Increasing Superconducting $T_c$’s by a Factor of 1000 with StripeLike Hopping Anisotropies

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We have studied the enhancement of the superconducting transition temperature, $T_c$, in a $t - J - U$ model of electrons moving on a square lattice in which anisotropic electronic hopping is introduced. The inclusion of such hopping mimics, in a approximate fashion, a potentially important characteristic of materials possessing stripelike charge and spin correlations. For this model we have calculated $T_c$ for singlet pairing using the non self-consistent Thouless criterion, and find a dramatic enhancement of $T_c$ induced by hopping anisotropies. Further, the maximum increase in $T_c$ is obtained when the system is pushed towards the extreme anisotropy limit, that is, when the hopping of electrons is confined to occur in $1 + 0^+$ dimensions. We demonstrate that in this limit the increase in $T_c$, with respect to the isotropic system, can be of the order of 1000. We have also determined that in the extreme anisotropy limit the superconducting gap is an equal mixture of $s$ and $d$ pairing symmetries (two choices of such a combination being $s + d$ and $s + id$) owing to the reduced (square to rectangular) symmetry of the system in the presence of hopping anisotropies. Thus, the presence of $d$-wave superconducting features in materials whose symmetry is very different from that of a two-dimensional square lattice, with the anisotropy produced by the appearance of stripes, is not unexpected.

I. INTRODUCTION

Strong support for the existence of stripes in high-$T_c$ cuprates, and other transition-metal oxides, has been provided by many experiments. This leads to the question: Do stripe correlations help, hinder, or even possibly create the pairing instability that leads to superconductivity? In this paper we demonstrate that at least one feature of stripelike correlations strongly enhances the superconducting transition temperature, $T_c$.

A previous examination of the magnetic properties of the very weakly doped cuprates modeled the observed experimental support for stripe correlations using an effective Hamiltonian in which a (spatially) anisotropic exchange interaction was implemented to represent the stripe-induced magnetic energy scales. That is, in the direction parallel to the stripes the full local $Cu – Cu$ exchange would be present, while perpendicular to the stripes a reduced exchange would be encountered across such stripes. Renormalized Hamiltonians of a similar simplifying spirit were also used in other studies of the doped cuprates.

In a recent paper we introduced a model that mimics one aspect of the stripe correlations by incorporating an anisotropic hopping Hamiltonian; that is, carriers are expected to be able to move much more readily along the direction of the stripes, so-called rivers of charge, than perpendicular to the stripes. Allowing the carriers to interact via Heisenberg superexchange (using a two-dimensional $t - J$ model), and excluding double occupancy ($U \to \infty$), we have found exact solutions for the two electron bound-state problem, viz., in the dilute electron density limit. Our calculations demonstrated how stripedlike hopping anisotropies can produce (i) a vanishing value for the threshold exchange coupling, $J_c/t$, that is required for the stabilization of two-particle bound states, and (ii) a dramatic increase in the two-electron binding energies. The physical interpretation of these results is particularly interesting — for the same problem in either one dimension, or in two dimensions with isotropic hopping, a critical superexchange of $J_c/t = 2$ is obtained. However, in the extreme anisotropy limit the electrons are confined to hop in only one lattice direction, and for such a system we found that an infinitesimal $J/t$ produces bound states. The explanation of this result follows from recognizing that in the bound state the two electrons will travel in opposite directions on near-neighbour “chains”, and when they are on near neighbour sites, and have anti-parallel spins, a $S^+ S^-$ spin exchange interaction flips the chains on which the electrons are travelling. An infinitesimal $J/t$ using this mechanism is sufficient to produce a two-electron pair. It is appropriate to think of this result as binding produced by dimensional confinement.

This interesting result naturally leaves us with the task of investigating the transition to a superconducting phase in a system with a nonzero electronic density as the system undergoes a crossover from a two-dimensional to a $1 + 0^+$-dimensional system induced by hopping anisotropies.

In this paper we present the results of our investigation on the effects of such stripedlike hopping anisotropies on $T_c$. We use the non self-consistent Thouless criterion to determine $T_c$, a procedure that is known to reproduce the.
BCS result for the superconducting transition temperature $T_c$. We find a dramatic enhancement of $T_c$ the greater the degree of hopping anisotropy, and the maximum $T_c$ obtained is found to saturate in the extreme anisotropy limit. For certain system parameters, this enhancement can be of the order of 1000! Thus, this simple model of hopping anisotropy, which may be an essential ingredient to stripe correlations, provides a robust demonstration supporting the conjecture that stripes can indeed augment pairing correlations.

II. MODEL HAMILTONIAN

We model stripelike hopping anisotropy in a square lattice of strongly interacting electrons using the following $t - J - U$ model:

$$H = - \sum_{\langle i,j \rangle, \sigma} t_{ij} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) + \sum_{\langle i,j \rangle} J_{ij} (S_i \cdot S_j - \frac{1}{4} n_i n_j) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} .$$  

In this Hamiltonian, the sites of a two-dimensional square lattice of size $L_x \times L_y$ with periodic boundary conditions are labeled by the indices $i$ and $j$, $t_{ij}$ and $J_{ij}$ are the hopping integrals and exchange couplings between sites $i$ and $j$, respectively, $c_{i,\sigma}$ is the annihilation operator for electrons at site $i$ of spin $\sigma$, $n_{i,\sigma}$ is the number operator for electrons at site $i$ with spin $\sigma$, and $U$ is the on-site Hubbard energy.

The most familiar strong-coupling variant of the Hubbard model is the $t - J$ model, and the physics of (square lattice) doped Mott insulators described by this model was reviewed by Dagotto. As emphasized by, e.g., Anderson, a vital component of the $t - J$ Hamiltonian is the constraint of no double occupancy. That is, in the $t - J$ model one does not use the electron creation and annihilation operators of Eq. (1), but rather one uses constrained creation and annihilation operators (for example, see the discussions in Ref. [10]). However, the above $t - J - U$ Hamiltonian can be used to accomplish this same mathematical projection by taking $U \to \infty$ — this simplifying approach has been noted by a variety of researchers (see, e.g., Refs. [12–14]), and will also be used by us.

In this paper we restrict $t_{ij}$ and $J_{ij}$ to be nonzero for near neighbors (NN) only. Further, as we did in Ref. [1], we allow the hopping integral in the $x$ direction, $t_x$, to be different than the hopping integral in the $y$ direction, $t_y$. We have also investigated the physics that arises when $J_x$ is allowed to be different than $J_y$, but find that no qualitatively new physics arises as long as both $J_x$ and $J_y$ remain nonzero. Thus, from now on we set $J \equiv J_x = J_y$, and we analyze the resulting hopping anisotropy problem in terms of

$$t_x \equiv t , \quad r = \frac{t_y}{t} .$$

Thus, we have three dimensionless energy scales in the problem, viz., $U/t$, $J/t$, and $r$; the $U/t \to \infty$ limit reduces this number to two.

III. IDENTIFYING $T_c$ IN THE LADDER APPROXIMATION

We use the non self consistent Thouless criterion [3] to identify the temperature at which our system becomes unstable with respect to a low temperature superconducting phase. To this end, we determine the equation for the two-particle vertex, or effective interaction, in the singlet channel. It is known that at low electron densities [13] one may evaluate the vertex function via the ladder approximation to the Bethe-Salpeter equation, and the lack of convergence of the sum of the ladder diagrams identifies the critical temperature, viz. when the sum converges the system should be in the normal state. The non self consistent formulation of the ladder approximation allows us to work exclusively in the normal state, and has been shown to lead to an identical transition temperature to that found in the BCS theory of superconductivity [3].

Thus, we focus on evaluating the effective interaction $\Gamma$ when all particle-particle diagrams are included. The integral equation for this function in this approximation can be written as (note that we only need to consider $\Gamma_{\uparrow\downarrow}^{\uparrow\downarrow}$ [4], and to eliminate the proliferation of spin indices in the equations that follow from now on we suppress all spin dependencies from our equations)

$$\Gamma(k, k', Q) = V(k - k') - \int \frac{d^3q}{(2\pi)^3} V(k - q) G^0(q) G^0(Q - q) \Gamma(q, k', Q) .$$

The above integral equation is known as the Bethe-Salpeter equation in the ladder approximation [5], and the various functions appearing in this equation are defined as follows: $G^0(q)$ is the zeroth order single-particle Greens function defined by,
\[ G^0(q) = G^0(q, i\omega_n) = \frac{1}{i\omega_n - (\varepsilon_q - \mu)} \quad ; \]

the fermionic Matsubara frequencies are given by \( \omega_n = (2n + 1)\frac{\pi}{\beta} \); for our anisotropic hopping model the single particle dispersion of non-interacting band electrons is given by,

\[ \varepsilon_q = -2t(\cos q_x + r \cos q_y) \quad ; \]

\( \mu \) is the chemical potential.

To proceed to the solution of the Bethe-Salpeter equation, we need to reduce it according to symmetries. That is, the anisotropy that is present in Eq. (1) when \( 0 \leq r < 1 \) reflects a lowering of the point group symmetry of the system from that of a square to that of a rectangle. Recall that the basis functions corresponding to the relevant irreducible representations of the two-dimensional square lattice are 1, \((\cos k_x + \cos k_y)\) and \((\cos k_x - \cos k_y)\), which correspond to on-site s-wave, extended s-wave, and d-wave gap symmetries, respectively. Then note that in our anisotropic model these symmetries are mixed and map onto the fully symmetric \( A_1 \) irreducible representation of the rectangular point group. As a result, it is helpful to decompose the interaction, in the singlet channel (even in \( k \)), according to the basis functions of \( A_1 \) of the rectangular point group symmetry. That is, we artificially set \( J_x \neq J_y \), analyze the resulting interaction in terms of a linear combination of the \( A_1 \) basis functions of 1, \( \cos k_x \), and \( \cos k_y \), and then, in the last step of the calculation, restore the square lattice symmetry of the superexchange interaction by resetting \( J_x = J_y \).

Following this prescription, and focussing on singlet pairing only, we write the bare interaction term \( V(k - k') \) as

\[ V(k - k') = U - 2J_x \phi_x(k)\phi_x(k') - 2J_y \phi_y(k)\phi_y(k') \quad , \]

where \( \phi_x(k) = \cos k_x \) and \( \phi_y(k) = \cos k_y \). Substituting Eq. (3) into Eq. (6) we obtain

\[ \Gamma(k, k', Q) = [U - 2J_x \phi_x(k)\phi_x(k') - 2J_y \phi_y(k)\phi_y(k')] \quad ; \]

\[ - \int \frac{d^2q}{(2\pi)^2} [U - 2J_x \phi_x(k)\phi_x(q') - 2J_y \phi_y(k)\phi_y(q)] G^0(q) G^0(Q - q') \Gamma(q, k', Q) \quad . \]

The above equation is an integral equation for the vertex \( \Gamma(q, k', Q) \), and demonstrates how the irreducible representations of the square lattice group point are mixed in the rectangular phase. To solve this equation we use a standard projection technique (e.g., see Ref. [23]), and setting the total centre-of-mass momentum \( Q = 0 \), we obtain the following set of equations:

\[ \begin{bmatrix} (1 + U\chi_0) - 2J_x \chi_x & -2J_y \chi_y \\ U\chi_x & (1 - 2J_x \chi_xx) - J_y \chi_yx \\ U\chi_y & -2J_x \chi_yx (1 - 2J_y \chi_yy) \end{bmatrix} \begin{bmatrix} C_0(k) \\ C_x(k) \\ C_y(k) \end{bmatrix} = \begin{bmatrix} \chi_0 - 2J_x \chi_x \phi_x(k) & -2J_y \chi_y \phi_y(k) \\ \chi_x (1 - 2J_x \chi_xx \phi_x(k)) & -2J_y \chi_yx \phi_y(k) \\ \chi_y (1 - 2J_x \chi_yx \phi_x(k)) & (1 - 2J_x \chi_yy \phi_y(k)) \end{bmatrix} \]

We will also discuss results obtained in the no double occupancy limit, \( U/t \to \infty \), and in this limit Eq. (8) becomes

\[ \begin{bmatrix} \chi_0 - 2J_x \chi_x & -2J_y \chi_y \\ \chi_x (1 - 2J_x \chi_xx) & -2J_y \chi_yx \\ \chi_y (1 - 2J_x \chi_yx) & (1 - 2J_y \chi_yy) \end{bmatrix} \begin{bmatrix} C_0(k) \\ C_x(k) \\ C_y(k) \end{bmatrix} = \begin{bmatrix} \chi_0 - 2J_x \chi_x \phi_x(k) & -2J_y \chi_y \phi_y(k) \\ \chi_x (1 - 2J_x \chi_xx \phi_x(k)) & -2J_y \chi_yx \phi_y(k) \\ \chi_y (1 - 2J_x \chi_yx \phi_x(k)) & (1 - 2J_x \chi_yy \phi_y(k)) \end{bmatrix} \]

The various functions appearing in the above two equations are defined as

\[ C_0 = \frac{1}{N} \sum_q G^0(q)G^0(\bar{q})\Gamma(q, k) \quad , \]

\[ C_x = \frac{1}{N} \sum_q \phi_x(q)G^0(q)G^0(-q)\Gamma(q, k) \quad , \]

\[ C_y = \frac{1}{N} \sum_q \phi_y(q)G^0(q)G^0(-q)\Gamma(q, k) \quad . \]
The various $\mathbf{Q} = 0$ susceptibilities are functions of $\mu$ and $T$, and are defined by

$$
\chi_0 = \frac{1}{N} \sum_k G^0(k)G^0(-k),
$$

$$
\chi_x = \frac{1}{N} \sum_k \phi_x(k)G^0(k)G^0(-k),
$$

$$
\chi_y = \frac{1}{N} \sum_k \phi_y(k)G^0(k)G^0(-k),
$$

$$
\chi_{xx} = \frac{1}{N} \sum_k \phi_x(k)G^0(k)G^0(-k),
$$

$$
\chi_{xy} = \frac{1}{N} \sum_k \phi_x(k)G^0(k)G^0(-k),
$$

$$
\chi_{yy} = \frac{1}{N} \sum_k \phi_y(k)G^0(k)G^0(-k).
$$

To study the pairing instability we determine the temperature at which a divergence of the vertex $\Gamma(q,k',Q)$ occurs. Clearly, $\Gamma(q,k',Q)$ depends upon the coefficients $C_0$, $C_x$ and $C_y$, defined by Eq. (10), and a singularity in them demands the vanishing of the determinant of the coefficient matrix appearing on the left hand side of Eq. (9); the vanishing of this determinant is thus a simple way in which we can identify the superconducting transition temperature, and hence $T_c$ is obtained numerically as a function of the chemical potential $\mu$. However, a different and perhaps more physical way of displaying our results is to determine $T_c$ as a function of the electron density per lattice site, $n$, and in the BCS approximation $n$ at $T_c$ is given by

$$
n(\mu, T_c) = \frac{2}{\pi} \sum_k \frac{1}{e^{-\beta_\epsilon\left(\epsilon_k - \mu\right)} + 1}.
$$

Below we use this latter equation to plot $T_c$ vs. $n$.

Figure 2 shows our results for $U/t = 0$ and $J/t = 1/3$ (similar results are found for other ratios of $J/t$) with a hopping anisotropy of $r = 0.1, 0.01$, and $0.001$. (We have set $t = 1$ $eV$ as a representative energy; also, this allows us to express $T_c$ in Kelvin.) As is known from the results corresponding to the isotropic case, for $U/t = 0$ the low density ($\mu \sim -4t$) region is dominated by (on-site) $s$-wave pairing; that is to say that the maximum $T_c$ is obtained for $s$-wave pairing, whereas near half filling ($\mu \sim 0$), the $d$-wave instability dominates. As $r$ deviates from the isotropic case, the two pairing symmetries mix and we find a decrease in the values of $T_c$ near half filling, and an enhancement in $T_c$ at low densities. For $r = 0.1$ we see that there still exists a signature of two broad transitions ($d$-wave and on-site $s$-wave). As $r$ decreases further the two transitions merge with a $T_c^{\text{max}} \sim 200K$.

Intermediate ratios of $U/t$ lead to results that smoothly interpolate between $U/t = 0$ and $U/t = \infty$, and in the interests of brevity we only show these two limiting values of $U/t$. $U/t = \infty$ excludes the possibility of an on-site $s$-wave order parameter, hence the pairing symmetry has predominantly extended $s$- and $d$-wave components (see the discussion and numerical results in the next section). Our $T_c$ vs. $n$ results for these parameters are shown in Fig. 2 for the same hopping anisotropies as in Fig. 1.

In both of these figures, it should be noted that when we take the hopping anisotropy to be even smaller than $r = 0.001$, no noticeable change occurs — thus, our numerical results for this ratio are representative of the $r \to 0$ extreme hopping anisotropy limit.

The maximum $T_c$ at low densities, viz. $T_c^{\text{max}} \sim 70K$ (again taking $t = 1eV$) occurs at about $n = 0.08$. As a striking demonstration of the effectiveness of stripelike hopping anisotropy in increasing $T_c$, note for isotropic hopping, $J/t = 1/3$, $U/t = \infty$, and a density of $n = 0.08$ electrons per site, we find that $T_c \sim 0.08K$. That is, we find an enhancement of $T_c$ due to hopping anisotropy of a factor of about 1000! Clearly, this dramatic increase in the superconducting transition temperature supports the conjecture that stripelike correlations can strongly affect pairing, and, at the very least, can greatly augment the stability of the superconducting phase at higher temperatures.
FIG. 1. The dependence of the superconducting transition temperature, \( T_c \), vs. the electronic density per lattice site, \( n \), for \( U/t = 0 \) and \( J/t = 1/3 \). We have set \( t = 1 \) eV and express \( T_c \) in Kelvin. The three curves correspond to anisotropic hopping ratios, \( r \), of \( r = 0.1, 0.01, \) and \( 0.001 \).

FIG. 2. The same as Fig. 1, where the limit \( U/t \rightarrow \infty \) has been implemented.

We note that results demonstrating an enhancement of \( T_c \) due to orthorhombic distortions have been given earlier by Li et al. [19], although the extreme anisotropy limit was not considered; the importance of this latter limit was made apparent to us in our study of the bound-state formation for the same Hamiltonian as in this paper, albeit for only two electrons [7].

We also note that the onset of superconducting pairing caused by interchain single particle tunnelling (IST) has been considered earlier by Bourbonnais and Caron [20]. Starting from a Luttinger Liquid model (a linear array of conducting chains separated by some distance), it was shown in the limit of small interchain hopping IST leads to an effective pair tunnelling which may eventually induce superconductivity in the singlet channel below a temperature \( T_x \) (signifying a crossover to a higher dimensionality, viz., a Luttinger Liquid to Fermi Liquid transition).

In the quasi one-dimensional systems studied in Ref. [20], it was also found the transition temperature, \( T_c \), approximately scaled as \( t_\perp \), the interchain hopping integral, (or as \( (t_\perp)^\alpha \) where \( \alpha (\geq 1) \) is a continuous function of the interaction parameter). Our Fig. 3 shows the variation of the maximum \( T_c \) (as a function of electron density \( n \) vs. hopping anisotropy, \( r \), for \( U/t = 0, 1/3 \) and \( \infty \), and for \( J/t = 1/3 \). The dependence is found to be roughly linear, thus providing some support for the conjecture made by Bourbonnais et al. [20].
FIG. 3. The maximum $T_c$, found as a function of electronic density for each hopping anisotropy $r$, for $U/t = 0, 1/3$ and $\infty$ and $J/t = 1/3$. As in Figs. 1 and 2, we have expressed $T_c$ in Kelvin using $t = 1$ eV.

IV. BCS GAP EQUATION

As mentioned earlier, anisotropic hopping couples the superconducting gaps in the $s$- and $d$-wave channels, and this leads one to think in terms of a mixing between the two symmetries having the following forms [19,21,22]: (i) an $s + id$ state, where there is a phase difference of $\pi/2$ between the gap functions in $s$- and $d$-channels, and (ii) an $s + d$ state, where the phase difference is zero.

We have evaluated the ratio of these gaps by solving the zero temperature BCS gap equation, which can be written as,

$$\Delta(k) = - \sum_{k'} V(k, k') \frac{\Delta(k')}{2E_{k'}} ,$$

(13)

where $E_k = \sqrt{(\varepsilon_k - \mu)^2 + |\Delta(k)|^2}$. Note that in the $U/t \to \infty$ limit, the on-site $s$-wave component is suppressed and one is left to consider only the extended $s$- and the $d$-wave symmetries. For simplicity, in this section we only report on this region of parameter space ($U/t \to \infty$). This allows us to write the trial gap function in $k$-space with arbitrary phase difference $\theta$ in the form,

$$\Delta(k) = \Delta_s f_s(k) + e^{i\theta} \Delta_d f_d(k) ,$$

(14)

with $\Delta_s$ and $\Delta_d$ representing the amplitudes of the gap functions, which are real, and

$$f_s(k) = \cos k_x + \cos k_y ,$$

(15)

$$f_d(k) = \cos k_x - \cos k_y .$$

Ignoring the on-site term, we write the interaction in terms of the above-defined basis functions:

$$V(k, k') = V(k - k') = -2J[\cos(k_x - k_x') + \cos(k_y - k_y')]$$

$$= -J[f_s(k)f_s(k') + f_d(k)f_d(k')] .$$

(16)

Using Eqs. (14-16) in Eq. (13), one can take the real and imaginary parts of Eq. (13), and thus obtain coupled equations for $\Delta_s$ and $\Delta_d$. We have solved these equations numerically for both choices of the relative phase $\theta$, viz. $\theta = \pi/2$ (corresponding to $s + id$) and $\theta = 0$ (corresponding to $s + d$).

Our numerical results for the ratio of gap amplitudes for $s + id$ are shown in Fig. 4 — since the results for $s + d$ are qualitatively very similar, for brevity we omit that plot. The $r = 0.1$ case corresponding to the $s + d$ symmetry shows...
a variation in the ratio $\Delta_s/\Delta_d$ from $\sim 0.8$ ($\sim 0.6$ for $s + d$) for electronic densities near half filling, to $\sim 1.3$ ($\sim 1.3$ for $s + d$) for $\mu \approx -2t(1 + r)$ (low densities). Thus, at low densities the extended $s$-wave contribution is somewhat larger, whereas near half filling the $d$-wave component is stronger. As the anisotropy is increased, the ratios $\Delta_s/\Delta_d$ for both $s + id$ and $s + d$ become almost equal to unity for all densities.

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We note that similar results have been obtained earlier using variational Monte Carlo studies using a $t - J$ model [19] where the authors found no distinguishable difference between $s + d$ and $s + id$ pairing symmetries. More generally, they found that this result was true for any arbitrary $\theta$ in Eq. (13).

At this stage we cannot ascertain which of the above pairing states is chosen by the system in presence of hopping anisotropy, so there is a necessity to calculate the condensation energies for these pairing symmetries using a microscopically derived Ginzburg-Landau free energy functional — we leave this problem for a future publication.

V. CONCLUSIONS

To conclude, we find a dramatic enhancement of the superconducting transition temperature, $T_c$ at low electronic densities due to stripelike hopping anisotropies. Also, we find that the maximum $T_c$ is found to saturate as $r \rightarrow 0$, that is, in the extreme anisotropy limit. In fact, one can show that $T_c$ tracks the electronic density of states, consistent with the fact that our determination of the superconducting instability is essentially a mean-field theory. As the hopping anisotropy mixes different pairing symmetries, such as on-site $s$-wave, extended $s$-wave, and $d$-wave, it is expected that the system may choose either a $s + d$, or $s + id$, or more generally a pairing of the form $\Delta_s(k) + e^{i\theta} \Delta_d(k)$, where $\theta$ may be a function of temperature and anisotropy. To shed some light on this issue we have solved the zero temperature BCS gap equation and have evaluated the ratio between the gap amplitudes. Our results demonstrate an equal mixing between the $s$ and $d$ gap functions in the extreme anisotropy limit.

We do not wish to give the impression that we believe that this model is an adequate way of modelling the effects that stripelike rivers of charge create. For example, we have ignored all features associated with the discreteness of the stripes. Also, although we are including a near-neighbour antiferromagnetic exchange, the ladder approximation that we are using to determine a pairing instability will not be adequate near half filling, and thus our theory is not just for a moderately doped antiferromagnet.

Nonetheless, the results that we published in Ref. [7] on two-electron bound state formation, as well as the substantial increase in $T_c$ that we are presenting in this paper, demonstrate the possible importance of including stripelike hopping anisotropies in realistic microscopic theories.
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