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## *p*-wave superconductivity in a two-dimensional generalized Hubbard model

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## Abstract

In this Letter, we consider a two-dimensional Hubbard model that includes a second-neighbor correlated hopping interaction, and we find a triplet *p*-wave superconducting ground state within the BCS formalism. A small distortion of the square-lattice right angles is introduced in order to break the degeneracy of  $k_x \pm k_y$  oriented *p*-wave pairing states. For the strong coupling limit, analytical results are obtained. An analysis of the superconducting critical temperature reveals the existence of an optimal electron density and the gap ratio exhibits a non-BCS behavior. Finally, the particular case of strontium ruthenate is examined. (© 2005 Elsevier B.V. All rights reserved.

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The Hubbard model is perhaps the most used starting point to study many correlated electronic phenomena, such as magnetism in solids [1], superconductivity [2], charge and spin density waves [3]. In particular, the negative-U Hubbard model only leads to *s*-symmetry superconductivity, and the introduction of a negative-V term, i.e., an attractive interaction be-

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tween nearest neighbors, can produce anisotropic superconducting states. However, this later model has an intrinsic defect in favouring phase separation, which inhibits the formation of the superconducting ground state as the strength of the attraction grows [4]. On the other hand, it has been shown [5] that the correlated first-neighbor hopping interaction can induce an extended *s*-wave superconducting ground state without attractive density–density interactions. Recently, we have found that a small correlated second-neighbor interaction can lead to a *d*-wave superconductivity

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in square lattices [6]. However, it has been stated that triplet *p*-wave pairing never occurs in the twodimensional Hubbard model [7]. In this Letter, we report for the first time a *p*-wave superconducting ground state induced by a small distortion of the square-lattice right angles within the Hubbard model. It would be worth mentioning that a structural distortion has been observed at the surface of the  $Sr_2RuO_4$ [8], a *p*-wave superconducting material, although it is not clear its occurrence in the bulk.

The *d*-wave superconductivity has also been obtained by using the spin fluctuation technique within the standard Hubbard model [9–11]. Nevertheless, the picture that strong ferromagnetic spin fluctuations mainly induce the *p*-wave superconductivity may not be appropriate [12,13], since the spin fluctuations have turned out to be more like antiferromagnetic than ferromagnetic [14]. Indeed, the spin-triplet superconductivity in Sr<sub>2</sub>RuO<sub>4</sub> can rather be considered as a natural result of electron correlations [15]. In this sense, the present work represents an alternative way to obtain *p*-wave superconduction by considering the correlated hopping interactions.

During the last years, the experimental evidence favors a spin-triplet superconducting state in Sr<sub>2</sub>RuO<sub>4</sub> [16]. More recently, phase sensitive measurements seems to indicate an odd parity superconducting state, most likely of the *p*-wave type [17]. In Sr<sub>2</sub>RuO<sub>4</sub>, electrons in the RuO<sub>2</sub> planes are expected to play the most important role for its electronic properties [16]. In general, the  $k_x \pm k_y$  oriented *p*-wave superconducting states are doubly degenerated in a square lattice and a small distortion in its right angles breaks this degeneracy, favouring one of the *p*-wave states in competition with s- and d-wave superconducting states. A singleband Hubbard model has been considered to describe the electron dynamics on the RuO<sub>2</sub> planes [13], which is often called  $\gamma$  band that plays the dominant role in the superconducting transition, and the pairing on the other two bands,  $\alpha$  and  $\beta$ , is induced passively through the inter-orbit couplings. The band structure obtained from the density functional theory can be reasonably well described in the vicinity of the Fermi level by a square-lattice single  $\gamma$ -band tight-binding model with first- and second-neighbor hoppings  $t_0 = 0.4$  eV and  $t'_0 = -0.12 \text{ eV}$ , respectively [19].

In order to analyze p-wave superconducting states, we consider a minimal two-dimensional interacting electron system, where a second-neighbor correlatedhopping interaction ( $\Delta t_3$ ) is thought as the relevant term, besides the on-site Coulomb interaction (U), the first- and second-neighbor single-electron hoppings, as appear in the standard Hubbard model. This generalized Hubbard Hamiltonian can be written as [6]

$$H = t_0 \sum_{\langle i,j \rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + t'_0 \sum_{\langle \langle i,j \rangle \rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \Delta t_3 \sum_{\langle i,l \rangle, \langle \langle j,l \rangle, \langle \langle \langle i,j \rangle \rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} n_l,$$
(1)

where  $c_{i,\sigma}^{\dagger}$  ( $c_{i,\sigma}$ ) is the creation (annihilation) operator with spin  $\sigma = \downarrow$  or  $\uparrow$  at site *i*,  $n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}$ ,  $n_i = n_{i,\uparrow} + n_{i,\downarrow}, \langle i, j \rangle$  and  $\langle \langle i, j \rangle \rangle$  denote respectively the nearest-neighbor and the second-neighbor sites. It is worth mentioning that the second-neighbor densitydensity interaction (V) could be negative if attractive indirect interactions through phonons or other bosonic excitations are included, as discussed in Refs. [2,20]. However, a negative V may cause a phase-separation ground state [4,6] and then, in this Letter we take V = 0. Moreover, the models that include the nearestneighbor correlated-hopping interaction ( $\Delta t$ ) and  $\Delta t_3$ can respectively lead to s- and d-wave hole superconducting ground states without negative V [6,21]. Therefore,  $\Delta t = 0$  and small  $\Delta t_3$  are considered in this study to analyze only *p*-wave superconducting states.

In addition, we consider a small distortion of the right angles in the square lattice, which leads to changes in  $t'_0$  and  $\Delta t_3$  terms of Eq. (1). The new values of these parameters are  $t'_{\pm} = t'_0 \pm \delta$  and  $\Delta t^{\pm}_3 = \Delta t_3 \pm \delta_3$ , where  $\pm$  refers to the  $\mathbf{x} \pm \mathbf{y}$  direction. Doing a Fourier transform,

$$c_{\mathbf{k},\sigma} = \frac{1}{\sqrt{N_s}} \sum_{j} e^{i\mathbf{k}\cdot\mathbf{R}_j} c_{j,\sigma},$$
(2)

and

$$c_{\mathbf{k},\sigma}^{\dagger} = \frac{1}{\sqrt{N_s}} \sum_{j} e^{i\mathbf{k}\cdot\mathbf{R}_j} c_{j,\sigma}^{\dagger},\tag{3}$$

the Hamiltonian (Eq. (1)) in the momentum space becomes

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{0}(\mathbf{k}) c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma}$$

$$+ \frac{1}{N_{s}} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{\mathbf{k}\mathbf{k}'\mathbf{q}} c_{\mathbf{k}+\mathbf{q},\uparrow}^{\dagger} c_{-\mathbf{k}+\mathbf{q},\downarrow}^{\dagger} c_{-\mathbf{k}'+\mathbf{q},\downarrow}^{\dagger} c_{\mathbf{k}'+\mathbf{q},\uparrow}$$

$$+ \frac{1}{N_{s}} \sum_{\substack{\mathbf{k},\mathbf{k}',\\\mathbf{q},\sigma}} W_{\mathbf{k}\mathbf{k}'\mathbf{q}} c_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger} c_{-\mathbf{k}+\mathbf{q},\sigma}^{\dagger} c_{-\mathbf{k}'+\mathbf{q},\sigma}^{\dagger} c_{\mathbf{k}'+\mathbf{q},\sigma}^{\dagger}, \qquad (4)$$

where  $N_s$  is the total number of sites,

$$\varepsilon_0(\mathbf{k}) = 2t_0 \Big[ \cos(k_x a) + \cos(k_y a) \Big] + 2t'_+ \cos(k_x + k_y) + 2t'_- \cos(k_x - k_y), \quad (5)$$

$$V_{\mathbf{k}\mathbf{k}'\mathbf{q}} = U + \Delta t_3^{-} [\gamma(\mathbf{k} + \mathbf{q}, \mathbf{k}' + \mathbf{q}) + \gamma(-\mathbf{k} + \mathbf{q}, -\mathbf{k}' + \mathbf{q})] + \Delta t_3^{-} [\zeta(\mathbf{k} + \mathbf{q}, \mathbf{k}' + \mathbf{q}) + \zeta(-\mathbf{k} + \mathbf{q}, -\mathbf{k}' + \mathbf{q})],$$
(6)

and

$$W_{\mathbf{k}\mathbf{k}'\mathbf{q}} = \Delta t_3^+ \gamma (\mathbf{k} + \mathbf{q}, \mathbf{k}' + \mathbf{q}) + \Delta t_3^- \zeta (\mathbf{k} + \mathbf{q}, \mathbf{k}' + \mathbf{q}),$$
(7)

being

$$\gamma(\mathbf{k}, \mathbf{k}') = 2\cos[a(k_x + k'_y)] + 2\cos[a(k'_x + k_y)], \qquad (8)$$

$$\zeta(\mathbf{k}, \mathbf{k}') = 2 \cos[a(k_x - k'_y)] + 2 \cos[a(k'_x - k_y)], \qquad (9)$$

and 2**q** is the wave vector of the pair center of mass. Notice that  $V_{\mathbf{k}\mathbf{k}'\mathbf{q}}$  and  $W_{\mathbf{k}\mathbf{k}'\mathbf{q}}$  respectively contribute to antiparallel and parallel spin pairings, and their main contributions come from  $\mathbf{q} = \mathbf{0}$  terms.

Within the standard Bardeen–Cooper–Schrieffer (BCS) formalism, a normal Hartree–Fock decoupling of the interaction terms in Eq. (4) leads to the following reduced Hamiltonian for parallel spins [22],

$$H - \mu N$$

$$= \sum_{\mathbf{k},\sigma} (\varepsilon(\mathbf{k}) - \mu) c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$

$$+ \frac{1}{N_s} \sum_{\mathbf{k},\mathbf{k}',\sigma} W_{\mathbf{k}\mathbf{k}'\mathbf{0}} c^{\dagger}_{\mathbf{k},\sigma} c^{\dagger}_{-\mathbf{k},\sigma} c_{-\mathbf{k}',\sigma} c_{\mathbf{k}',\sigma}, \qquad (10)$$

where  $\mu$  is the chemical potential, N is the number of electrons, and

$$\varepsilon(\mathbf{k}) = \frac{U}{2}n + 2t_0 [\cos(k_x a) + \cos(k_y a)] + 2(t'_+ + 2n\Delta t^+_3)\cos(k_x + k_y) + 2(t'_- + 2n\Delta t^-_3)\cos(k_x - k_y),$$
(11)

being *n* the density of electrons per site. Notice that the single-electron dispersion relation  $\varepsilon(\mathbf{k})$  is now modified by adding terms  $\frac{U}{2}n$  and  $2n\Delta t_3^{\pm}$  to the self-energy and the second neighbor hoppings, respectively.

At finite temperature T, the equations that determine the superconducting gap  $(\Delta_k)$  and the chemical potential  $(\mu)$  for the case of parallel spins are similar to the singlet one [6], and they are

$$\Delta_{\mathbf{k}} = -\frac{1}{N_s} \sum_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'\mathbf{0}} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2k_BT}\right),\tag{12}$$

and

$$n-1 = -\frac{1}{N_s} \sum_{\mathbf{k}'} \frac{\varepsilon(\mathbf{k}') - \mu}{E_{\mathbf{k}'}} \tanh\left(\frac{E_{\mathbf{k}'}}{2k_B T}\right), \quad (13)$$

where the single-excitation energy  $(E_k)$  is given by

$$E_{\mathbf{k}} = \sqrt{(\varepsilon(\mathbf{k}) - \mu)^2 + \Delta_{\mathbf{k}}^2}.$$
(14)

It is worth mentioning that for the pairs with spin function  $(|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle)/\sqrt{2}$ , corresponding to triplet (+) and singlet (-), the same equations (12) and (13) are obtained except that  $V_{\mathbf{kk'0}}$  replaces  $W_{\mathbf{kk'0}}$ . In this work, the *p*-wave superconducting gap is given by  $\Delta_{\mathbf{k}} = \Delta_p[\sin(k_x a) \pm \sin(k_y a)]$ , and Eq. (12) can be written as

$$l = \pm \frac{4\delta_3}{N_s} \times \sum_{\mathbf{k}} \frac{\sin^2 a k_x \pm \sin a k_x \sin a k_y}{E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T}\right),$$
(15)

where  $\delta_3 = (\Delta t_3^+ - \Delta t_3^-)/2$ . Notice that given *n* and *T*, Eqs. (13) and (15) have to be solved together for  $\mu$  and  $\Delta_p$ . In particular, the critical temperature  $(T_c)$  is determined by  $\Delta_p(T_c) = 0$ . For the case of triplets with  $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$  and  $\mathbf{q} = \mathbf{0}$ , the term *U* in Eq. (6) is an even function in the *k'* space and  $\Delta_{\mathbf{k}} = \Delta_p[\sin(k_x a) \pm \sin(k_y a)]$  is odd, and then the sum over the first Brillouin zone of the product of them is zero. Furthermore, the terms  $\Delta t_3^{\pm}$  reduce to those of  $W_{\mathbf{kk'0}}$ , except for a factor of 2. However, due to the sum over  $\sigma$  in the third term of Eq. (4), it turns out that triplets



Fig. 1. Critical temperature  $(T_c)$  versus electron density (n) obtained with a mean-field chemical potential approximation for  $\Delta t_3 = \delta = 0$ ,  $t'_0 = -0.3|t_0|$ ,  $\delta_3 = 0.5|t_0|$  (open squares),  $0.375|t_0|$  (open circles),  $0.25|t_0|$  (open up triangles),  $0.2|t_0|$  (open down triangles),  $0.125|t_0|$  (open rhombus) and arbitrary U. The solid lines indicate the self-consistent solutions of equations (13) and (15). Inset:  $T_c$  versus  $\Delta t_3$  for p- and d-channel superconducting states with n = 0.61 (n = 0.5) respectively presented as open and solid black (gray) circles for  $\delta_3 = 0.375|t_0|$ , as well as open and solid black (gray) down triangles for  $\delta_3 = 0.2|t_0|$ .

with antiparallel spins obey the same equations (13) and (15), in consequence the three types of triplets with different total spin projections have the same superconducting behavior [23].

In order to reach very low  $T_c$ , instead of solving two coupled integral equations (13) and (15), we have calculated  $\mu$  directly from the mean-field density of states, obtained from Eq. (11). The results of this calculation are shown in Fig. 1 for  $\delta_3 = 0.5|t_0|$  (open squares),  $0.375|t_0|$  (open circles),  $0.25|t_0|$  (open up triangles),  $0.2|t_0|$  (open down triangles) and  $0.125|t_0|$ (open rhombus) for  $\Delta t_3 = \delta = 0$ ,  $t'_0 = -0.3|t_0|$ , in comparison with the solutions of self-consistent equations (13) and (15) indicated by solid lines for the cases of  $\delta_3 = 0.5|t_0|$  and  $0.375|t_0|$ . This agreement is somewhat expected since it has been shown that the Fermi energy calculated from the correlated density of states coincides with the chemical potential obtained from Eq. (13) [24]. Also, notice that there are changes of  $T_c$  up to 4 orders of magnitude in a narrow range of electronic density. In the inset of Fig. 1 the  $T_c$  of p- and d-channel superconducting states with



Fig. 2. The variations of (a) maximum critical temperature  $(T_c^{\text{max}})$  and (b) optimal density  $(n_{\text{op}})$  as functions of  $\delta_3$ .

n = 0.61 (n = 0.5) as a function of  $\Delta t_3$  are respectively exhibited as open and solid black (gray) circles for  $\delta_3 = 0.375|t_0|$ , as well as open and solid black (gray) down triangles for  $\delta_3 = 0.2|t_0|$ . Observe that for large  $\Delta t_3$  the *p*-wave superconductivity is suppressed by *d*-channel superconducting states, where the latter depend slightly on the values of  $\delta_3$  (see solid circles and solid down triangles in the inset) because  $\delta_3$  only modifies  $\varepsilon(\mathbf{k})$  in Eq. (10) of Ref. [6]. In fact, for  $n \ll 1$ , the *d*-wave superconductivity is suppressed and then *p*-channel superconducting states become the ground state even for  $\delta_3 \ll \Delta t_3$ . In addition, the results show the existence of a maximum critical temperature  $(T_c^{\text{max}})$  at an optimal electron density  $(n_{\text{op}})$ , which are respectively plotted in Fig. 2(a) and (b), both as functions of  $\delta_3$ . Notice that  $T_c^{\text{max}}$  increases and  $n_{\text{op}}$  decreases when  $\delta_3$  grows, where the limit when  $\delta_3 \rightarrow 0$ corresponds to  $n_{\rm op} \simeq 1.3$ , very close to the expected  $\gamma$ -band filling of Sr<sub>2</sub>RuO<sub>4</sub> [25,26].

Moreover, the *p*-wave superconducting states are analyzed by looking at their gap strength  $(\Delta_p)$  and the single-excitation energy gap  $(\Delta_0)$ , which is defined as the minimum value of  $E_{\mathbf{k}}$  given by Eq. (14), with  $\Delta_{\mathbf{k}} = \Delta_p[\sin(k_x a) + \sin(k_y a)]$  evaluated at the antinode [6]. In the limit  $t_0, t'_0, \Delta t_3, \delta \rightarrow 0$ , analytical solutions have been obtained for the low density



Fig. 3. Numerical results (open circles) of (a) the *p*-channel superconducting gap  $(\Delta_p)$ , (b) critical temperature  $(T_c)$ , and (c) gap ratio  $[2\Delta_0/(k_BT_c)]$  versus the electron concentration (*n*), for  $\delta_3 \neq 0$  and the other parameters equal to zero, in comparison with the analytical solutions (dashed lines) valid for  $n \rightarrow 0$ .

regime  $(n \rightarrow 0)$  and they are

$$\Delta_p = 2\delta_3 \sqrt{2n} \left( 1 - \frac{9n}{4} \right),\tag{16}$$

$$k_B T_c = \frac{(1-n)\delta_3}{\tanh^{-1}(1-n)},$$
(17)

and

$$\frac{2\Delta_0}{k_B T_c} = \frac{2\ln(\frac{2-n}{n})}{(1-n)} \left(1 - \frac{9n}{4}\right).$$
 (18)

In Fig. 3(a)–(c), numerical results of  $\Delta_p/\delta_3$ ,  $T_c/\delta_3$ , and the gap ratio  $(2\Delta_0/k_BT_c)$  versus *n* are respectively shown with the rest of parameters equal to zero, where the universal analytical solutions (Eqs. (16)–(18)) are indicated by dashed lines. Note that the gap ratio in the dilute limit is independent of the interaction parameters, as found in Refs. [6,21]. Furthermore, in Fig. 3(c) it is observed that at the low density limit the gap ratio reaches very high values in comparison with the value



Fig. 4. Temperature dependence of the gap ratio  $[2\Delta_0/(k_BT_c)]$  for the *p*-wave case (open circles) with  $\Delta t_3 = \delta = 0$ ,  $t'_0 = -0.3|t_0|$ ,  $\delta_3 = 0.375|t_0|$  and n = 0.61, and the *s*-wave case (solid line) with  $U = -2.5|t_0|$ , and  $t'_0 = -0.3|t_0|$ .

of 3.57 predicted by the BCS theory and it decreases as the electron density grows. It is important to mention that in Fig. 3 the unique parameter taken different to zero is  $\delta_3$  and in this case the real strong-coupling limit is obtained only when  $n \rightarrow 0$ , since the kinetic energy (Eq. (11)) is proportional to  $n\delta_3$ .

The temperature dependence of the gap ratio  $(2\Delta_0/k_BT_c)$  for one of the systems in Fig. 1, with  $\delta_3 = 0.375|t_0|$  (open circles) and n = 0.61, is shown in Fig. 4 in comparison with the *s*-wave superconducting state obtained from a negative-*U* Hubbard model [2] with  $U = -2.5|t_0|$ ,  $t'_0 = -0.3|t_0|$  and n = 0.61 (solid line). In the inset of Fig. 4, the normalized gap ratios  $[\Delta_0(T)/\Delta_0(0)]$  for the same systems of the main plot are comparatively shown. Observe that the *p*-wave  $2\Delta_0/k_BT_c$  is larger than the *s*-wave one and the corresponding normalized gap ratio has a different behavior from the BCS theory.

Finally, in Fig. 5 the excitation energy of the quasiparticles ( $\Delta_0$ ) for the *p*-channel superconducting state is plotted as a function of the polar angle  $\theta = \tan^{-1}(k_y/k_x)$  for the same system as in Fig. 4, where  $\Delta_0$  is calculated around ( $\pi, \pi$ ) point in the **k** space since the minimum of  $E_{\mathbf{k}}$  is located there (see Eq. (14)). Observe a clear *p*-symmetry gap and the orientation of  $\Delta_0$  is determined by the sign of  $\delta_3$ .

In summary, we have demonstrated that the *p*-wave superconductivity can be obtained within a



Fig. 5. Calculated single-particle excitation energy gap ( $\Delta_0$ ) as a function of the polar angle for the same *p*-wave superconducting system as in Fig. 4.

two-dimensional generalized Hubbard model and the BCS framework. We have verified that in the studied regime, i.e.,  $U/|t_0| \gg 1$ ,  $\Delta t_3 = \delta = 0$ , the truly ground state has *p*-symmetry, since *s*- and *d*-wave superconducting states are inhibited by large U [21] and the condition  $\Delta t_3 = 0$  [6], respectively. In fact, for finite  $\Delta t_3$ , the *p*-channel superconductivity still survives in competition with the *d*-channel when  $\delta_3 \ll \Delta t_3$  in the low carrier region ( $n \ll n_{op}$ ), as shown in the inset of Fig. 1, similar to the two-particle behavior [18]. One of the main features of the *p*-wave superconducting state is the existence of an optimal electron density for  $T_c$  and  $\Delta_p$ , as shown in Fig. 1 and Eq. (16), because the attractive interaction grows with the Fermi surface size but at the same time, the increase of electron density reduces the potential energy, given by  $\langle W_{\mathbf{k},\mathbf{k}'}\rangle =$  $\sum_{\mathbf{k},\mathbf{k}'} (W_{\mathbf{k},\mathbf{k}'} - W_{\mathbf{k},-\mathbf{k}'}) u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}$  [22]. Also, we have proven that a tiny distortion of the square lattice generates *p*-wave superconducting states and one of them becomes the ground state even in competition with sand d-wave superconducting states for certain parameter regions. In the limit of tiny distortion the optimal electronic density tends to 1.3, in agreement with the Fermi energy position estimated by the band theory for Sr<sub>2</sub>RuO<sub>4</sub> [25,26]. Moreover, we have observed that the Fermi energy obtained from the mean-field density of states could be a good candidate for the real chemical potential, which simplifies the numerical calculations enormously. Finally, the Hamiltonian

used in this Letter can be further addressed beyond the BCS formalism, for example, by using the spin fluctuation technique or the density-matrix renormalization approach [27], as done for the Kubo conductivity [28] and its extension to multidimensional systems [29].

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