from the spinon background causes the effective holon–holon interaction: ——, holon propagators; - - -, spinon propagators.

The fermion (holon) part of the mean-field Hamiltonian contains only a hopping term and is easily diagonalized in momentum space

$$H_{02} = \sum_k \varepsilon_k^{\mathrm{h}} e_k^+ e_k - 8NPQt \tag{16}$$

where $\varepsilon_k^{\mathrm{h}} = \mu + 4tP(\cos k_x + \cos k_y)$ is the kinetic energy of holons. After dropping irrelative terms in (8), we obtain an interaction part between the holons and spinons:

$$H'_{12} = \frac{t}{N}\sum_k \sum_{k'} \sum_q \sum_\sigma g(q) e^+_{q+k'} e_{q+k} s^+_{k\sigma} s_{k'\sigma}. \tag{17}$$

Here $g(k) = \Sigma_\tau \exp(\mathrm{i}k \cdot \tau)$, where τ is the nearest-neighbour vector.

We shall use a canonical transformation to obtain the effective holon–holon interaction. It is well known that

$$\mathcal{H} = \tfrac{1}{2}\langle 0|[H'_{12}, S]|0\rangle \tag{18}$$

where S is the generating function, and $|0\rangle$ is the spinon ground state. We choose S to satisfy the equation $H'_{12} = [S, H_{01} + H_{02}]$. Because the spinons have Bose condensation at $k = \{\kappa\}$, when $T = 0$, the expression for the generating function S is more complicated than that in the slave-boson method. For effective holon–holon interaction, we should discuss the following three cases.

(i) Two holons exchange two spinons, which are not in the condensate.

As discussed by Wang [17], in the slave-boson method, the generating function contains two parts. One corresponds to the so-called 'normal' part which does not contribute to the effective holon–holon interaction, and the other corresponds to the 'anomalous' part which contributes to the effective holon–holon interaction. We have found that S_1 also has two parts, and only the 'anomalous' part, which is shown in figure 1, needs to be kept. The situation is very similar to that in the slave-boson scheme.

It is not difficult to obtain S_1:

$$S_1 = -\frac{t}{N}\sum_q {\sum_k}' {\sum_{k'}}' \varphi_0(q, k, k')(e^+_{q+k'} e_{q+k} \beta_{k'} \alpha_{-k} - \mathrm{HC}) \tag{19}$$

where

$$\varphi_0(q, k, k') = [g(q) u_{k'} v_k + g(q + k + k') u_k v_{k'}]/(\varepsilon^{\mathrm{h}}_{q+k} - \varepsilon^{\mathrm{h}}_{q+k'} + E_k + E_{k'}). \tag{20}$$

By evaluating equation (18), we obtain the effective Hamiltonian of the holon–holon interaction:

$$\mathcal{H}_1 = \frac{1}{2N}\sum_q \sum_k \sum_{k'} V_1(q, k, k') e^+_{k'-q} e_{k'} e^+_{k+q} e_k \tag{21}$$

where

$$V_1(q,k,k') = -\frac{t^2}{N}\sum_p{}' \{[g(k'-q-p)u_{p+q}v_p + g(k'+p)u_p v_{p+q}] \times \varphi_0(k-p,p,p+q) + [g(k-p)u_{p+q}v_p + g(k+p+q)u_p v_{p+q}] \times \varphi_0(k'-q-p,p,p+q)\}. \tag{22}$$

The pairing potential, which we are interested in, is attractive for the holon Cooper pairs as shown by the following:

$$\mathcal{V}_1(k,-k) = -\frac{t^2}{N}\sum_p{}' \frac{[g(k-p)+g(k+p)]^2|\lambda_p|^2}{4E_p^3}. \tag{23}$$

From equation (23), we see that the most important contributions to $\mathcal{V}_1(k,-k)$ come from the terms with momentum q near the condensation momentum κ, because E_q takes its minimum value at κ.

(ii) Two holons exchange two spinons, with only one spinon being in the condensate, and the other not.

We choose the generating function S_2 as follows:

$$S_2 = -\frac{t}{N}\sum_q\sum_k{}'\sum_\kappa \{e^+_{q+\kappa}e_{q+k}[\varphi_1(q,k,\kappa)\beta^+_k\xi^+_{-\kappa} + \varphi_2(q,k,\kappa)\beta^+_k\eta^+_{-\kappa} + \varphi_3(q,k,\kappa)\alpha_{-k}\xi^+_{-\kappa} + \varphi_4(q,k,\kappa)\alpha_{-k}\eta^+_{-\kappa}] - \text{HC}\}. \tag{24}$$

We define

$$\begin{aligned}
\varphi_1(q,k,\kappa) &= [1/(\varepsilon^{\rm h}_{q+k} - \varepsilon^{\rm h}_{q+\kappa} - E_k)][g_1(q,k,\kappa) \\
&\quad + 2\varepsilon^{\rm s}_\kappa g_2(q,k,\kappa)/(\varepsilon^{\rm h}_{q+k} - \varepsilon^{\rm h}_{q+\kappa} - E_k)] \\
\varphi_2(q,k,\kappa) &= g_2(q,k,\kappa)/(\varepsilon^{\rm h}_{q+k} - \varepsilon^{\rm h}_{q+\kappa} - E_k) \\
\varphi_3(q,k,\kappa) &= [1/(\varepsilon^{\rm h}_{q+k} - \varepsilon^{\rm h}_{q+\kappa} + E_k)][g_3(q,k,\kappa) \\
&\quad + 2\varepsilon^{\rm s}_\kappa g_4(q,k,\kappa)/(\varepsilon^{\rm h}_{q+k} + \varepsilon^{\rm h}_{q+\kappa} + E_k)] \\
\varphi_4(q,k,\kappa) &= g_4(q,k,\kappa)/(\varepsilon^{\rm h}_{q+k} - \varepsilon^{\rm h}_{q+\kappa} + E_k)
\end{aligned} \tag{25}$$

where

$$\begin{aligned}
g_1(q,k,\kappa) &= g(q)u_k - g(q+k+\kappa)v_k \\
g_2(q,k,\kappa) &= -g(q)u_k - g(q+k+\kappa)v_k \\
g_3(q,k,\kappa) &= -g(q)v_k + g(q+k+\kappa)u_k \\
g_4(q,k,\kappa) &= g(q)v_k + g(q+k+\kappa)u_k.
\end{aligned} \tag{26}$$

By evaluating equation (18), we obtain

$$\mathcal{H}_2 = \frac{1}{2N}\sum_q{}'\sum_k\sum_{k'} V_2(q,k,k')e^+_{k'-q}e_{k'}e^+_{k+q}e_k \tag{27}$$

where Σ'_q does not include $q = 0, \pm 2\kappa$. Here

$$V_2(q,k,k') = -\frac{t^2}{2N}n_0\sum_\kappa \{g_4(k'-\kappa,\kappa-q,\kappa)g_4(k+q-\kappa,\kappa-q,\kappa) \times \left(\frac{1}{\varepsilon^{\rm h}_k - \varepsilon^{\rm h}_{q+k} + E_{\kappa-q}} + \frac{1}{\varepsilon^{\rm h}_{k'-q} - \varepsilon^{\rm h}_{k'} + E_{\kappa-q}}\right)$$

$$- g_2(k' - \kappa, \kappa - q, \kappa) g_2(k + q - \kappa, \kappa - q, \kappa)$$

$$\times \left(\frac{1}{\varepsilon^{\rm h}_{k} - \varepsilon^{\rm h}_{k+q} - E_{\kappa-q}} + \frac{1}{\varepsilon^{\rm h}_{k'-q} - \varepsilon^{\rm h}_{k'} - E_{\kappa-q}} \right) \tag{28}$$

and $n_0 = \langle \eta^+_\kappa \eta_\kappa \rangle$. In this case, the pairing potential is also attractive for the holon Cooper pairs:

$$\mathcal{V}_2(k, -k) = -\frac{2t^2}{N} n_0 \sum_\kappa \frac{g^2(k + \kappa)(u_{\kappa+2k} + v_{\kappa+2k})^2}{E_{\kappa+2k}}. \tag{29}$$

(iii) Two holons exchange two spinons, both of which are in the condensate. This causes effective repulsion rather than attractive interaction between holons.

Here we have to emphasize that the three cases that we have just discussed can never appear simultaneously. There are three totally different possibilities or channels for the pairing of the two holons by exchange of the two spinons due to the existence of the spinon condensate. When the temperature $T \neq 0$, there is no spinon condensate, and so only case (i) can appear. At $T = 0$, because of the existence of the spinon condensate, all three cases can appear with their own definite probabilities. As demonstrated by Yoshioka [11], the fraction n_0/N of spinon condensate is only about 0.3–0.4 depending on the value of δ. So the probability that two spinons are in the condensate can only be about 0.1. This means that the probability for case (iii) is about 0.1. From this point of view, although spinon condensation reduces the possibility of the holon pairing, it has only a little effect on the pairing. Because the spinon condensation at $T = 0$ means the presence of the long-range antiferromagnetic order (when $\Delta_\tau \neq 0$), our result means that long-range order will be harmful to holon pairing, i.e. to the superconductivity. On the other hand, our result also means that even when antiferromagnetic order exists, because of the spinon condensation, two holons can still be paired by exchanging the spinons. So, it means that superconductivity can coexist with the antiferromagnetic long-range order, just as others have discussed [18–20].

$\mathcal{V}_1(k, -k)$ and $\mathcal{V}_2(k, -k)$ include an s-wave-like component and a d-wave-like component. Their relative strength depends on the RVB-state order parameter Δ_τ. For different symmetry cases, we obtain different λ_k by equation (12) as follows for s waves,

$$\lambda_k = {\rm i}2J(\sin k_x + \sin k_y)\Delta_x \tag{30a}$$

and, for d waves,

$$\lambda_k = {\rm i}2J(\sin k_x - \sin k_y)\Delta_x. \tag{30b}$$

Substituting these λ_k into the expressions for E_k, u_k and v_k, we can get corresponding expressions of the attractive interaction for s waves and d waves.

Because the model Hamiltonian that we are treating is exactly two dimensional, the Bose condensation of the spinons can occur only at $T = 0$, therefore, so long as $T \neq 0$, $n_0 = 0$ and $\mathcal{V}_2(k, -k)$ will be equal to zero. Only $\mathcal{V}_1(k, -k)$ will be able to survive. Since Δ_τ and E_k depend on temperature, the attractive interaction $\mathcal{V}_1(k, -k)$ is also temperature dependent. With increase in temperature, $\Delta_\tau \to 0$, and correspondingly $\mathcal{V}_1(k, -k) \to 0$.

The real system, however, cannot be exactly 2D and is, at most, quasi-2D. If we include coupling between different CuO_2 planes, the system can have spinon Bose condensation at higher temperatures $T \neq 0$. The coupling effect on the Bose condensation and the bare holon–holon attractive interaction is an interesting problem and will be discussed in a forthcoming paper.

The superconductivity arising from the 2D charged fermions pairing has been widely discussed in the literature [21, 22]. Of course, the pairing mechanism is very different and the attractive interaction between the two fermions may be produced by exchanging various kinds of quasi-particles, e.g. phonons, magnons, excitons and plasmons. Here because of reversal of the statistics of the holons and spinon, we also show that the fermion-type spinless holons can attract each other by exchanging the boson-type spinons, which contrasts with the slave-boson formalism of the boson-type holon pairing discussed by Wang [17]. It seems to us that the fermion's Cooper pairing mechanism is more reasonable and natural than the boson's Cooper pairing and, for the RVB model, the slave-fermion scheme is better than the slave-boson scheme. More theoretical and experimental work has to be done to identify which scheme is correct and better.

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