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# Spectral Representations and Description of a Superconducting State with *S*-Type Order Parameter Δ(k)

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The inclusion of a singular contribution to the spectral intensity of the anomalous correlation function is shown to regain the sum rule and remove the unjustified forbidding of the *S*-symmetry order parameter in superconductors with strong correlations. For the order parameter of this symmetry, the solution to the self-consistency equation is analyzed beyond the nearest-neighbor approximation. © *2003 MAIK "Nauka/Interperiodica"*.

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**1.** Among the models describing the main features of a superconducting transition through the nonphonon Cooper pairing mechanism in an electron system with strong correlations, the Hubbard model and the *t–J* model obtained on its basis are most frequently used. It was the Hubbard model that was invoked in [1] to discover a kinematic pairing mechanism for the formation (at $U \longrightarrow \infty$) of a superconducting phase with the order parameter $\Delta_0$ independent of quasimomentum. However, more recently, the possibility of forming such a state was questioned by some theorists, because the solution to the self-consistent equation for the order parameter $\Delta(\mathbf{k}) = \Delta_0$ violates, in their opinion, the requirement that the on-site anomalous mean $\langle X_f^{0\sigma} X_f^{0\bar{\sigma}} \rangle$ of the product of Hubbard operators must be zero.

In this communication, the above statement is analyzed using the spectral representations of the time-dependent anomalous correlation functions. The new point is that the spectral intensity of the anomalous correlation function constructed from Hubbard operators contains, apart from the usual regular part, an additional singular component. It is shown that, after the inclusion of the singular component, the necessary requirements for one-time on-site correlations are fulfilled, on the one hand, and, on the other, neither the equations of motion for the Green's functions nor the self-consistent equation for the superconducting order parameter are affected. The *S*-type superconducting phase will be considered in the non-nearest-neighbor approximation, and it will be shown that the superconducting order parameter (OP) with this symmetry may, in principle, go to zero.

**2.** In the standard notation, the Hubbard Hamiltonian has the form [2]

$$H = \sum_{f\sigma} (\varepsilon - \mu) a_{f\sigma}^{+} a_{f\sigma} + \sum_{fm} t_{fm} a_{f\sigma}^{+} a_{m\sigma} + U \sum_{f} \hat{n}_{f\uparrow} \hat{n}_{f\downarrow}, \tag{1}$$

The scattering amplitude in the strong-correlation regime was calculated for model (1) in [3]. It was found that, in the Cooper scattering channel, this amplitude has a singularity corresponding to the instability against the superconducting transition (Zaĭtsev kinematic mechanism). A set of four equations for the normal and anomalous Green's functions describing the superconducting state in model (1) with a finite *U* was obtained and solved in [4]. In [4], the pairing was caused not only by the electron motion in the lower Hubbard band but also by the electron transitions from the lower to the upper Hubbard subband and by the charge-carrier motion in the upper subband.

At the same time, the superconducting phase with strong correlations can be studied using the effective Hamiltonian [5] constructed in the operator form of the perturbation theory for a small parameter $|t_{fm}|/U \ll 1$. It is known that the corresponding Hilbert space $\tilde{L}$ for $H_{\text{eff}}$ does not contain binary states. As a result, only the anomalous means $\langle X_f^{0\sigma} X_m^{0\bar{\sigma}} \rangle$ appear in the theory of superconducting state, and they must go to zero for the coinciding site indices. The opinion that this phase could not be realized rested on the difficulties caused by the necessity of satisfying this requirement in a superconducting phase with the *S*-symmetry OP.

Leaving aside the physical interpretation of the "strangeness" of the above-mentioned forbidding, we rather analyze the mathematical aspect of the problem. For this purpose, we consider the spectral representations of the temporal anomalous correlation functions and their relation to the Fourier transform of the anomalous two-time Green's function.

First of all, there is a fundamental difference between the anomalous Green's functions in the BCS theory and in the theory of high-$T_c$ superconductivity with the electronic pairing mechanism. The anomalous Green's function of the standard Fermi second-quantization operators

$$F_{\sigma\bar{\sigma}}(ft;gt') = -i\theta(t-t')\langle\{a^+_{f\sigma}(t), a^+_{g\bar{\sigma}}(t')\}\rangle$$

is zero at $t = t' + \delta$ ($\delta \longrightarrow +0$). This is caused by the fact that the creation operators anticommute at the coinciding times. At the same time, the means $\langle a^+_{f\sigma}(t)a^+_{g\bar{\sigma}}(t)\rangle$ and $\langle a^+_{g\bar{\sigma}}(t)a^+_{f\sigma}(t)\rangle$ are nonzero in the superconducting phase even for $f = g$:

$$\langle a^+_{f\sigma}a^+_{f\bar{\sigma}}\rangle = \eta(\sigma)\langle X^{20}_f\rangle, \quad \langle a^+_{f\bar{\sigma}}a^+_{f\sigma}\rangle = -\eta(\sigma)\langle X^{20}_f\rangle.$$

A different situation occurs for the anomalous Green's function with the Hubbard operators:

$$\begin{aligned}&\langle\langle X^{\bar{\sigma}0}_f(t)|X^{\sigma0}_g(t')\rangle\rangle \\ &= -i\theta(t-t')\langle\{X^{\bar{\sigma}0}_f(t), X^{\sigma0}_g(t')\}\rangle.\end{aligned} \quad (2)$$

In this case at $t \longrightarrow t' + 0$, the means $\langle X^{\bar{\sigma}0}_f X^{\sigma0}_g\rangle$ and $\langle X^{\sigma0}_g X^{\bar{\sigma}0}_f\rangle$ are identical zeros for the coinciding site indices. It is essential that this is so not due to the properties of the physical system but due to the multiplication algebra for Hubbard operators. The fact that Eq. (2) is valid regardless of the particular physical system allows it to be explicitly taken into account using the spectral representation.

With this property in mind, the spectral intensity $\tilde{J}^{\sigma\bar{\sigma}}_{gf}(\omega)$ in the spectral representation

$$\langle X^{\sigma0}_g(t')X^{\bar{\sigma}0}_f(t)\rangle = \int d\omega\exp\{-i\omega(t-t')\}\tilde{J}^{\sigma\bar{\sigma}}_{gf}(\omega) \quad (3)$$

can be written in the form

$$\begin{aligned}\tilde{J}^{\sigma\bar{\sigma}}_{gf}(\omega) &= \tilde{J}^{\sigma\bar{\sigma}}_{gf} - \delta(\omega)\delta_{fg}\int d\omega_1 J^{\sigma\bar{\sigma}}_{gf}(\omega_1)\exp(-i\omega_1\delta), \\ &\delta \longrightarrow +0,\end{aligned} \quad (4)$$

providing a zero value for the right-hand side of Eq. (3) at $t = t' + \delta$ ($\delta \longrightarrow +0$) if $f = g$. This is the main distinction between the introduced spectral representation and the representation used in the theory of two-time temperature Green's functions [6].

The following fact is of fundamental importance. The singular component of the spectral intensity cannot be determined solely from the known Fourier transform of the analytic continuation of the anomalous Green's function in the upper complex half plane. This fact provides one more example of the known problem of ambiguous reproduction of the spectral intensity of correlation function from the spectral theorem. The discussion of particular examples of this kind is given, e.g., by Yu.G. Rudoĭ in [7] and in original works [8, 9]. In practice, the inclusion of the singular component is necessary for obtaining the correct limiting values for the correlators.

To prove this statement, we use Eq. (3) to construct the spectral representation for the anomalous correlation function $\langle X^{\bar{\sigma}0}_f(t)X^{\sigma0}_g(t')\rangle$. After the cyclic permutation of operators under the trace sign, one obtains from Eq. (3)

$$\begin{aligned}\langle X^{\bar{\sigma}0}_f(t)X^{\sigma0}_g(t')\rangle &= \int d\omega\exp\{-i\omega(t-t')\} \\ &\times\{J^{\sigma\bar{\sigma}}_{gf}(\omega)\exp(\beta\omega) - \delta(\omega)\delta_{fg}S^{\bar{\sigma}\sigma}_{fg}\},\end{aligned} \quad (5)$$

where

$$\begin{aligned}S^{\bar{\sigma}\sigma}_{gf} &= \int d\omega_1 J^{\sigma\bar{\sigma}}_{gf}(\omega_1)\exp(\beta\omega_1)\exp(-i\omega_1\delta), \\ &\beta = 1/T, \quad \delta \longrightarrow +0.\end{aligned} \quad (6)$$

One can see that the right-hand side turns to zero at $t \longrightarrow t' + 0$ and $f = g$, as it must, and $\langle X^{\bar{\sigma}0}_f X^{\sigma0}_f\rangle = 0$.

By using spectral representations (3) and (5), one obtains the following expression for the average value of the anticommutator appearing in the definition of the anomalous Green's function:

$$\begin{aligned}\langle\{X^{\bar{\sigma}0}_f(t), X^{\sigma0}_g(t')\}_+\rangle &= \int d\omega\exp\{-i\omega(t-t')\} \\ &\times\{J^{\sigma\bar{\sigma}}_{gf}(\omega)[\exp(\beta\omega)+1] - \delta(\omega)\delta_{fg}\Sigma^{\sigma\bar{\sigma}}_{gf}\},\end{aligned} \quad (7)$$

where

$$\begin{aligned}\Sigma^{\sigma\bar{\sigma}}_{gf} &= \int d\omega_1 J^{\sigma\bar{\sigma}}_{gf}(\omega_1)[\exp(\beta\omega_1)+1]\exp(-i\omega_1\delta), \\ &\delta \longrightarrow +0.\end{aligned} \quad (8)$$

From definition (2) and using Eq. (7), one gets for the Fourier transform of the anomalous Green's function:

$$\begin{aligned}\langle\langle X^{\bar{\sigma}0}_f|X^{\sigma0}_g\rangle\rangle_\omega &= \int\frac{d\omega_1}{\omega-\omega_1+i\delta} \\ &\times\{J^{\sigma\bar{\sigma}}_{gf}(\omega)\exp((\beta\omega)+1) - \delta(\omega)\delta_{fg}\Sigma^{\sigma\bar{\sigma}}_{gf}\}.\end{aligned} \quad (9)$$

Consequently, the spectral theorem [6] in our case takes the form of the integral equation for $J^{\sigma\bar{\sigma}}_{gf}(\omega)$:

$$\begin{aligned}-\frac{1}{\pi}\frac{\mathrm{Im}\langle\langle X^{\bar{\sigma}0}_f|X^{\sigma0}_g\rangle\rangle_{\omega+i\delta}}{\exp(\beta\omega)+1} &= J^{\sigma\bar{\sigma}}_{gf}(\omega) - \frac{\delta(\omega)\delta_{fg}}{\exp(\beta\omega)+1} \\ &\times\int d\omega_1 J^{\sigma\bar{\sigma}}_{gf}(\omega_1)[\exp(\beta\omega_1)+1]\exp(-i\omega_1\delta).\end{aligned} \quad (10)$$

One can readily verify that

$$J_{gf}^{\sigma\bar{\sigma}}(\omega) = R_{gf}^{\sigma\bar{\sigma}}(\omega) + \delta(\omega)\delta_{fg}\frac{A_{ff}^{\sigma\bar{\sigma}}}{\exp(\beta\omega)+1}, \quad (11)$$

with

$$R_{gf}^{\sigma\bar{\sigma}}(\omega) = -\frac{1}{\pi}\frac{\mathrm{Im}\langle\langle X_f^{\bar{\sigma}0}|X_g^{\sigma 0}\rangle\rangle_{\omega+i\delta}}{\exp(\beta\omega)+1}$$

satisfies the integral equation for an arbitrary $A_{ff}^{\sigma\bar{\sigma}}$. Here, it is taken into account that the equality

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

being the particular case of a more general relation

$$\langle\langle X_f^{\bar{\sigma}0}(t)|X_g^{\sigma 0}(t')\rangle\rangle_{(t\to t'+\delta)} = \int d\omega \exp(-i\omega\delta)\langle\langle X_f^{\bar{\sigma}0}|X_g^{\sigma 0}\rangle\rangle_{\omega+i\delta} = 0, \quad (13)$$
$$\delta \longrightarrow +0,$$

is valid. The uncertainty in $A_{ff}^{\sigma\bar{\sigma}}$ is immaterial, because the total spectral intensity $\tilde{J}_{gf}^{\sigma\bar{\sigma}}(\omega)$ is independent of $A_{ff}^{\sigma\bar{\sigma}}$. Indeed, substituting solution (11) into definition (4), one obtains

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

Thus, the analytically continued Fourier transform of the anomalous Green's function determines only the regular part $R_{gf}^{\sigma\bar{\sigma}}(\omega)$ of the total spectral intensity $\tilde{J}_{gf}^{\sigma\bar{\sigma}}(\omega)$. In turn, its singular component is uniquely expressed through $R_{gf}^{\sigma\bar{\sigma}}(\omega)$, providing the correct values for the correlators in the limiting cases.

This analysis demonstrates that the above-mentioned forbidding of the superconducting phase with the *S*-symmetry OP is caused by ignoring the singular component of the correlation function, and not by any physical principle. The inclusion of the singular part removes this forbidenness without changing the form of all equations obtained in the theory of superconducting state in strongly correlated systems.

To confirm the statement about the invariability of the self- consistent equations, we note that Eq. (3) leads to the following expression for the one-time correlators:

$$\langle X_f^{0\sigma}X_g^{0\bar{\sigma}}\rangle = S_{gf}^{\bar{\sigma}\sigma} - \delta_{fg}S_{gf}^{\bar{\sigma}\sigma} = \frac{1}{N}\sum_q \exp\{iq(f-g)\}\left\{S_q^{\bar{\sigma}\sigma} - \frac{1}{N}\sum_k S_k^{\bar{\sigma}\sigma}\right\}. \quad (15)$$

This means that, in the quasimomentum representation,

$$\langle X_{q\sigma}X_{-q\bar{\sigma}}\rangle = \sum_{(f-g)}\exp\{-iq(f-g)\}\langle X_f^{0\sigma}X_g^{0\bar{\sigma}}\rangle = S_q^{\bar{\sigma}\sigma} - \frac{1}{N}\sum_k S_k^{\bar{\sigma}\sigma}.$$

It follows that the equation for the superconducting order parameter in the *t*–*J** model (three-center interactions are taken into account) [10, 11]

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

does not change its form after the singular component of spectral intensity is taken into account, because

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

Let us consider the solution to Eq. (16) for the *S*-symmetry OP. Beyond the nearest-neighbor approximation (with the three nonzero hopping parameters), one has

$$t_{\mathbf{k}} = t_1S_1(\mathbf{k}) + t_2S_2(\mathbf{k}) + t_3S_3(\mathbf{k}),$$
$$J_{\mathbf{k}} = J_1S_1(\mathbf{k}) + J_2S_2(\mathbf{k}) + J_3S_3(\mathbf{k}), \quad (17)$$
$$J_i = 2t_i^2/U.$$

Here, $S_i(\mathbf{k})$ are the square-lattice invariants:

$$S_1(\mathbf{k}) = (\cos k_x a + \cos k_y a)/2,$$
$$S_2(\mathbf{k}) = \cos(k_x a)\cos(k_y a),$$
$$S_3(\mathbf{k}) = (\cos 2k_x a + \cos 2k_y a)/2.$$

Taking into account the relation

$$\langle X_{q\sigma}X_{-q\bar{\sigma}}\rangle = \left(\frac{\Delta_{\mathbf{q}}}{2E_{\mathbf{q}}}\right)\tanh\left(\frac{E_{\mathbf{q}}}{2T}\right),$$

one finds that the quasimomentum dependence of the OP in the *S* phase has the form

$$\Delta_{\mathbf{k}} = \Delta_0 + \Delta_1S_1(\mathbf{k}) + \Delta_2S_2(\mathbf{k}) + \Delta_3S_3(\mathbf{k}). \quad (18)$$

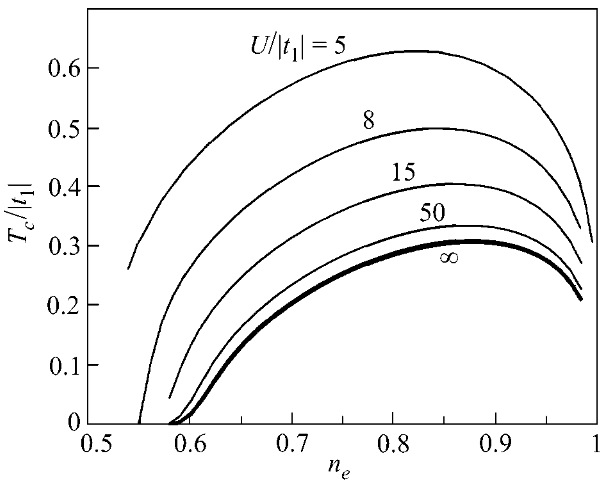


**Fig. 1.** Concentration dependence of the critical temperature for the superconducting transition to the *S* phase with allowance for three hopping integrals.

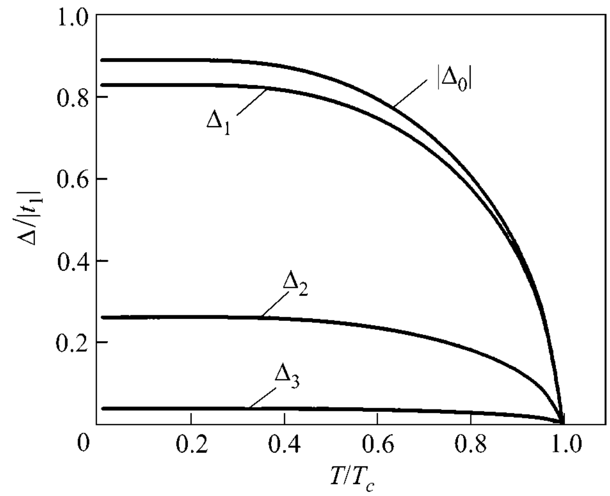


**Fig. 2.** Temperature dependence of the amplitudes $\Delta_i$ ($i$ = 0, 1, 2, 3) of the *S*-symmetry order parameter $\Delta(\mathbf{k})$.

The coefficients $\Delta_i$ ($i$ = 0, 1, 2, 3) are found from the solution to the following set of four equations:

$$\Delta_0 = \sum_{l=0}^{3}\left\{\sum_{j=1}^{3} 2G_{lj}T_j + \frac{n}{2}J_0G_l - \frac{n}{U}\sum_{i,j=1}^{3} G_{lij}T_iT_j\right\}\Delta_l$$

$$(T_j = -4t_j, \quad j = 1, 2, 3),$$

$$\Delta_m = 4\sum_{l=0}^{3}\left\{nJ_mG_{ml} + (1-n/2)T_m\sum_{i=1}^{3} G_{li}T_i/U\right\}\Delta_l, \qquad (19)$$

$$m = 1, 2, 3,$$

where

$$G_i = G_{i00}, \quad G_{ij} = G_{ij0},$$

and

$$G_{ijl} = \frac{1}{N}\sum_{\mathbf{q}} S_i(\mathbf{q})S_j(\mathbf{q})S_l(\mathbf{q})\Psi_{\mathbf{q}},$$

$$\Psi_{\mathbf{q}} = \frac{\tanh(E_{\mathbf{q}}/2T)}{2E_{\mathbf{q}}}, \quad S_0(\mathbf{k}) = 1.$$

The results of the numerical analysis of the superconducting transition temperature as a function of electron concentration is shown in Fig. 1 for various values of the Coulomb repulsion parameter $U$. For finite $U$, the superconducting state is formed through both the Zaĭtsev kinematic [3, 1] and magnetic pairing mechanisms. As $U$ increases, the region of superconducting state diminishes (the magnetic pairing mechanism is suppressed). In the limit of large $U$, only the kinematic mechanism is retained (thick curve). In the calculations, the following values of hopping integrals were used: $t_2/|t_1| = -0.35$ and $t_3/|t_1| = -0.05$.

The temperature behavior of the parameters $\Delta_i$ ($i$ = 0, 1, 2, 3) is demonstrated in Fig. 2 for the same values of hopping integrals, $U/|t_1| = 5$, and $n_e = 0.82$. The chosen electron concentration corresponded to the optimal doping ($T_c/|t_1| = 0.64$). One can see that the absolute values of $\Delta_0$ and $\Delta_1$ are close and nearly compensate each other ($\Delta_0 < 0$). In such a situation, the third term in $\Delta_{\mathbf{k}}$ comes into play. Note also that, due to a complex quasimomentum dependence of $\Delta_{\mathbf{k}}$ and the close values of parameters $\Delta_i$ ($i$ = 0, 1, 2, 3), $\Delta_{\mathbf{k}}$ turns to zero at certain lines in the Brillouin zone. This fact is of interest because it opens up the possibility to obtain the spectrum of elementary excitations in the superconducting phase with the *S*-type symmetry of order parameter and a narrow, or even zero, energy gap. Our preliminary calculations corroborate this assumption; however, because of limited space, the corresponding results will be reported elsewhere.

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## REFERENCES

1. R. O. Zaĭtsev and V. A. Ivanov, Pis'ma Zh. Éksp. Teor. Fiz. **46**, 140 (1987) [JETP Lett. **46**, S116 (1987)].
2. J. C. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1963).
3. R. O. Zaĭtsev, Zh. Éksp. Teor. Fiz. **70**, 1100 (1976) [Sov. Phys. JETP **43**, 574 (1976)].

4. R. O. Zaĭtsev, V. A. Ivanov, and Yu. V. Mikhaĭlova, Fiz. Met. Metalloved. **68**, 1108 (1989).
5. Yu. A. Izyumov, Usp. Fiz. Nauk **167**, 465 (1997) [Phys. Usp. **40**, 445 (1997)].
6. D. N. Zubarev, *Nonequilibrium Statistical Thermodynamics* (Nauka, Moscow, 1971; Consultants Bureau, New York, 1974).
7. *Statistical Physics and the Quantum Theory of Field*, Ed. by N. N. Bogolyubov (Nauka, Moscow, 1973).
8. H. Callen, R. H. Swendsen, and R. Tahir-Kheli, Phys. Lett. A **25**, 505 (1967).
9. P. E. Bloomfield and N. Nafari, Phys. Rev. A **5**, 806 (1972).
10. V. Yu. Yushankhay, G. M. Vujicic, and R. B. Zakula, Phys. Lett. A **151**, 254 (1990).
11. V. V. Val'kov, T. A. Val'kova, D. M. Dzebisashvili, and S. G. Ovchinnikov, Pis'ma Zh. Éksp. Teor. Fiz. **75**, 450 (2002) [JETP Lett. **75**, 378 (2002)].

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