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Effective holon-holon interaction in the resonating-valence-bond state

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The effective holon-holon interaction mediated by the spinon background is derived in the framework of the resonating-valence-bond model. The interaction is present only after the spinons undergo a transition to a spin superfluid state and is attractive for the holon Cooper pairs. The latter property of the holon-holon interaction gives further support to the conjecture that the two-dimensional Hubbard model by itself in the large-U limit could lead to superconductivity.

The two-dimensional (2D) Hubbard model in the large-U limit has attracted increasing attention because of its possible connection with high-temperature superconductivity in the copper oxide superconductors. An intriguing question is whether the 2D large-U Hubbard model by itself, without introducing other external coupling sources such as phonons or interlayer tunneling of the underlying electrons, can lead to superconductivity. In this paper we study this problem within the framework of the resonating-valence-bond (RVB) model developed by Anderson[1] and his collaborators.[2,3] We find that the RVB background can naturally provide an attractive pairing interaction between the charged excitations, and which, combining with the result that the 2D ideal boson gas with an *arbitrarily weak* pair attraction is unstable with respect to pair condensation,[4,5] supports the proposal that the superconductivity in the doped Mott-Hubbard insulator arises from the BCS-like pairing of the charged excitations.

In the RVB model of the 2D large-U Hubbard model the elementary excitations[2,6] are the neutral spin-$\frac{1}{2}$ solitons, called "spinons," and the charged particles called "holons." These excitations are fundamentally different from those in the regular Fermi liquid in the sense that here the spin degrees and the charge degrees of freedom are separated. A coupled holon-spinon Hamiltonian has been derived by Zou and Anderson[2] in the limit that the double occupancy of the electrons at the same site is eliminated:

$$H=-t\sum_{\langle i,j\rangle\sigma} e_j^\dagger e_i S_{i\sigma}^\dagger S_{j\sigma} - J\sum_{\langle i,j\rangle}(S_{i\uparrow}^\dagger S_{j\downarrow}^\dagger S_{j\downarrow}S_{i\uparrow}+S_{i\uparrow}^\dagger S_{j\uparrow}S_{j\downarrow}^\dagger S_{i\downarrow})+\tilde{\mu}\sum_i e_i^\dagger e_i\,, \tag{1}$$

where $e_i(S_i)$ and $e_i^\dagger$ $(S_i^\dagger)$ are the holon (spinon) annihilation and creation operators at site i. t is the hopping integral and $J=4t^2/U$. The chemical potential $\tilde{\mu}$ is added to conserve the total number of holons.

The holon operators obey Bose statistics, i.e., $[e_i,e_j^\dagger]=\delta_{ij}$, and the spinon operators obey Fermi statistics, i.e., $[S_{i\sigma},S_{j\sigma'}^\dagger]_+=\delta_{ij}\delta_{\sigma\sigma'}$. They are not, however, free to operate since they are subjected to the local restrictions:

$$\sum_\sigma S_{i\sigma}^\dagger S_{i\sigma}+e_i^\dagger e_i=1\,. \tag{2}$$

The restrictions can be removed by using a set of Lagrangian multipliers, $\{\lambda_i\}$. In this paper we shall derive the effective interaction between holons mediated by the spinon background in the limit[7,8] that both the holons and the spinons are sufficiently delocalized so that λ_i can be replaced by a site-independent variable, λ. We find that the interaction is present only if the spinons are in the spin superfluid (RVB) state.

The total Hamiltonian (for a 2D square lattice) thus can be written as

$$H=H_{01}+H_{02}+H_{12}\,, \tag{3}$$

where

$$H_{01}=-tQ\sum_{\langle i,j\rangle\sigma}S_{i\sigma}^\dagger S_{j\sigma} - J\sum_{\langle i,j\rangle}(S_{i\uparrow}^\dagger S_{j\downarrow}^\dagger S_{j\downarrow}S_{i\uparrow}+S_{i\uparrow}^\dagger S_{j\uparrow}S_{j\downarrow}^\dagger S_{i\downarrow})+\lambda\sum_{i\sigma}S_{i\sigma}^\dagger S_{i\sigma}\,, \tag{4}$$

$$H_{02}=-2tP\sum_{\langle i,j\rangle}e_j^\dagger e_i+\mu\sum_i e_i^\dagger e_i+\sum_i V_\infty e_i^\dagger e_i e_i^\dagger e_i+8NPQt\,, \tag{5}$$

and

$$H_{12}=-t\sum_{\langle i,j\rangle\sigma}(e_j^\dagger e_i-Q)(S_{i\sigma}^\dagger S_{j\sigma}-P)\,. \tag{6}$$

Here $P=\langle S_{i\sigma}^\dagger S_{j\sigma}\rangle$ and $Q=\langle e_j^\dagger e_i\rangle$. μ is the redefined chemical potential for holons. The on-site repulsion V_∞ in Eq. (5) is added explicitly to prevent double occupation of the holons at the same site, and thus to eliminate the unphysical result caused by the replacement of λ_i by λ. The origin of V_∞ can be traced to the original electron operators, for which double occupation at the same site is eliminated because of the Pauli exclusion principle and the largeness of the U in the Hubbard model. One can solve H_{01} in the mean-field approximation, as originally done by Baskaran, Zou, and Anderson.[3] In this approximation H_{01} can be diagonalized using the standard Bogoliubov transformation to give

$$H_{01}=\sum_{\mathbf{k}}E_{\mathbf{k}}(\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}+\beta_{-\mathbf{k}}^{\dagger}\beta_{-\mathbf{k}})-\sum_{\mathbf{k}}(E_K-\varepsilon_{\mathbf{k}}^s)+4NJ(P^2+n_s^2)+J\sum_{\langle i,j\rangle}|\Delta_{ij}|^2 . \quad (7)$$

The new particle operators $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ are related to the spinon operators by

$$S_{\mathbf{k}\uparrow}=u_{\mathbf{k}}\alpha_{\mathbf{k}}+v_{\mathbf{k}}\beta_{-\mathbf{k}}^{\dagger} , \quad (8)$$

and

$$S_{\mathbf{k}\downarrow}=u_{\mathbf{k}}\beta_{\mathbf{k}}-v_{\mathbf{k}}\alpha_{-\mathbf{k}}^{\dagger} , \quad (9)$$

where $u_{\mathbf{k}}^2=\frac{1}{2}(1+\varepsilon_{\mathbf{k}}^s/E_{\mathbf{k}})$ and $v_{\mathbf{k}}^2=\frac{1}{2}(1-\varepsilon_{\mathbf{k}}^s/E_{\mathbf{k}})$. $\varepsilon_{\mathbf{k}}^s$ is the kinetic energy of the spinons:

$$\varepsilon_{\mathbf{k}}^s=\lambda-4Jn_s-2(tQ+JP)(\cos k_x+\cos k_y) . \quad (10)$$

$E_{\mathbf{k}}=[(\varepsilon_{\mathbf{k}}^s)^2+\Delta_{\mathbf{k}}^2]^{1/2}$ is the quasiparticle excitation energy, and $\Delta_{\mathbf{k}}$ is the order parameter for the spin superfluid state,

$$\Delta_{\mathbf{k}}=\frac{1}{N}\sum_{\mathbf{p}}\frac{\Delta_{\mathbf{p}}V_{\mathbf{kp}}}{2E_{\mathbf{p}}}\tanh(E_{\mathbf{p}}/2k_BT) . \quad (11)$$

where $V_{\mathbf{kp}}=4J[\cos(p_x-k_x)+\cos(p_y-k_y)]$. Finally, $n_s=\langle S_{i\sigma}^{\dagger}S_{i\sigma}\rangle$ and $\Delta_{ij}=\langle S_{j\downarrow}S_{i\uparrow}\rangle$ in Eq. (7).

The structure of the spin superfluid order parameter $\Delta_{\mathbf{k}}$ is a fascinating subject. Because of the symmetry of the kernel $V_{\mathbf{kp}}$, $\Delta_{\mathbf{k}}$ can have s-wave-like,[3] d-wave-like,[9,10] and $(s+id)$-wave-like[10,11] solutions. Transitions between the different phases have also been proposed.[10,12]

When the spinons are in the normal state, there is no holon-holon interaction caused by the scattering from the spinon background, at least to second order. Diagrammatically, as shown in Fig. 1, the terms represented by Fig. 1(a) which have momentum flowing $-\mathbf{q}$ from left to right, will be canceled by the terms having momentum flowing $\mathbf{q}$ from right to left [Fig. 1(b)]. After the spinons undergo a transition to the superfluid state, there are scattering events such as terms shown in Fig. 1(c) in addition to those in Figs. 1(a) and 1(b). Terms represented by Figs. 1(a) and 1(b) also cancel each other in the spin superfluid state, leaving only the terms represented by Fig. 1(c). Thus, the presence and the structure of the spin superfluid state can dramatically affect the holon dynamics.

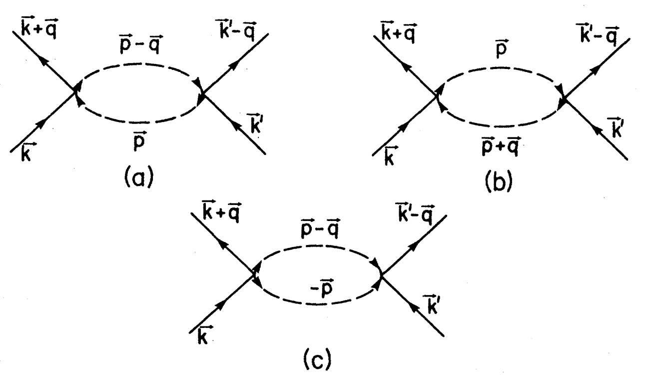

FIG. 1. Diagrams representing the holon-holon interaction mediated by the spinon background. The solid lines represent the holon propagators and the dashed lines represent the spinon propagators. The anomalous diagram (c) is present only in the spin superfluid state.

We shall use a canonical transformation[13,14] to obtain the effective holon-holon interaction. In this method,

$$H_{\text{eff}}=\frac{1}{2}\langle 0|[H_{12},S]|0\rangle , \quad (12)$$

where S is the generating function, and $|0\rangle$ is the spinon ground state. S can be easily found, since it satisfies the equation $H_{12}+[H_{01}+H_{02},S]=0$. S contains two parts. The first part corresponds to the "normal" diagrams, namely those in Figs. 1(a) and 1(b), and does not contribute to the effective holon-holon interaction. The second part corresponds to the relevant "anomalous" diagrams, i.e., those represented by Fig. 1(c), and is

$$S=-\frac{t}{N}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\frac{g(\mathbf{q})u_{\mathbf{k}'}v_{\mathbf{k}}+g(\mathbf{q}+\mathbf{k}+\mathbf{k}')u_{\mathbf{k}}v_{\mathbf{k}'}}{\varepsilon_{\mathbf{q}+\mathbf{k}}^h-\varepsilon_{\mathbf{q}+\mathbf{k}'}^h+(E_{\mathbf{k}}+E_{\mathbf{k}'})}\times(e_{\mathbf{q}+\mathbf{k}'}^{\dagger}e_{\mathbf{q}+\mathbf{k}}\beta_{-\mathbf{k}}\alpha_{\mathbf{k}'}-\text{H.c.}) , \quad (13)$$

where $\varepsilon_{\mathbf{k}}^h$ is the holon kinetic energy

$$\varepsilon_{\mathbf{k}}^h=\mu-4tP(\cos k_x+\cos k_y) , \quad (14)$$

and $g(\mathbf{k})=\sum_{\delta}e^{i\mathbf{k}\cdot\delta}$ (δ is the nearest-neighbor vector).

By evaluating Eq. (12), we obtain

$$H_{\text{eff}}=\frac{1}{2N}\sum_{\mathbf{kk'q}}V(\mathbf{kk'q})e_{\mathbf{k}+\mathbf{q}}^{\dagger}e_{\mathbf{k}}e_{\mathbf{k}'-\mathbf{q}}^{\dagger}e_{\mathbf{k}'} . \quad (15)$$

The matrix element $V(\mathbf{kk'q})$ is

$$V(\mathbf{kk'q})=\frac{t^2}{N}\sum_{\mathbf{p}}\left(\frac{F_2(\mathbf{k},\mathbf{p},\mathbf{q})F_2(\mathbf{k}'-\mathbf{q},\mathbf{p},\mathbf{q})}{\varepsilon_{\mathbf{k}'-\mathbf{q}}^h-\varepsilon_{\mathbf{k}'}^h-(E_{\mathbf{p}}+E_{\mathbf{p}+\mathbf{q}})}-\frac{F_1(\mathbf{k},\mathbf{p},\mathbf{q})F_1(\mathbf{k}'-\mathbf{q},\mathbf{p},\mathbf{q})}{\varepsilon_{\mathbf{k}'-\mathbf{q}}^h-\varepsilon_{\mathbf{k}'}^h+(E_{\mathbf{p}}+E_{\mathbf{p}+\mathbf{q}})}\right) , \quad (16)$$

where $F_1(\mathbf{k},\mathbf{p},\mathbf{q})$ and $F_2(\mathbf{k},\mathbf{p},\mathbf{q})$ are the vertex functions:

$$F_1(\mathbf{k},\mathbf{p},\mathbf{q})=g(\mathbf{k}-\mathbf{p})u_{\mathbf{p}+\mathbf{q}}v_{\mathbf{p}}+g(\mathbf{k}+\mathbf{p}+\mathbf{q})u_{\mathbf{p}}v_{\mathbf{p}+\mathbf{q}} , \quad (17)$$

and

$$F_2(\mathbf{k},\mathbf{p},\mathbf{q})=g(\mathbf{k}-\mathbf{p})u_{\mathbf{p}}v_{\mathbf{p}+\mathbf{q}}+g(\mathbf{k}+\mathbf{p}+\mathbf{q})u_{\mathbf{p}+\mathbf{q}}v_{\mathbf{p}} . \quad (18)$$

The Hamiltonian governing the holon dynamics will have H_{eff} added to Eq. (5).

It is especially interesting to note that Eq. (16) implies a pairing potential, $V(\mathbf{k},-\mathbf{k}')$,

$$V(\mathbf{k},-\mathbf{k}')=\frac{t^2}{N}\sum_{\mathbf{q}}F_1(\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{k})F_2(\mathbf{k},\mathbf{k}+\mathbf{q},\mathbf{k}'-\mathbf{k})\times\frac{2(E_{\mathbf{k}+\mathbf{q}}+E_{\mathbf{k}'+\mathbf{q}})}{(\varepsilon_{\mathbf{k}'}^h-\varepsilon_{\mathbf{k}}^h)^2-(E_{\mathbf{k}+\mathbf{q}}+E_{\mathbf{k}'+\mathbf{q}})^2} , \quad (19)$$

which is attractive for the holon Cooper pairs,

$$V(\mathbf{k},-\mathbf{k})=-\frac{t^2}{N}\sum_{\mathbf{q}}[g(\mathbf{q}-\mathbf{k})+g(\mathbf{q}+\mathbf{k})]^2u_{\mathbf{q}}^2v_{\mathbf{q}}^2/E_{\mathbf{q}} . \quad (20)$$

The range of such attractive interactions is on the order of the spinon energy. The interaction will be screened in the usual way when the holon dynamics is considered.

Superconductivity arising from 2D charged bosons has been discussed in the literature.[4,5,6] In particular, it has been shown[4] that the ideal 2D boson gas with an arbitrarily weak pair attractive interaction is unstable toward a BCS-like pair condensation. The result given in Eq. (20) shows that the model Hamiltonian, defined by Eqs. (3)-(6), can support holon pair condensation, which thus suggests that the 2D Hubbard model by itself could lead to superconductivity provided that the RVB model is a good approximation of the Hubbard model in the large-U limit. If the superconductivity in the copper oxide materials comes from the mechanism discussed above, our results have an interesting experimental implication, namely that the superconductivity transition in these materials will always be accompanied by, and after, the phase transition of the spinons to the spin superfluid state.

$V(\mathbf{k},-\mathbf{k}')$ has a nonvanishing s-wave component. Higher-order components are also present in $V(\mathbf{k},-\mathbf{k}')$. The relative strength of the different components depends on the structure of the spin superfluid state. $V(\mathbf{k},-\mathbf{k}')$ is also temperature dependent. In the case that the superconducting state has s-wave symmetry, the relatively important holon Cooper pairs are those at the bottom of the holon band, i.e., those with small $\mathbf{k}$. For these pairs, the bare pair attractive interaction is

$$V(T)\simeq -t^2(1/N)\sum_{\mathbf{q}} g^2(\mathbf{q})\Delta_{\mathbf{q}}^2/E_{\mathbf{q}}^3 .$$

If the spin superfluid state also has s-wave symmetry, and the quasiparticle excitation spectrum of the spin superfluid state is gapless, as suggested by Zou and Anderson,[2] then $V(T)\propto -\Delta_0^2(T)/[A^2+\Delta_0^2(T)]^{3/2}$, where $\Delta_0(T)$ is the amplitude of $\Delta_{\mathbf{k}}$, and $A=2(tQ+JP)$.

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