Composite operators for a BCS superconductor

J. Bonča

Theoretical Division, T-11, Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM 87545, and J. Stefan Institute, University of Ljubljana, 61111 Ljubljana, Slovenia

A. V. Balatsky

Center for Materials Science and Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, and Landau Institute for Theoretical Physics, Moscow, Russia

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A new form of the composite operator which generalizes the Cooper pairs for a BCS superconductor is introduced. This approach is similar to the derivation of the composite operator of the odd-frequency superconductors. Examples of the $d_{x^2-y^2}$, d_{xy}, and p-wave composite operators for a 2D t–J model are given.

Recently the notion of a composite operator as a generalization of the Cooper pair in the theory of superconductivity has been proposed.[1–4] Examples of the composite operators are

$$\Delta=\begin{cases}\langle \mathbf{S}(\mathbf{i})c_\alpha(\mathbf{j})c_\beta(\mathbf{k})\rangle(i\sigma^y\vec{\sigma})_{\alpha\beta}; & S=0\\ \langle \mathbf{S}(\mathbf{i})c_\alpha(\mathbf{j})c_\beta(\mathbf{k})\rangle(\sigma^x\vec{\sigma})_{\alpha\beta}; & S=1,\quad S_x=0\end{cases}. \tag{1}$$

These composite operators describe the bound state of the spin excitation at site **i** and a triplet or a singlet Cooper pair at sites **j** and **k**. Clearly, these operators carry a charge $2e$ and thus describe the superconducting ordering. This type of condensate is inherent in the odd-frequency superconductors[1–4] which might be found in strongly correlated systems such as t–J and the Hubbard models. It has been argued that frustration of the magnetic degrees of freedom by carriers may produce enhanced composite pairing correlations for the operators similar[2] to Eq. (1).

The composite operator in the theory of superconductivity represents a new level in the hierarchy of the possible superconducting condensate. Any number of particle-hole (i.e., neutral) operators, together with a Cooper pair operator, have a charge $2e$ and thus can, in principle, describe a superconducting state.[5] Because of this general argument, we point out that the composite operators are possible for BCS superconductors and for odd-frequency superconductors.

The purpose of this note is to show that composite operators similar to Eq. (1) can be constructed in the case of BCS pairing. As an example we consider a 2D t–J model on a square lattice. Previously, a composite operator for the particular case of $d_{x^2-y^2}$ symmetry in a 2D t–J model was considered by Poilblanc.[8] The most relevant for a possible BCS (even-gap) superconductivity in this model are singlets: an extended s-wave (identity representations of D_4 point group symmetry), a $d_{x^2-y^2}$-wave (B_2), and a d_{xy}-wave (B_1). We find that in addition to the standard choice of the pairing state in these channels: $\Delta_{x^2-y^2} = \langle c_{\uparrow \mathbf{k}} c_{\downarrow -\mathbf{k}} \rangle \propto \cos k_x - \cos k_y$; $\Delta_{xy} \propto \sin k_x \sin k_y$, there is a set of composite operators which satisfies all the requirements of the symmetry and spin eigenvalues:

$$\Delta_{R=\sqrt{2}}^{d_{x^2-y^2}} = \sum_{\mathbf{i}} \{ (\mathbf{S}_{\mathbf{i}+\hat{\mathbf{x}}} - \mathbf{S}_{\mathbf{i}+\hat{\mathbf{y}}}) \mathbf{T}_{\mathbf{i},\mathbf{i}+\hat{\mathbf{x}}+\hat{\mathbf{y}}} + (\mathbf{S}_{\mathbf{i}-\hat{\mathbf{x}}} - \mathbf{S}_{\mathbf{i}-\hat{\mathbf{y}}}) \mathbf{T}_{\mathbf{i},\mathbf{i}-\hat{\mathbf{x}}-\hat{\mathbf{y}}} + (\mathbf{S}_{\mathbf{i}+\hat{\mathbf{x}}} - \mathbf{S}_{\mathbf{i}-\hat{\mathbf{y}}}) \mathbf{T}_{\mathbf{i},\mathbf{i}+\hat{\mathbf{x}}-\hat{\mathbf{y}}} + (\mathbf{S}_{\mathbf{i}-\hat{\mathbf{x}}} - \mathbf{S}_{\mathbf{i}+\hat{\mathbf{y}}}) \mathbf{T}_{\mathbf{i},\mathbf{i}-\hat{\mathbf{x}}+\hat{\mathbf{y}}} \},$$

$$\Delta_{R=1}^{d_{xy}} = \sum_{\mathbf{i}} \{ (\mathbf{S}_{\mathbf{i}+\hat{\mathbf{x}}+\hat{\mathbf{y}}} - \mathbf{S}_{\mathbf{i}+\hat{\mathbf{x}}-\hat{\mathbf{y}}}) \mathbf{T}_{\mathbf{i},\mathbf{i}+\hat{\mathbf{x}}} - (\mathbf{S}_{\mathbf{i}-\hat{\mathbf{x}}+\hat{\mathbf{y}}} - \mathbf{S}_{\mathbf{i}-\hat{\mathbf{x}}-\hat{\mathbf{y}}}) \mathbf{T}_{\mathbf{i},\mathbf{i}-\hat{\mathbf{x}}} + (\mathbf{S}_{\mathbf{i}+\hat{\mathbf{x}}+\hat{\mathbf{y}}} - \mathbf{S}_{\mathbf{i}-\hat{\mathbf{x}}+\hat{\mathbf{y}}}) \mathbf{T}_{\mathbf{i},\mathbf{i}+\hat{\mathbf{y}}} - (\mathbf{S}_{\mathbf{i}+\hat{\mathbf{x}}-\hat{\mathbf{y}}} - \mathbf{S}_{\mathbf{i}-\hat{\mathbf{x}}-\hat{\mathbf{y}}}) \mathbf{T}_{\mathbf{i},\mathbf{i}-\hat{\mathbf{y}}} \}, \tag{2}$$

$$\Delta_{R=1}^{p_x} = \sum_{\mathbf{i}} (\mathbf{S}_{\mathbf{i}+\hat{\mathbf{x}}} - \mathbf{S}_{\mathbf{i}-\hat{\mathbf{x}}}) (\mathbf{P}_{\mathbf{i},\mathbf{i}+\hat{y}} + \mathbf{P}_{\mathbf{i},\mathbf{i}-\hat{\mathbf{y}}}) \},$$

where $\mathbf{T}_{\mathbf{i},\mathbf{j}} = \frac{1}{i} c_{\mathbf{i},\sigma} (\sigma^y \vec{\sigma})_{\sigma\sigma'} c_{\mathbf{j},\sigma'}$ and $\mathbf{P}_{\mathbf{i},\mathbf{j}} = c_{\mathbf{i},\sigma} (\sigma^x \vec{\sigma})_{\sigma\sigma'} c_{\mathbf{j},\sigma'}$. We used real space representation with $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ being unit vectors in the x and y directions, respectively. In the last of the three equations in (2) we present for completeness the p_x-wave triplet $S_z=0$ composite operator. It is interesting to note that Cooper pairs in Eqs. (2) lie on the symmetry axes of given symmetries, i.e., $x^2-y^2=0$, $xy=0$, $x=0$, respectively.

The symmetry of the above order parameters is exactly the same as that of the standard operators and corresponds to one of the symmetry representations on the square lattice.[7] To describe the derivation of the composite operators of Eq. (2) for a BCS superconductor, we will review the derivation of the composite operators for odd-gap superconductors.[1–4] The general form of the two-particle gap function can be written as

$$\Delta_{\mathbf{ij}}(t) = \langle T_t c_{\mathbf{i}\alpha}(t) c_{\mathbf{j}\beta}(0) \rangle \sigma^y_{\alpha\beta}. \tag{3}$$

Assuming analyticity of the gap function at small $t \to 0$, the latter can be expanded for odd-frequency and BCS channels as[2]

$$\Delta_{\mathbf{ij}}^{\mathrm{odd}}(t) = \Delta_{\mathbf{ij}}^{(1)} t + \mathcal{O}(t^3) \tag{4}$$

$$\Delta_{\mathbf{ij}}^{\mathrm{even}}(t) = \Delta_{\mathbf{ij}}^{(0)} + \frac{1}{2} \Delta_{\mathbf{ij}}^{(2)} t^2 + \mathcal{O}(t^4). \tag{5}$$

For odd-frequency pairing after taking the time derivative

$$\left. \frac{\partial \Delta_{\mathbf{ij}}^{\mathrm{odd}}(t)}{\partial t} \right|_{t=0} = \Delta_{\mathbf{ij}}^{(1)} \propto \langle [H, c_{\mathbf{i}\alpha}] c_{\mathbf{j}\beta} \rangle \sigma^y_{\alpha\beta}$$

we obtain the composite operator. Here we restrict the analysis to the singlet case. The generic form of the composite operator is always as in Eq. (1); however, the details will depend on the Hamiltonian H (for more details in the case of the t–J model see, for example, Ref. 2).

To obtain the composite operators for even frequency or BCS pairing (2), we must to take the second-order time derivative

$$\Delta_{ij}^{(2)} = \frac{\partial^2 \Delta_{ij}^{\text{even}}(t)}{\partial t^2}\bigg|_{t=0} \propto \langle [H,(H,c_{i\alpha})] c_{j\beta}\rangle \sigma^{y}_{\alpha\beta}. \tag{6}$$

We obtain the composite operator in the form of Eq. (2) by taking as the first commutator the hopping term $H_t = t\Sigma_{ij} c^{\dagger}_{i\sigma} c_{j\sigma}$ and as the second commutator the Heisenberg term $H_j = J\Sigma_{ij} \mathbf{S}_i \mathbf{S}_j$. The commutator $[H_t, c_{i\alpha}]$ moves the particle to the neighboring site which may lie on the main symmetry axis. The second commutator with $[H_J,(H_t,c_{i\alpha})]$ produces an extra spin operator. From $[\mathbf{S}_i, c_{i\alpha}] = (-\frac{1}{2})\vec{\sigma}_{\alpha\nu} c_{i\nu}$ we find $[H_J, c_{i\alpha}] = -J\Sigma_{\langle ik\rangle} \mathbf{S}_k \vec{\sigma}_{\alpha\nu} c_{i\nu}$, from which directly follows the general structure of the operators in Eq. (2) as the composite operators of a Cooper pair with an attached spin operator. A direct check reveals that these composite operators satisfy the required symmetry conditions under D_4 point group transformations.

In conclusion, we present the list of composite operators for BCS (even-frequency) pairing, using a 2D *t–J* model as an example. The structure of these composite operators is analogous to the composite operators introduced for the odd-frequency pairing. An important difference between these operators for odd-frequency and BCS pairing is that the composite operator for BCS pairing comes from the dressing of the quasiparticle operator under the assumption that standard equal-time BCS gap function is nonzero. Although this dressing might improve the overlap with the ground state, it does not represent new physics. The situation changes drastically if the usual BCS gap function has a very small or even zero expectation value. In this case the composite BCS operator corresponds to the real "pairing" processes. For the odd-frequency pairing the composite operator represents the equal-time "pairing" in odd-frequency superconductors. It was pointed out in Ref. 2 that the closeness to the instability in the *t–J* model helps the composite channel because of the presence of soft spin fluctuations in the system. Presumably the same situation holds for the composite BCS channels in the frustrated correlated systems.

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[7] We note that the $d_{x^2-y^2}$ form of the composite operator was previously derived by Poilblanc.[8]

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