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PHYSICS

On Calculating Spectral Intensities for Anomalous Average Values in the Theory of Superconductors with Strong Electron Correlations

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In this paper, we show that allowance for properties of the Hubbard operator algebra leads to the appearance of a singular (at $\omega = 0$) component in the total spectral intensity of the anomalous correlation function of superconductors that possess the electron pairing mechanism. In this case, the spectral theorem acquires the form of a singular integral equation. Taking these features into account, we can eliminate previously claimed forbidding of realization of the superconducting phase with the *S*-type symmetry of the order parameter.

1. While constructing a theory of high-temperature superconductors which is based on the electron pairing mechanism, the two following methods are most widely employed. The first approach uses the diagram technique for Hubbard operators [1, 2]. The second one is based on the formalism of irreversible retarded two-time Green's functions [3]. Previously, the scattering amplitude calculated for the Hubbard model [4] in the regime of strong electron correlations [1] was analyzed in the paramagnetic phase. It was shown that in the Cooper channel, this amplitude has a singularity corresponding to the transition into the superconducting phase (Zaĭtsev mechanism) [2]. While analyzing this phase on the basis of retarded Green's functions, the spectral theorem [5] was used, which made it possible to obtain self-consistency equations for calculating normal and anomalous average values. It turned out that at $f = g$, the anomalous average values $\langle X_{\mathbf{g}}^{0\sigma} X_{\mathbf{f}}^{0\bar{\sigma}}\rangle$, ($X_{\mathbf{g}}^{0\sigma}$ and $X_{\mathbf{f}}^{0\bar{\sigma}}$ are Hubbard operators [6]) calculated according to this rule for the superconducting phase with the *S*-type symmetry of the order parameter do not satisfy the evident requirement $\langle X_{\mathbf{f}}^{0\sigma} X_{\mathbf{f}}^{0\bar{\sigma}}\rangle = 0$ [3]. This violation of the sum rule has constituted the statement on forbidding the superconducting state of the *S*-type.

We now show that the origin of this forbidding is exclusively associated with ignoring the singular (at $\omega = 0$) component of the spectral intensity of the anomalous correlation function $\langle X_{\mathbf{g}}^{0\sigma}(t') X_{\mathbf{f}}^{0\bar{\sigma}}(t)\rangle$. With this statement taken into account, we can satisfy necessary requirements for anomalous correlators in limiting cases without any variation of the form of the previously obtained self-consistency equations for the superconducting phase. The approach developed allows us to overcome problems that arise when describing the superconducting phase with the *S*-type symmetry of the order parameter.

2. Before analyzing features of spectral representations for the correlation functions $\langle X_{\mathbf{g}}^{0\sigma}(t') X_{\mathbf{f}}^{0\bar{\sigma}}(t)\rangle$, we pay attention to the fundamental distinction between the anomalous Green's function in the BCS theory and the anomalous Green's function in the theory of high-temperature superconductivity based on the electron pairing mechanism. The anomalous Green's function constructed on usual Fermi operators of secondary quantization

$$F_{\sigma\bar{\sigma}}(\mathbf{f}t; \mathbf{g}t') = -i\theta(t-t')\langle\{a_{\mathbf{f}\sigma}^{+}(t), a_{\mathbf{g}\bar{\sigma}}^{+}(t')\}\rangle$$

is zero when $t = t' + \delta$, $\delta \to +0$. This is associated with the anti-commutativity of Fermi production operators at coinciding times. At the same time, the time-average values $\langle a_{\mathbf{f}\sigma}^{+}(t) a_{\mathbf{g}\bar{\sigma}}^{+}(t)\rangle$ and $\langle a_{\mathbf{g}\bar{\sigma}}^{+}(t) a_{\mathbf{f}\sigma}^{+}(t)\rangle$ in the superconducting phase can be nonzero in their own right (and opposite in their signs) even at $\mathbf{f} = \mathbf{g}$:

$$\langle a_{\mathbf{f}\sigma}^{+} a_{\mathbf{f}\bar{\sigma}}^{+}\rangle = \eta(\sigma)\langle X_{\mathbf{f}}^{20}\rangle, \quad \langle a_{\mathbf{f}\bar{\sigma}}^{+} a_{\mathbf{f}\sigma}^{+}\rangle = -\eta(\sigma)\langle X_{\mathbf{f}}^{20}\rangle,$$
$$\eta(\sigma) = 2\sigma.$$

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Another situation takes place for the anomalous Green's function constructed on Hubbard operators,

$$\langle\langle X_{\mathbf{f}}^{\bar\sigma 0}(t)|X_{\mathbf{g}}^{\sigma 0}(t')\rangle\rangle = -i\theta(t-t')\langle\{X_{\mathbf{f}}^{\bar\sigma 0}(t), X_{\mathbf{g}}^{\sigma 0}(t')\}\rangle. \quad (1)$$

In this case, for $t \to t' + 0$, the average values $\langle X_{\mathbf{f}}^{\bar\sigma 0}X_{\mathbf{g}}^{\sigma 0}\rangle$ and $\langle X_{\mathbf{g}}^{\sigma 0}X_{\mathbf{f}}^{\bar\sigma 0}\rangle$ entering into the definition of the Green's function identically vanish as long as the site indices turn out to be equal. It is important that such a situation occurs not by virtue of features of a physical system but as a result of the algebra of the Hubbard operator multiplication. The independence of this fact of particular physical conditions makes it possible to explicitly take it into account at the spectral-representation level.

Keeping in mind this feature, we can write out the spectral intensity $\tilde J_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega)$ in the spectral representation

$$\langle X_{\mathbf{g}}^{\sigma 0}(t')X_{\mathbf{f}}^{\bar\sigma 0}(t)\rangle = \int d\omega \exp\{-i\omega(t-t')\}\tilde J_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega), \quad (2)$$

as

$$\tilde J_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega) = J_{\mathbf{gf}}^{\sigma\bar\sigma} - \delta(\omega)\delta_{\mathbf{fg}}\int d\omega_1 J_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega_1)\exp(-i\omega_1\delta), \quad \delta \to +0. \quad (3)$$

This form ensures the elimination of the right-hand side in expression (2) at $t = t' + \delta$, $\delta \to +0$ as far as $\mathbf{f} = \mathbf{g}$ and provides the basic distinction of the introduced spectral representation form that usually is applied in the theory of two-time temperature Green's functions [5].

We now on the basis of representation (2) are able construct the spectral representation of the anomalous correlation function $\langle X_{\mathbf{f}}^{\bar\sigma 0}(t), X_{\mathbf{g}}^{\sigma 0}(t')\rangle$. In this case, using the property of cyclic transpositivity of operators under the trace sign, we obtain from representation (2)

$$\langle X_{\mathbf{f}}^{\bar\sigma 0}(t)X_{\mathbf{g}}^{\sigma 0}(t')\rangle = \int d\omega \exp\{-i\omega(t-t')\} \times\{J_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega)\exp(\beta\omega) - \delta(\omega)\delta_{\mathbf{fg}}S_{\mathbf{fg}}^{\bar\sigma\sigma}\}, \quad (4)$$

$$S_{\mathbf{fg}}^{\bar\sigma\sigma} = \int d\omega_1 J_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega_1)\exp(\beta\omega_1)\exp(-i\omega_1\delta), \quad \beta = \frac{1}{T}, \quad \delta \to +0. \quad (5)$$

It is seen that also in this case, for $\mathbf{f} = \mathbf{g}$ and $t \to t' + 0$, as it must, the right-hand side vanishes, and $\langle X_{\mathbf{f}}^{\bar\sigma 0}X_{\mathbf{f}}^{\sigma 0}\rangle = 0$.

Applying spectral representations (2) and (4), we find the expression for the average value of the anticommutator entering into the definition of the anomalous Green's function:

$$\langle\{X_{\mathbf{f}}^{\bar\sigma 0}(t), X_{\mathbf{g}}^{\sigma 0}(t')\}_+\rangle = \int d\omega \exp\{-i\omega(t-t')\} \times\{J_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega)[\exp(\beta\omega)+1] - \delta(\omega)\delta_{\mathbf{fg}}\Sigma_{\mathbf{gf}}^{\sigma\bar\sigma}\}, \quad (6)$$

where

$$\Sigma_{\mathbf{gf}}^{\sigma\bar\sigma} = \int d\omega_1 J_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega_1)[\exp(\beta\omega_1)+1] \times\exp(-i\omega_1\delta), \quad \delta \to +0. \quad (7)$$

From definition (1) with allowance for (6), we find the Fourier transform of the anomalous Green's function

$$\langle\langle X_{\mathbf{f}}^{\bar\sigma 0}|X_{\mathbf{g}}^{\sigma 0}\rangle\rangle_\omega = \int \frac{d\omega_1}{\omega - \omega_1 + i\delta} \times\{J_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega)(\exp(\beta\omega)+1) - \delta(\omega)\delta_{\mathbf{fg}}\Sigma_{\mathbf{gf}}^{\sigma\bar\sigma}\}. \quad (8)$$

Hence in this case, the spectral theorem [5] acquires the form of the integral equation with respect to $J_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega)$

$$-\frac{1}{\pi}\frac{\mathrm{Im}\langle\langle X_{\mathbf{f}}^{\bar\sigma 0}|X_{\mathbf{g}}^{\sigma 0}\rangle\rangle_{\omega+i\delta}}{\exp(\beta\omega)+1} = J_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega) - \frac{\partial(\omega)\delta_{\mathbf{fg}}}{\exp(\beta\omega)+1} \times\int d\omega_1 J_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega_1)[\exp(\beta\omega_1)+1]\exp(-i\omega_1\delta). \quad (9)$$

It is easy to see that the solution to this equation can be written out in the form

$$J_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega) = R_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega) + \delta(\omega)\delta_{\mathbf{fg}}\frac{A_{\mathbf{ff}}^{\sigma\bar\sigma}}{\exp(\beta\omega)+1}, \quad (10)$$

where

$$R_{\mathbf{gf}}^{\sigma\bar\sigma}(\omega) = -\frac{1}{\pi}\frac{\mathrm{Im}\langle\langle X_{\mathbf{f}}^{\bar\sigma 0}|X_{\mathbf{g}}^{\sigma 0}\rangle\rangle_{\omega+i\delta}}{\exp(\beta\omega)+1}, \quad (11)$$

and $A_{\mathbf{ff}}^{\sigma\bar\sigma}$ is an arbitrary constant. When deriving (10), we took into account that the equality

$$\int d\omega \exp(-i\omega\delta)\mathrm{Im}\langle\langle X_{\mathbf{f}}^{\bar\sigma 0}|X_{\mathbf{g}}^{\sigma 0}\rangle\rangle_{\omega+i\delta} = 0, \quad (12)$$

which is a part of more generally evident relation

$$\langle\langle X_{\mathbf{f}}^{\bar\sigma 0}(t)|X_{\mathbf{g}}^{\sigma 0}(t')\rangle\rangle_{(t\to t'+\delta)} = \int d\omega \exp(-i\omega\delta)\langle\langle X_{\mathbf{f}}^{\bar\sigma 0}|X_{\mathbf{g}}^{\sigma 0}\rangle\rangle_{\omega+i\delta} = 0 \quad \delta \to +0 \quad (13)$$

takes place.

The ambiguity of the quantity $A_{\mathbf{ff}}^{\sigma\bar{\sigma}}$ is inessential because the total spectral intensity $\tilde{J}_{\mathbf{gf}}^{\sigma\bar{\sigma}}(\omega)$ turns out to be independent of $A_{\mathbf{ff}}^{\sigma\bar{\sigma}}$. Indeed, substituting solution (10) into definition (3), we arrive at

$$\tilde{J}_{\mathbf{gf}}^{\sigma\bar{\sigma}}(\omega) = R_{\mathbf{gf}}^{\sigma\bar{\sigma}}(\omega) - \delta(\omega)\delta_{\mathbf{fg}}\int d\omega_1 R_{\mathbf{gf}}^{\sigma\bar{\sigma}}(\omega_1)\exp(-i\omega_1\delta). \quad (14)$$

In view of this property and also of the fact that according to its form written in (3), $J_{\mathbf{gf}}^{\sigma\bar{\sigma}}(\omega)$ must not contain a singular component at $\omega = 0$, we obtain that the constant $A_{\mathbf{ff}}^{\sigma\bar{\sigma}}$ can be taken to be zero. Thus, it is seen that the analytically continued Fourier transform of the anomalous Green's function determines only the regular part $R_{\mathbf{gf}}^{\sigma\bar{\sigma}}(\omega)$ of the total spectral intensity $\tilde{J}_{\mathbf{gf}}^{\sigma\bar{\sigma}}(\omega)$. In turn, the singular (at $\omega = 0$) component of the total spectral intensity $\tilde{J}_{\mathbf{gf}}^{\sigma\bar{\sigma}}(\omega)$ is unambiguously expressed in terms of $R_{\mathbf{gf}}^{\sigma\bar{\sigma}}(\omega)$, thereby ensuring true values of correlators in limiting cases.

The following fact is of fundamental importance. The singular (at $\omega = 0$) component of the total spectral intensity cannot be determined only from the knowledge of the Fourier transform of the anomalous Green's function, which is analytically continued to the upper complex half-plane. This fact, in essence, is one further example that illustrates the well-known problem of ambiguously reconstructing the spectral intensity of the correlation function according to the spectral theorem. A discussion of particularly relevant examples can be found, e.g., in the review by Rudoĭ, which has entered into the collection of papers [7], as well as in original papers [8, 9]. Practically, the allowance for singular (at $\omega = 0$) components turns out to be necessary in order to obtain true limiting correlator values.

The analysis performed shows that the origin of above-mentioned forbidding for the existence of the superconducting phase with *S*-type symmetry of the order parameter is exclusively caused by the loss of the singular (at $\omega = 0$) component of the correlation function but not by a principle having a certain actual physical content. Consequently, introducing a singular addition overcomes the indicated forbidding without changing the forms of all previously derived equations in the theory of the superconducting state for strongly correlated systems.

Aimed at confirming the statement on the invariability of the self-consistent equations, we note that representation (2) leads to the following expression for simultaneous correlators:

$$\langle X_{\mathbf{f}}^{0\sigma}X_{\mathbf{g}}^{0\bar{\sigma}}\rangle = S_{\mathbf{gf}}^{\sigma\bar{\sigma}} - \delta_{\mathbf{fg}}S_{\mathbf{gf}}^{\sigma\bar{\sigma}}$$
$$= \frac{1}{N}\sum_{\mathbf{q}}\exp\{i\mathbf{q}(\mathbf{f}-\mathbf{g})\}\left\{S_{\mathbf{q}}^{\bar{\sigma}\sigma} - \frac{1}{N}\sum_{\mathbf{k}}S_{\mathbf{k}}^{\bar{\sigma}\sigma}\right\}. \quad (15)$$

This implies that in the quasi-momentum representation, we have

$$\langle X_{\mathbf{q}\sigma}X_{-\mathbf{q}\bar{\sigma}}\rangle = \sum_{(\mathbf{f}-\mathbf{g})}\exp\{-i\mathbf{q}(\mathbf{f}-\mathbf{g})\}\langle X_{\mathbf{f}}^{0\sigma}X_{\mathbf{g}}^{0\bar{\sigma}}\rangle$$
$$= S_{\mathbf{q}}^{\bar{\sigma}\sigma} - \frac{1}{N}\sum_{\mathbf{k}}S_{\mathbf{k}}^{\bar{\sigma}\sigma}.$$

Hence, it follows that the equation

$$\Delta_{\mathbf{k}} = \frac{1}{N}\sum_{\mathbf{q}}\left\{2t_{\mathbf{q}} + \frac{n}{2}(J_{\mathbf{k}+\mathbf{q}} + J_{\mathbf{k}-\mathbf{q}}) + 4\left(1-\frac{n}{2}\right)\frac{t_{\mathbf{k}}t_{\mathbf{q}}}{U} - n\left(\frac{t_{\mathbf{q}}^2}{U} - \frac{J_0}{2}\right)\right\}\langle X_{\mathbf{q}\sigma}X_{-\mathbf{q}\bar{\sigma}}\rangle \quad (16)$$

for the superconducting order parameter *t* – *J** of the model (with due regard to three-center interactions) [10, 11] does not vary with allowance for the singular component of the spectral intensity of the correlation function because

$$\frac{1}{N}\sum_{\mathbf{q}}\left\{\left[2t_{\mathbf{q}} + \frac{n}{2}(J_{\mathbf{k}+\mathbf{q}} + J_{\mathbf{k}-\mathbf{q}}) + 4\left(1-\frac{n}{2}\right)\frac{t_{\mathbf{k}}t_{\mathbf{q}}}{U} - n\left(\frac{t_{\mathbf{q}}^2}{U} - \frac{J_0}{2}\right)\right]\left[\frac{1}{N}\sum_{\mathbf{p}}S_{\mathbf{p}}^{\bar{\sigma}\sigma}\right]\right\} \equiv 0.$$

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