Comment on “High-Spin Polaron in Lightly Doped CuO$_2$ Planes”

In a recent Letter, Lau, et al. [1] investigated the single hole problem in an effective model containing Cu d and O 2p orbitals by exact diagonalization on clusters composed of 32 CuO$_2$ unit cells. With full quantum fluctuations due to the antiferromagnetic (AFM) background, they found that spin-polaron solutions with spin 3/2 become lowest energy solutions in certain region of Brillouin zone (BZ), which they claimed no similar solutions were obtained in other models or approximations before. In this Comment, we would like to point out that such high-spin polaron solutions have been found in our previous Letter [2] published in 2003 and many of features described by Lau et al. have in fact been seen in our Letter.

Starting from the single-band $t-J$ model, we constructed the variational wave function (VWF) for low energy states with single-hole in the AFM background as:

$$|\Psi_1(q_h)\rangle = P_d \sum_{|k| \neq q_h} (A_k a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger + B_k b_{k\uparrow}^\dagger b_{-k\downarrow}^\dagger)|N_{s/2}\rangle^{-1}|0\rangle,$$

(1)

Detailed description of the symbols used in Eq. (1) can be found in our Letter [2]. $q_h$ denotes the hole momentum which is excluded from the sum if $q_h$ is within the spin BZ, otherwise $q_h - Q$ is excluded where $Q = (\pi, \pi)$ is the AFM wave vector. $q_s$ is the momentum of unpaired spin which is present due to the creation of a single hole. $P_d$ here enforces the constraint of no doubly occupied sites.

As shown in Refs. [2, 3], the quasi-particle (QP) states with finite spectral weight can be obtained from Eq. (1) by setting $q_h = q_s$. Energy dispersion of these QP states is quite consistent with the exact solutions of 32 sites for the $t-J$ model [4] and extended $t-J$ model [5, 6]. Comparing the energy dispersion and the spectral weight presented in Figs. 2 and 4 in Ref. [3] with those shown in Fig. 2 in Lau’s Letter [1], it is clear that these two results also agree with each other nicely. Especially, the features that QP states have the lowest energy at $(\pi/2, \pi)$ and smallest spectral weight at $(\pi, \pi)$ are well-captured by our VWFs.

In addition to QP states, we obtained another different set of states, namely the spin-bag (SB) states, by choosing $q_h \neq q_s$. As explained in our Letter [2], the SB states can be viewed as exciting a spin wave with momentum $k' = q_s - q_h$ on top of a QP state with momentum $q_h$. These SB states carrying almost negligible spectral weight was also discussed in the paper. This construction is in complete agreement with the concept of high-spin polaron 3/2 states presented in Lau’s Letter.

Furthermore, we found that the spin-bag states could be the lowest energy states in certain region of BZ, and interestingly the discussion given in Lau’s Letter about the energy difference between spin 3/2 and 1/2 states along the direction from (0, 0) to $(\pi/2, \pi)$ and then to $e(π, π)$ matches almost perfectly with our results on QP and SB states shown in Fig. 1 in our Letter [2].

By assuming that a Zhang-Rice singlet [6] could be formed by superimposing the weight of four nearest neighbor oxygen, we could calculate the spin-spin correlations based on Lau’s Fig. 3(a). The values of -0.225 and -0.273 are obtained for the e and d bonds defined in the inset of Fig. 2 in [2]. These are fairly compatible with our data of -0.215 and -0.224 respectively, although different parameters were used in the two calculations.

Since almost all the low energy states presented by Lau et al. are consistent with our results on a single-band $t-J$ model, the claim of the breakdown of Zhang-Rice singlet is not convincing. In our viewpoints, the smoking gun signature proving the breakdown of Zhang-Rice singlet should be a calculation showing that non-bonding state of Cu spin with its four neighboring oxygen holes indeed has lower or comparable energy with the Zhang-Rice singlet. Such a calculation, up to our knowledge, has never been reported to date.

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