Comment on “Odd-parity singlet pairing in the positive-U Hubbard model”

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Comment on "Odd-Parity Singlet Pairing in the Positive-U Hubbard Model"

In a recent Letter [1], Scalettar, Singh, and Zhang (SSZ) proposed a form of pairing state in the doped paramagnetic 2D Hubbard model based on a pairing operator

$$\Delta_x^\eta = 2\sum_{\mathbf{k}} \sin(k_x) c_{\mathbf{k}\uparrow} c_{-\mathbf{k}+\mathbf{Q}\downarrow} \tag{1}$$

having net center-of-mass momentum $\mathbf{Q}=(\pi,\pi)$ and spin zero. This anomalous pairing was motivated by Monte Carlo results for a 4×4 lattice which exhibits enhancement of the correlation $\langle \Delta_x^{\eta\dagger} \Delta_x^\eta \rangle$ more strongly than other channels previously considered. It was stated that such a pairing state breaks both parity and time-reversal symmetries.

In this Comment, we point out that when proper account is taken of the quasiparticle dressing in the normal phase (a large energy compared to the superconducting condensation energy) the ground state will exhibit conventional $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ pairing, with $(\mathbf{k}\uparrow, -\mathbf{k}+\mathbf{Q}\downarrow)$ leading to an exponentially lower T_c.

The BCS theory is based on pairing of quasiparticles of the normal phase [2]. Recently [3], it has been shown how quasiparticle (hole) operators can be constructed in such systems as

$$\gamma_{\mathbf{k}s} = v_{\mathbf{k}} c_{\mathbf{k}s} + \frac{1}{\sqrt{N}} \sum_{\mathbf{q},s'} u_{\mathbf{k}\mathbf{q}}^{ss'} c_{\mathbf{k}+\mathbf{q},s'} (\boldsymbol{\sigma}\cdot\mathbf{S}_{\mathbf{q}})^{s's} + \cdots . \tag{2}$$

$\mathbf{S}_{\mathbf{q}}$ is the spin-density operator defined as $\mathbf{S}_{\mathbf{q}} = (1/\sqrt{N})\sum_{\mathbf{m}} e^{i\mathbf{m}\cdot\mathbf{q}} \mathbf{S}_{\mathbf{m}}$, where $\mathbf{m}$ labels sites of a lattice of N sites and $u_{\mathbf{k}\mathbf{q}}^{ss'}$ are numbers of order 1. The rest of the notation is standard. The spin degrees of freedom should be thought of as a collective excitation obtained from the Hubbard model, e.g., in the RPA approximation. In the mean-field commensurate antiferromagnet [4], $\mathbf{S}_{\mathbf{q}}$ is taken to be a c number $\sqrt{N}\langle S_{\mathbf{m}}^z\rangle \delta_{\mathbf{q},\mathbf{Q}} (\sigma^z)^{s's}$, i.e., proportional to $\sqrt{N}$.

However, in the paramagnet, matrix elements of $\mathbf{S}_{\mathbf{q}}$ are of order unity for all $\mathbf{q}$. Then, it follows that the admixture of bare states $\mathbf{k}+\mathbf{q}$ into $\mathbf{k}$ is of order $1/\sqrt{N}$ in the paramagnet for any value of $\mathbf{q}$, including $\mathbf{Q}$.

Conventional time-reversal-invariant quasiparticle pairing is given by the operator

$$\Delta_\phi = \sum_{\mathbf{k}} \phi_{\mathbf{k}} \gamma_{\mathbf{k}\uparrow} \gamma_{-\mathbf{k}\downarrow} , \tag{3}$$

where $\phi_{\mathbf{k}}$ is the pair orbital wave function. Inserting Eq. (2) into Eq. (3) one finds

$$\Delta_\phi = \sum_{\mathbf{k}} \phi_{\mathbf{k}} \left[v_{\mathbf{k}} v_{-\mathbf{k}} c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} + \frac{v_{-\mathbf{k}}}{\sqrt{N}} \sum_{\mathbf{q},s'} u_{\mathbf{k}\mathbf{q}}^{\uparrow s'} (\boldsymbol{\sigma}\cdot\mathbf{S}_{\mathbf{q}})^{s'\uparrow} c_{\mathbf{k}+\mathbf{q},s'} c_{-\mathbf{k}\downarrow} + \cdots \right] . \tag{4}$$

The cross terms are similar to those of SSZ except that all $\mathbf{q}$'s enter, each with weight $1/\sqrt{N}$. Using the expansion equation (4) to calculate the correlation function $\langle \Delta_\phi^\dagger \Delta_\phi \rangle$, one finds anomalous pairing fluctuations involving terms proportional to, for example,

$$(1/\sqrt{N}) \langle c_{\mathbf{k}+\mathbf{q}\uparrow} c_{-\mathbf{k}\downarrow} c_{-\mathbf{k}\uparrow} c_{\mathbf{k}+\mathbf{q}'\downarrow} S_{\mathbf{q}'}^z S_{\mathbf{q}}^z \rangle . \tag{5}$$

Using the fact that the matrix elements of $c_{\mathbf{k}s}$ and $S_{\mathbf{q}}^z$ are of order 1, one sees that while this anomalous correlation function is finite for small N, it vanishes when $N \to \infty$. This behavior is supported by numerical studies in the Hubbard model.

A second possibility is to pair γ's rather than c's in Eq. (1). While this prescription is fully equivalent to the $\gamma_{\mathbf{k}\uparrow}\gamma_{-\mathbf{k}\downarrow}$ pairing in the ordered antiferromagnet, where $-\mathbf{k}$, and $-\mathbf{k}+\mathbf{Q}$ are the identical state, this is no longer true in the paramagnet. In fact, the $-\mathbf{k}+\mathbf{Q}$ state is a shadow band state [6] whose residue in the propagator is weaker than that of $-\mathbf{k}$ in the actual band. This leads to a weaker pairing attraction for the pairing (1) and a lower T_c. Further model and numerical studies will be helpful in substantiating this result.

In conclusion, when the BCS prescription of pairing quasiparticles $\gamma_{\mathbf{k},s}$ of the normal phase is maintained, T_c is maximized and the anomalous nonzero drift momentum of pairs proposed by SSZ in the paramagnetic phase vanishes. We find, instead, steady pair drift, the center of mass of bare electron $c_{\mathbf{k}s}$ pairs appears to recoil as spin fluctuations are emitted and absorbed, with a range of momenta $\mathbf{q}$ spread by an amount $\sim 1/L_{ss}$ about the nesting wave vector $\mathbf{Q}$ of the antiferromagnet.

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