

# Discrete-lattice model approach to the tunneling between d-wave superconductors: interference of tunnel bonds

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The Josephson current between d-wave superconductors is investigated in the framework of tight-binding lattice model. The junction is modelled by a small number of connecting bonds. It is obtained that the Josephson current through one bond vanishes when at least one of the superconductors has (110) interface-to-crystal orientation. Interference between the nearest bonds is appeared to be very important. In particular, it is the interference term that leads to the nonzero Josephson current for (110) orientation. Also, interference of two connecting bonds manifests itself in non-monotonic behavior of the critical Josephson current in dependence on the distance between the bonds.

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Electronic transport through the junctions between high- $T_c$  cuprate superconductors has been the object of interest for many years. In particular, the dc Josephson effect has been intensively studied theoretically [1–5]. These investigations were inspired by the fact that superconducting order parameter dominantly exhibits d-wave symmetry in high- $T_c$  cuprates. This was established by SQUID-like experiments [6] and the tricrystal experiment [7]. Theoretical investigations predicted a number of results, which are the consequences of d-wave nature of superconducting order parameter. For example, the zero-energy Andreev bound state (ZES) is formed at junction interfaces [8], what gives rise to anomalous enhancement of the critical Josephson current in d-wave superconductor junctions at low temperatures [1–3]. Also, for a mirror junction, where the order parameter on the both sides of the junction is rotated by the same angle in opposite directions, a non-monotonic temperature dependence of the critical current was predicted [1–3]. The temperature dependence of the critical current was studied experimentally on the grain boundaries with well-defined lattice orientation [9–12]. For mirror junctions the non-monotonic behavior was found in [12], whereas in other cases a monotonic behavior was reported [9–11]. In addition, for the  $45^\circ$  asymmetric junction a  $\sin 2\varphi$ -like current-phase relation was predicted [3]. However, in the experiments on the asymmetric junctions not all samples exhibit the predicted  $\sin 2\varphi$ -like current-phase relation [12–14].

The theoretical investigations of the Josephson current for the junctions between d-wave superconductors were carried out on the basic of continuous approach

[1–3] as well as making use of tight-binding lattice model [5]. The main results of these methods are consistent with each other for the case of planar junctions. However, the lattice-model approach can not only give a more realistic description of the electronic structure of the copper oxide planes of high- $T_c$  superconductors and allows to mimic the corresponding Fermi surfaces, but it also gives the possibility to study electronic transport through quantum point contacts of various types. The recent advances in the fabrication of nanoscale devices [15–18] (for a review see [19]) has provoked a renewed interest in the detailed analysis of models involving a few conducting channels. Josephson current through quantum point contacts has been investigated in a number of papers since the pioneer work by Beenakker and van Houten [20]. The theory describing a single-mode quantum point contact between two s-wave superconductors in a site representation has been developed in [21–23]. In particular, in [23] single-mode quantum point contact is modelled by the only bond connecting two s-wave superconductors. At the same time, to the best of my knowledge, the junctions between d-wave superconductors through a few connecting bonds have not been considered yet. Also, interference of the connecting bonds has not been investigated by now.

The present paper is devoted to these issues. I consider two d-wave superconductors in a mean-field site representation connected by the only bond or by several bonds in the tunnel limit. It is shown that for the case of several connecting bonds their interference is very important and leads to the non-monotonic (oscillating) behavior of the critical current in dependence on the distance between the bonds. Furthermore, it is found that for the (110) interface-to-crystal orientation

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of at least one of the superconductors the Josephson current through each separate bond vanishes due to the symmetry and the current is entirely determined by the interference term.

The principal scheme of the junction under consideration is shown on the Fig.1. Two superconductors are

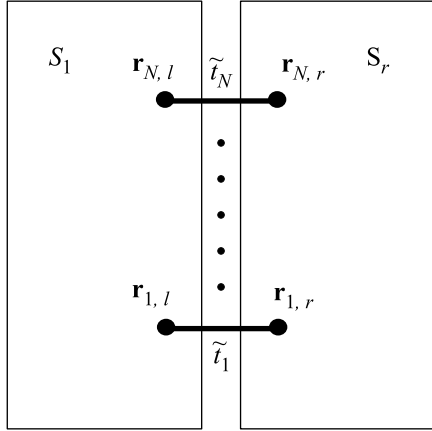


Fig.1. The scheme of the considered junction. Left and right superconductors  $S_l$  and  $S_r$  are connected by the  $N$  bonds with appropriate hopping elements  $\tilde{t}_1, \dots, \tilde{t}_N$

connected by the  $N$  bonds with appropriate hopping elements  $\tilde{t}_1, \dots, \tilde{t}_N$ . Then the full Hamiltonian of the system takes the form

$$\mathcal{H} = \mathcal{H}_l + \mathcal{H}_r + \mathcal{V}, \quad (1)$$

where  $\mathcal{H}_{l,r}$  correspond to the separate half-spaces and  $\mathcal{V}$  contains coupling between them. For the each separate half-space we can use the usual mean-field lattice Hamiltonian in the tight-binding model

$$\mathcal{H}_{l,r} = - \sum_{\mathbf{r},\sigma} \mu c_\sigma^\dagger(\mathbf{r}) c_\sigma(\mathbf{r}) - \sum_{\mathbf{r} \neq \mathbf{r}',\sigma} t_{\mathbf{r},\mathbf{r}'} c_\sigma^\dagger(\mathbf{r}) c_\sigma(\mathbf{r}') + \sum_{\mathbf{r},\mathbf{r}'} \{ \Delta_{\mathbf{r},\mathbf{r}'} c_\uparrow^\dagger(\mathbf{r}) c_\downarrow^\dagger(\mathbf{r}') + h.c. \}. \quad (2)$$

Here  $\mu$  is the chemical potential;  $t_{|\mathbf{r} \neq \mathbf{r}'}$  are the hopping elements. For  $d$ -wave superconductors pairing is assumed to be nonzero only for the nearest neighbors  $\Delta_{\mathbf{r},\mathbf{r} \pm \mathbf{a}} = -\Delta_{\mathbf{r},\mathbf{r} \pm \mathbf{b}} = \Delta_0$ . Here  $\mathbf{r}$  - are the site positions;  $\mathbf{a}$ ,  $\mathbf{b}$  - are the basic lattice vectors ( $|\mathbf{a}| = |\mathbf{b}| = 1$ ). The coupling  $\mathcal{V}$  between the superconductors is modelled by

$$\mathcal{V} = - \sum_{\sigma,i=1 \dots N} \{ \tilde{t}_{\mathbf{r}_{i,l},\mathbf{r}_{i,r}} c_\sigma^\dagger(\mathbf{r}_{i,l}) c_\sigma(\mathbf{r}_{i,r}) + h.c. \}. \quad (3)$$

As we are interested in the Josephson current in such a system, the phase difference  $\phi$  between the supercon-

ductors should be taken into account. It is convenient to include it into the coupling term  $\mathcal{V}$ :

$$\tilde{t}_{\mathbf{r}_{i,l},\mathbf{r}_{i,r}} = \tilde{t}_i e^{i\phi/2}, \quad \tilde{t}_{\mathbf{r}_{i,r},\mathbf{r}_{i,l}} = \tilde{t}_i e^{-i\phi/2}. \quad (4)$$

Then we can assume the superconducting gaps  $\Delta_{l,r}$  and hopping elements  $\tilde{t}_i$  to be real numbers in the whole system.

Let  $\hat{G}(\mathbf{r}, \mathbf{r}') \equiv \hat{G}(\mathbf{x}, \mathbf{x}', \omega_m)$  be the Green's function of the whole system;  $\hat{G}_0(\mathbf{r}, \mathbf{r}')$  is the Green's function of the uncoupled superconductors;  $\hat{G}_b(\mathbf{r}, \mathbf{r}') = \hat{G}_b(\mathbf{r} - \mathbf{r}')$  is the Green's function in the bulk of the superconductors. Then we can represent  $\hat{G}$  via  $\hat{G}_0$  and  $\hat{T}$ -matrix:

$$\hat{G}(\mathbf{r}, \mathbf{r}') = \hat{G}_0(\mathbf{r}, \mathbf{r}') + \sum_{\substack{\alpha,\beta=l,r \\ i,j=1 \dots N}} \hat{G}_0(\mathbf{r}, \mathbf{r}_{i,\alpha}) \hat{T}_{i,j}^{\alpha,\beta} \hat{G}_0(\mathbf{r}_{j,\beta}, \mathbf{r}'). \quad (5)$$

Here all elements are  $2 \times 2$  matrices in particle-hole space. Then it can be derived making use of Eq.(3) that  $T$ -matrix obeys the following equation:

$$\hat{T}_{i,j}^{\alpha,\beta} - \hat{t}_i^\alpha \sum_{\substack{\gamma=l,r \\ k=1 \dots N}} \hat{G}_0(\mathbf{r}_{i,\alpha}, \mathbf{r}_{k,\gamma}) \hat{T}_{k,j}^{\gamma,\beta} = \hat{t}_i^\alpha \delta_{i,j} \delta_{\alpha,\beta}. \quad (6)$$

Here  $\bar{l} = r$ ,  $\bar{r} = l$ , and matrices  $\hat{t}_i^\alpha$  are defined by

$$\hat{t}_i^\alpha = (\hat{t}_i^r)^\alpha = \begin{pmatrix} \tilde{t}_i e^{i\phi/2} & 0 \\ 0 & -\tilde{t}_i e^{-i\phi/2} \end{pmatrix}. \quad (7)$$

By the definition the Green's function  $\hat{G}_0(\mathbf{r}, \mathbf{r}')$  corresponds to the uncoupled superconducting half-spaces. Then we can write

$$\hat{G}_0(\mathbf{r}_l, \mathbf{r}_r) = 0, \quad \hat{G}_0(\mathbf{r}_r, \mathbf{r}_l) = 0, \quad (8)$$

for any  $\mathbf{r}_l \in S_l$  and  $\mathbf{r}_r \in S_r$ . After doing this, we can resolve Eq.(6) in  $(l, r)$ -space:

$$\begin{pmatrix} \check{T}^{r,r} & \check{T}^{r,l} \\ \check{T}^{l,r} & \check{T}^{l,l} \end{pmatrix} = \begin{pmatrix} \check{G}_0^l (1 - \check{G}_0^r \check{G}_0^l)^{-1} \check{t} & (1 - \check{G}_0^l \check{G}_0^r)^{-1} \check{t}^* \\ (1 - \check{G}_0^r \check{G}_0^l)^{-1} \check{t} & \check{G}_0^r (1 - \check{G}_0^l \check{G}_0^r)^{-1} \check{t}^* \end{pmatrix}. \quad (9)$$

Here symbols with the check are  $2N \times 2N$  matrices in particle-hole and  $i, j = 1 \dots N$  spaces. Namely  $\check{T}^{\alpha,\beta} \equiv \hat{T}_{i,j}^{\alpha,\beta}$ ,  $\check{t} = \hat{t}_i^\alpha \delta_{i,j}$  and  $\check{G}_0^\alpha \equiv \hat{t}_i^\alpha \hat{G}_0(\mathbf{r}_{i,\alpha}, \mathbf{r}_{j,\alpha})$ .

Let the  $y$ -axis be along the surface in the  $(a, b)$ -crystal plane and the  $x$ -axis be the normal to surface. Then the functions  $\hat{G}_0^\alpha_{i,j} \equiv \hat{G}_0(\mathbf{r}_{i,\alpha}, \mathbf{r}_{j,\alpha})$  can also be obtained from  $\hat{G}_b$  by the  $\hat{T}$ -matrix technique[24]:

$$\hat{G}_0(x, x', k_y) = \hat{G}_b(x - x', k_y) - \hat{G}_b(x - x_0, k_y) \left[ \hat{G}_b(0, k_y) \right]^{-1} \hat{G}_b(x_0 - x', k_y). \quad (10)$$

Here  $x_0$  is the position of isolating barrier between the superconductors (see [24] for details) and  $\hat{G}_b(x, k_y)$  is the Fourier transform with respect to  $k_x$  of the bulk Green's function  $\hat{G}_b(\mathbf{k})$  ( $\hbar = 1$ ):

$$\hat{G}_b(n, k_y) = \frac{d}{2\pi} \int_{k_x = -\pi/d}^{\pi/d} \hat{G}_b(k_x, k_y) e^{ik_x x d} dk_x. \quad (11)$$

I only consider two possible interface-to-crystal orientations of superconductors: (100) and (110). Then  $d = 1$  for (100) orientation and  $d = 1/\sqrt{2}$  for (110) orientation. Instead of the usual square Brillouin zone  $k_a = [-\pi, \pi]$ ,  $k_b = [-\pi, \pi]$  I now use the surface-adapted Brillouin zone given by  $k_x = [-\pi/d, \pi/d]$  and  $k_y = [-\pi d, \pi d]$ . Then for the following calculations we should transform the Green's function  $\hat{G}_0(x, x', k_y)$  into the full coordinate representation  $\hat{G}_0(\mathbf{r}, \mathbf{r}') = \hat{G}_0(x, x', y - y')$ .

The Josephson current through the barrier can be expressed by ( $G$  - is the upper left part of  $\hat{G}$ ,  $\omega_m = (2m + 1)\pi T$ )

$$J(\phi) = -2ieT \sum_{\omega_m} \sum_{i=1\dots N} (\tilde{t}_{\mathbf{r}_{i,1}, \mathbf{r}_{i,r}} G(\mathbf{r}_{i,r}, \mathbf{r}_{i,1}) - \tilde{t}_{\mathbf{r}_{i,r}, \mathbf{r}_{i,1}} G(\mathbf{r}_{i,1}, \mathbf{r}_{i,r})). \quad (12)$$

Taking into account Eq.(8) it can be obtained from Eq.(5) that

$$\begin{aligned} \hat{G}(\mathbf{r}_{i,r}, \mathbf{r}_{i,1}) &= \sum_{j,k=1\dots N} \hat{G}_0^r{}_{i,j} \hat{T}_{j,k}^{r,l} \hat{G}_0^l{}_{k,i}, \\ \hat{G}(\mathbf{r}_{i,1}, \mathbf{r}_{i,r}) &= \sum_{j,k=1\dots N} \hat{G}_0^l{}_{i,j} \hat{T}_{j,k}^{l,r} \hat{G}_0^r{}_{k,i}. \end{aligned} \quad (13)$$

Then for calculating the Josephson current we only need  $T^{l,r}$  and  $T^{r,l}$  elements of  $T$ -matrix.

Let us consider now the case of one connecting bond (i.e.  $N = 1$ ). Then Eq.(12) can be easily written explicitly (the analogous expression for the case of  $s$ -wave superconductors has been derived in [21]):

$$J(\phi) = 2ieT \sum_{\omega_m} \tilde{t}^2 \frac{F_0^r \bar{F}_0^l e^{i\phi} - \bar{F}_0^r F_0^l e^{-i\phi}}{Z(\tilde{t}, \phi)}, \quad (14)$$

where  $F_0^{l,r}$  and  $\bar{F}_0^{l,r}$  are the off-diagonal elements of  $\hat{G}_0^l$  and  $\hat{G}_0^r$  in particle-hole space:

$$\hat{G}_0^\alpha = \begin{pmatrix} G_0^\alpha & F_0^\alpha \\ \bar{F}_0^\alpha & \bar{G}_0^\alpha \end{pmatrix}. \quad (15)$$

The denominator in Eq.(14) takes the form

$$Z(\tilde{t}, \phi) = 1 - \tilde{t}^2 (G_0^r G_0^l + \bar{G}_0^r \bar{G}_0^l - F_0^r \bar{F}_0^l e^{i\phi} - \bar{F}_0^r F_0^l e^{-i\phi}) + \tilde{t}^4 (G_0^r \bar{G}_0^r - F_0^r \bar{F}_0^r) (G_0^l \bar{G}_0^l - F_0^l \bar{F}_0^l). \quad (16)$$

This denominator leads to high-order powers of transparency (more then first order in  $D \sim |\tilde{t}|^2$ ) and

is responsible for the deviation of the Josephson current from the sinusoidal behavior  $J(\phi) \sim \sin(\phi)$ . But for the particular problem it is more important to consider the numerator of Eq.(14). It includes the anomalous Green's functions of the coinciding space arguments  $F_0^\alpha \equiv F_0(\mathbf{r}^\alpha, \mathbf{r}^\alpha)$  and  $\bar{F}_0^\alpha$  (with  $\alpha = l, r$ ), for uncoupled superconductors. Here  $\mathbf{r}^l$  and  $\mathbf{r}^r$  - are left and right ends of the bond connecting two superconductors. But it is easy to obtain, that for d-wave superconductor with (110) (i.e.  $45^\circ$ ) smooth surface these Green's functions are zero:  $F(\mathbf{r}, \mathbf{r}) = \bar{F}(\mathbf{r}, \mathbf{r}) = 0$ . This takes place due to the symmetry of sites positions and appropriate hopping elements with respect to the reflection  $(y - y_i) \rightarrow -(y - y_i)$  near the considered site  $(x_i, y_i)$  and simultaneous changing sign of order parameter under the reflection. These symmetry relations result in impossibility of flowing the Josephson current through one-bond contact if at least one of the superconductors is a d-wave superconductor with (110) orientation.

The vanishing of one-bond Josephson current between (110) d-superconductors is a consequence of d-wave symmetry of order parameter and has no analogue for the junctions between s-wave superconductors, where the current is nonzero for one-bond contact.

Any reasons which do not change the above symmetry of the system (for example, surface pair breaking) cannot change this statement. But if the symmetry is destroyed, the nonzero one-bond Josephson current arises. If asymmetry is small, then current is small also. The possible reasons, giving the nonzero Josephson current through one-bond contact between (110) d-wave superconductors are: 1) not smooth surface of the superconductor (ends of facets or surface roughness) at the distance of the order of  $\xi_0$  from the bond between the superconductors; 2) the impurities in the bulk or at the surface of the superconductor, also placed not far then  $\xi_0$  from the bond; 3) nonzero  $is$ -component of the order parameter or magnetic field.

Let us consider the tunnel limit, i.e. only take into account the first order of the barrier transparency  $D \sim \tilde{t}^2$ . This means that values  $\tilde{t}_i$  are sufficiently small and we can neglect  $\check{G}_0^\alpha$  in comparison with  $\check{t}$  in Eq.(9). It is worth to note that this approximation fails at sufficiently low temperatures due to the divergence of the Green's function  $\hat{G}_0$  at  $\omega_m \rightarrow 0$  if the particular surface-to-crystal orientation of d-wave superconductor leads to the formation of zero-energy surface bound states.

In the tunnel limit ( $\tilde{t} \ll t$ ; the temperature is not too low in the presence of ZES)

$$\check{T}^{r,l} = \check{t}^*, \quad \check{T}^{l,r} = \check{t}. \quad (17)$$

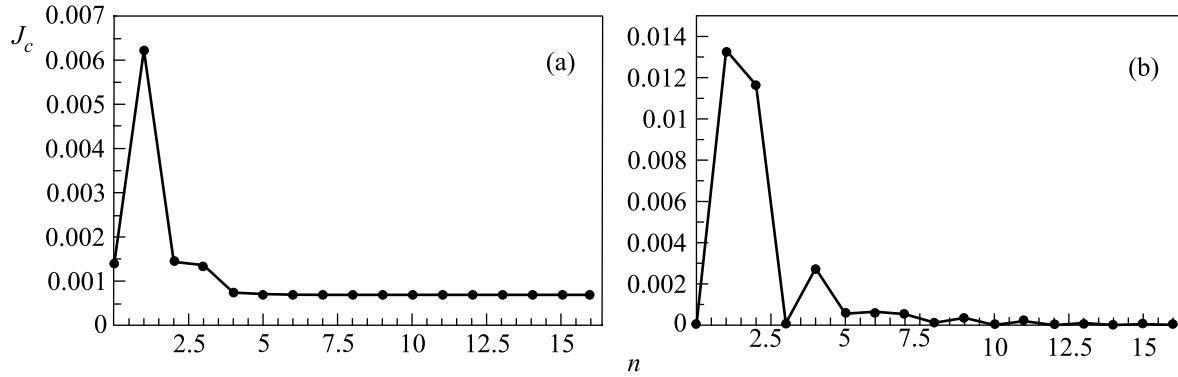


Fig.2. The critical Josephson current in two-bond contact (in units of  $e\Delta_0(T=0)/\hbar$ ) plotted as a function of the distance  $L = nd_y$  between the bonds.  $T = 0.6T_c$ , where  $T_c$  is the superconducting critical temperature. (a) Junction between superconductors with (100) orientation (b) The same for (110) orientation

Then the expression for the Josephson current takes the form:

$$J(\phi) = 2ieT \sum_{\omega_m} \sum_{i,j=1\dots N} \bar{t}_i \bar{t}_j (F_{0,i,j}^r \bar{F}_{0,j,i}^l e^{i\phi} - \bar{F}_{0,j,i}^r F_{0,i,j}^l e^{-i\phi}). \quad (18)$$

It can be seen that Eq.(18) contains two physically different parts. First of them is the sum of the terms, which are proportional to  $\bar{t}_i^2$ . It represents the simple algebraic sum of currents through each bond separately (compare with Eq.(14)). But the other terms are proportional to  $\bar{t}_i \bar{t}_j$  and give the interference part of the current. For the case of the junction with (110)-orientation the interference part is the only non-vanishing term.

Now I turn to the case  $N = 2$ . This is the simplest case for studying of the effects caused by the interference between the connecting bonds. The results are presented for junctions between d-wave superconductors with (100) and (110) orientations. In following the superconducting order parameter is assumed to be spatially constant. Although surface pair breaking is large for (110) surface orientation, this simplification does not change my results qualitatively.

In order to calculate the Josephson current Eq.(18) we need the Green's functions  $F(x, x', y - y')$  and  $\bar{F}(x, x', y - y')$ . They are obtained in the model of nearest neighbors with the parameters  $\Delta_0(T=0) = 0.1t$ ,  $\mu = 0.5t$ . For this set of parameters  $T_c \approx 0.173t$  and  $\Delta_{\max}(T=0) \approx 0.35t$ . I present the results for  $T \approx 0.6T_c$ , where  $\Delta_0(0.6T_c) \approx 0.9\Delta_0(T=0)$ . The hopping parameters for the tunneling bonds are taken to be equal  $t_1 = t_2 = 0.1t$  and the bonds are placed at the distance  $L = nd_y$  from each other. Here  $d_y = d^{-1}$  is the period of lattice along the surface. For (100) orientation  $d_y = 1$  and for (110) orientation  $d_y = \sqrt{2}$ . Bonds

$\bar{t}$  connect the last surface layers of sites of both superconductors, therefore we should take  $x = x' = x_l^{\text{surf}}$  or  $x = x' = x_r^{\text{surf}}$ , where  $x_{l,r}^{\text{surf}}$  are the  $x$ -coordinates of the positions of the last layers in left/right superconductor. The value  $y - y'$  equals 0 for non-interference terms and  $y - y' = \pm L$  for interference terms. Then the critical Josephson current can be written as:

$$J_c = 8eT\bar{t}^2 \sum_{\omega_m} (|F_0|^2 + |F_L|^2). \quad (19)$$

Here the term with  $F_0 \equiv F(y - y' = 0)$  corresponds to the current through each bond separately, while the term with  $F_L \equiv F(y - y' = L)$  corresponds to the interference part of the current. The critical Josephson current described by Eq.(19) is presented on Fig.2. As the current for (110) orientation is entirely due to the interference term, it goes to zero with increasing of the distance between the bonds. At the same time for (100) orientation the current tends to the value determined by the sum of two independent bonds. The interference part of the current oscillates and decays with increasing  $L$  due to the vanishing  $|F_L|$  at  $L \rightarrow \infty$ . It can be seen from Fig.2 that the characteristic distance between the bonds to consider them to be independent is  $\xi_0 \sim t/\Delta_0$ . It is worth to note that the interference part of the critical current is always positive for both orientations considered.

In conclusion, in this paper I have studied the Josephson current through a contact with small number of connecting bonds between two d-wave superconductors. It is obtained that the Josephson current cannot flow through one-bond contact connecting d-wave superconductors of (110) surface-to-crystal orientation with smooth surfaces. The expression for the Josephson current in the junction with arbitrary number of bonds in tunnel limit is found. It is shown that the interfer-

ence between the nearest bonds is very important. The Josephson current in two-bond junction is calculated. It is obtained that the interference of two connecting bonds manifests itself in non-monotonic behavior of the critical Josephson current in dependence on the distance between the bonds and leads to the nonzero Josephson current for (110) orientation.

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