Comment on "Quantum Monte Carlo Evidence for Superconductivity in the Three-Band Hubbard Model in Two Dimensions"

In a recent Letter, Kuroki and Aoki [1] presented quantum Monte Carlo (QMC) results for pairing correlations in the three-band Hubbard model, which describes the Cu-$d_{x^2-y^2}$ and O-$p_{x,y}$ orbitals present in the CuO_2 planes of high-T_c materials. In this Comment we concentrate on the parameter set $U_d = 3.2t_{pd}, \Delta = 2.7t_{pd}, t_{pp} = -0.4t_{pd}$. For this parameter choice, Kuroki and Aoki see a maximal increase in the $d_{x^2-y^2}$ pairing correlations which they associate with a signature of off-diagonal long-range order (ODLRO). We argue that:

(i) The above parameter set is not appropriate for the description of high-T_c materials since it does *not satisfy the minimal requirement of a charge-transfer gap at half-filling.* To illustrate this point, we have calculated with QMC methods the average hole number as a function of the chemical potential: $\langle n\rangle(\mu)$. Our results, which are plotted in Fig. 1, show a vanishingly small charge-transfer gap (i.e., $\Delta_{\rm ct} < 0.07t_{pd}$). In contrast, for a physical parameter set [2], one obtains a sizable charge-transfer gap which is detectable from the plateau in the $\langle n\rangle(\mu)$ curve (see inset, Fig. 1). For the latter parameter set, a number of normal state properties were shown to successfully reproduce experimental data [3]. However, despite intensive numerical efforts, no ODLRO was unambiguously detected [4].

(ii) *The observed increase in the $d_{x^2-y^2}$ channel* (Fig. 2 in Ref. [1]) *is dominantly produced by the pair-field correlations without the vertex part* [5]. To prove this point we have calculated the pair-field correlations in the d-wave channel summed over distances $\mathbf{r}$ with $|r_x|, |r_y| < R$ $[S_d(R)]$ [see Fig. 2(a)]. As in Ref. [1], an increase as a function of R can be seen. However, the vertex contribution to the pair-field correlations, which is the relevant quantity, is an order of magnitude smaller and shows—within our numerical accuray—no significant increase as a function of R [see Fig. 2(b)]. Hence the claim of evidence of ODLRO is not justified.

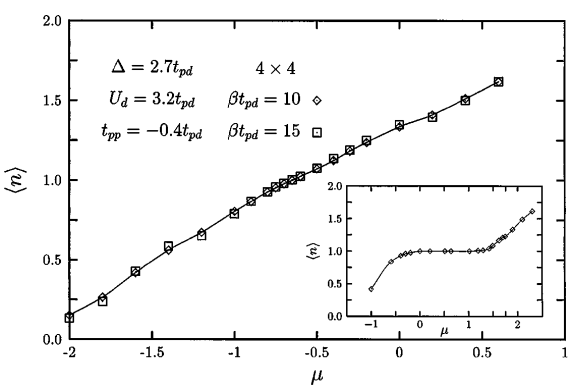

FIG. 1. $\langle n\rangle(\mu)$ on a 4×4 lattice at $\beta t_{pd} = 10, 15$ for the parameter set $U_d = 3.2t_{pd}, \Delta = 2.7t_{pd}, t_{pp} = -0.4t_{pd}$. Inset: $\langle n\rangle(\mu)$ on a 4×4 lattice at $\beta t_{pd} = 10$ for $U_d = 6t_{pd}, \Delta = 4t_{pd}, t_{pp} = 0.0$ [2].

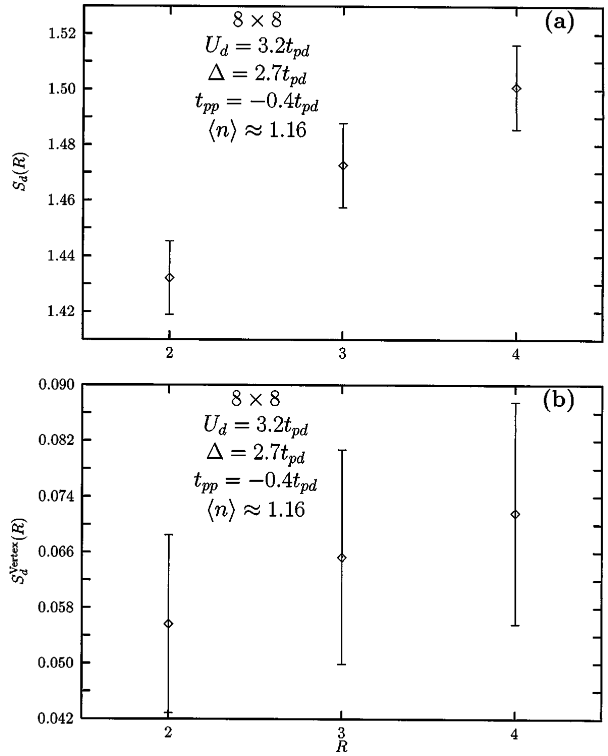

FIG. 2. (a) $S_d(R)$ on an 8×8 lattice at zero temperature and $U_4 = 3.2t_{pd}, \Delta = 2.7t_{pd}, t_{pp} = -0.4t_{pd}$. (b) Vertex contribution to $S_d(R)$ shown in (a).

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H. Endres,[1] W. Hanke,[1,2] H. G. Evertz,[1] and F. F. Assaad[2]
[1]Physikalisches Institut
Universität Würzburg
97074 Würzburg, Germany
[2]Department of Physics
University of California, Santa Barbara
Santa Barbara, California 93106-9530

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