# **Temperature-doping phase diagram of layered superconductors**

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The superconducting properties of a layered system are analyzed for the cases of zero and nonzero angular momenta of the pairs. The effective thermodynamic potential for the quasi-two-dimensional XY model for the gradients of the phase of the order parameter is derived from the microscopic superconducting Hamiltonian. The dependence of the superconducting critical temperature  $T_c$  on doping, or carrier density, is studied at different values of coupling and interlayer hopping. It is shown that the critical temperature  $T_c$  of the layered system can be lower than the critical temperature of the two-dimensional Berezinskii-Kosterlitz-Thouless transition  $T_{BKT}$  at some values of the model parameters, contrary to the case in which the parameters of the XY model do not depend on the microscopic Hamiltonian parameters.

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# I. INTRODUCTION

Theoretical description of the doping dependence of the superconducting properties of high-temperature superconductors (HTSCs) is one of the most difficult problems of modern condensed-matter physics. Generally speaking, the complicated crystal structure of these materials, low-dimensional (quasi-two-dimensional) transport properties, the superconducting order-parameter anisotropy, strong correlations, and other properties result in the fact that many years after the discovery the microscopic mechanism of HTSC's is not understood yet.

During the last years many models which take into account some of the cuprate properties have been proposed. The doping dependence of the superconducting properties at T=0 in the s-wave pairing channel was studied for the threedimensional (3D) case in Refs. 1-3 and, particularly, for the quasi-2D case.<sup>4</sup> For the 2D case this problem was studied at T=0 (when a long-range superconducting order is still possible in a 2D system<sup>6</sup>), for the case of local attraction, in Refs. 1, 2, and 5, and for the phonon-mediated model<sup>7</sup> (for a review, see Ref. 8, for example). The *d*-wave pairing along with the s-wave one at T=0 for the case of the extended Hubbard model with next-nearest-neighbor attraction was studied in Refs. 9 and 10 and for a 2D continuum model with short-range attraction and electron correlations, in Ref. 11. The properties of a model with doping-dependent correlation length were studied recently in Ref. 12.

The 2D *s*-wave pairing at finite temperatures, when the Berezinskii-Kosterlitz-Thouless (BKT) transition can take place in a superconducting system, was considered in Refs. 13 and 14 for the case of the model with local attraction and in Refs. 15 and 16 for the case of electron-phonon pairing. The problem of *s*-wave superconductivity with a fluctuating order-parameter phase in the 3D case was analyzed in Refs. 14 and 17. The effective action for a slowly fluctuating *d*-wave superconducting order parameter for the 2D case was also analyzed in Refs. 18,19,21,20.

However, it is known that long-range order is impossible

in 1D and 2D systems with an order parameter that has a continuous symmetry.<sup>6</sup> Therefore, to obtain a real phase transition with long-range order and a homogeneous order parameter one needs to take into account the interlayer coupling  $t_z$ . Layered superconductivity is much more complicated since the possibility of interlayer fluxon and intralayer vortex phase transitions with corresponding critical temperatures  $T_f$  and  $T_v$  must be analyzed. It was already shown<sup>22-25</sup> that there is only one phase transition in such a system with the critical temperature  $T_c$  and  $T_v < T_c < T_f$  $\simeq 8T_v$ . The critical temperature  $T_c$  is equal to  $T_v$ , or, what is equivalent, to the temperature  $T_{BKT}$  of the 2D BKT phase transition at  $t_z = 0$ . Then, this temperature value increases to the value  $T_f$  with interlayer hopping  $t_z$  growth. In Refs. 22-25 the phase order-parameter effective Hamiltonian was studied in the presence of an external magnetic field and this model was mapped on the quasi-2D XY model. The *XY*-model parameters  $J_{\parallel}$  and  $J_{\perp}$  were considered as phenomenological constants. It was shown that  $T_{BKT} = \pi/2J_{\parallel}$  and  $T_f \approx 8T_{BKT}$ .

In this paper we derive the effective *XY* Hamiltonian from the initial Hamiltonian for the layered system of attracting fermions. In this case the parameters  $J_{\parallel}$  and  $J_{\perp}$  depend on the bare parameters of charge-carrier density, coupling, pair angular momentum, temperature, and the interlayer hopping. As is shown below, this leads to the nontrivial dependence of the superconducting critical temperature  $T_c$  on the model parameters. In particular, in general, this temperature is different from the critical temperature of the 2D BKT transition and  $T_c < T_{BKT}$  at some values of the model parameters, contrary to the results for the case in which parameters  $J_{\parallel}$ and  $J_{\perp}$  don't depend on the parameters of the microscopic Hamiltonian, and when the relation  $T_c < T_{BKT}$  always holds at  $J_{\perp} > 0$ .<sup>22–25</sup>

# II. THE MODEL AND THE THERMODYNAMIC POTENTIAL

The model Hamiltonian for a layered superconducting system can be written as

$$H(\tau) = \sum_{\sigma,j} \int d^2 r \psi_{j\sigma}^{\dagger}(\tau, \mathbf{r}) \left[ -\frac{\vec{\nabla}^2}{2m} + 2t_z - \mu \right] \psi_{j\sigma}(\tau, \mathbf{r}) - \sum_{\sigma, j_1, j_2} t_{mn} \int d^2 r \psi_{j_1\sigma}^{\dagger}(\tau, \mathbf{r}) \psi_{j_2\sigma}(\tau, \mathbf{r}) - \frac{1}{2} \sum_{\sigma, j} \int d^2 r_1 d^2 r_2 \psi_{j\sigma}^{\dagger}(\tau, \mathbf{r}_2) \psi_{j\sigma}^{\dagger}(\tau, \mathbf{r}_1) V(\mathbf{r}_1, \mathbf{r}_2) \times \psi_{j\sigma}(\tau, \mathbf{r}_1) \psi_{j\sigma}(\tau, \mathbf{r}_2),$$
(1)

where  $\psi_{j\sigma}(\tau, \mathbf{r})$  is a Fermi field with mass *m* and spin  $\sigma = \uparrow$  and  $\downarrow$ ,  $\tau$  is an imaginary time, and *j*,  $\mathbf{r}$  are layer number and intralayer coordinate, correspondingly;  $t_{j_1j_2} = t_z(\delta_{j_2,j_1+1} + \delta_{j_2,j_1-1})$  corresponds to the nearest interplane hopping. The free fermion dispersion relation in momentum space has the following form:

$$\xi(\mathbf{k},k_z) = \frac{\mathbf{k}^2}{2m} + 2t_z - 2t_z \cos(ak_z) - \mu, \qquad (2)$$

where **k** is a 2D wave vector with a bandwidth *W*, and  $k_z$  is the momentum in the interlayer (z) direction (it changes in the interval  $[0,2\pi/a]$ , where *a* is the interlayer spacing);  $\mu$ is the chemical potential of the system. In Eq. (1) interaction  $V(\mathbf{r}_1, \mathbf{r}_2)$  describes a nonretarded in-plane fermion attraction.

The partition function of the system is

$$Z = \int D\psi^{\dagger} D\psi e^{-S} \tag{3}$$

with the action

$$S = \int_{0}^{\beta} d\tau \left[ \sum_{\sigma,j} \int d^{2}r \psi_{j\sigma}^{\dagger}(\tau,\mathbf{r}) \partial_{\tau} \psi_{j\sigma}(\tau,\mathbf{r}) + H(\tau) \right].$$
(4)

To study the superconducting properties of the system with an arbitrary pairing symmetry the Hubbard-Stratonovich transformation with bilocal fields  $\phi_j(\tau, \mathbf{r}_1, \mathbf{r}_2)$ and  $\phi_j^{\dagger}(\tau, \mathbf{r}_1, \mathbf{r}_2)$  can be applied:<sup>26</sup>

$$\exp\left[\psi_{j\uparrow}^{\dagger}(\tau,\mathbf{r}_{2})\psi_{j\downarrow}^{\dagger}(\tau,\mathbf{r}_{1})V(\mathbf{r}_{1},\mathbf{r}_{2})\psi_{j\downarrow}(\tau,\mathbf{r}_{1})\psi_{j\uparrow}(\tau,\mathbf{r}_{2})\right]$$

$$=\int D\phi^{\dagger}D\phi\exp\left\{-\int_{0}^{\beta}d\tau\sum_{j}\int d^{2}r_{1}d^{2}r_{2}$$

$$\times\left[\frac{|\phi_{j}(\tau,\mathbf{r}_{1},\mathbf{r}_{2})|^{2}}{V(\mathbf{r}_{1},\mathbf{r}_{2})}-\phi_{j}^{\dagger}(\tau,\mathbf{r}_{1},\mathbf{r}_{2})\psi_{j\downarrow}(\tau,\mathbf{r}_{1})\psi_{j\uparrow}(\tau,\mathbf{r}_{2})\right]$$

$$-\psi_{j\uparrow}^{\dagger}(\tau,\mathbf{r}_{1})\psi_{j\downarrow}^{\dagger}(\tau,\mathbf{r}_{2})\phi_{j}(\tau,\mathbf{r}_{1},\mathbf{r}_{2})\left]\right\}.$$
(5)

Let us introduce the Nambu spinor:

$$\Psi_{j}(\tau,\mathbf{r}) = \begin{bmatrix} \psi_{j\uparrow}(\tau,\mathbf{r}) \\ \psi_{j\downarrow}^{\dagger}(\tau,\mathbf{r}) \end{bmatrix}, \quad \Psi_{j}^{\dagger}(\tau,\mathbf{r}) = \begin{bmatrix} \psi_{j\uparrow}^{\dagger}(\tau,\mathbf{r}), \psi_{j\downarrow}(\tau,\mathbf{r}) \end{bmatrix}.$$

In this case the partition function can be written as

$$Z = \int D\psi^{\dagger} D\psi D\phi^{\dagger} D\phi e^{-\overline{S}(\psi^{\dagger},\psi,\phi^{\dagger},\phi)}, \qquad (6)$$

where

$$\begin{split} \bar{S}(\psi^{\dagger},\psi,\phi^{\dagger},\phi) &= \int_{0}^{\beta} d\tau \sum_{j_{1},j_{2}} \int d^{2}r_{1} \int d^{2}r_{2} \\ &\times \left\{ \delta_{j_{1}j_{2}} \frac{|\phi_{j_{1}}(\tau,\mathbf{r}_{1},\mathbf{r}_{2})|^{2}}{V(\mathbf{r}_{1},\mathbf{r}_{2})} \\ &- \delta_{j_{1}j_{2}} \Psi_{j_{1}}^{\dagger}(\tau,\mathbf{r}_{1}) \left[ -\partial_{\tau} - \tau_{z} \left( \frac{\vec{\nabla}_{\mathbf{r}_{1}}^{2}}{2m} + 2t_{z} - \mu \right) \right] \right] \\ &\times \Psi_{j_{1}}(\tau,\mathbf{r}_{2}) \, \delta(\mathbf{r}_{1} - \mathbf{r}_{2}) \\ &+ t_{j_{1}j_{2}} \Psi_{j_{1}}^{\dagger}(\tau,\mathbf{r}_{1}) \tau_{z} \Psi_{j_{2}}(\tau,\mathbf{r}_{2}) \, \delta(\mathbf{r}_{1} - \mathbf{r}_{2}) \\ &- \delta_{j_{1}j_{2}} \phi_{j_{1}}^{\dagger}(\tau,\mathbf{r}_{1},\mathbf{r}_{2}) \Psi_{j_{1}}^{\dagger}(\tau,\mathbf{r}_{1}) \tau_{-} \Psi_{j_{1}}(\tau,\mathbf{r}_{2}) \\ &- \delta_{j_{1}j_{2}} \Psi_{n}^{\dagger}(\tau,\mathbf{r}_{1}) \tau_{+} \Psi_{j_{1}}(\tau,\mathbf{r}_{2}) \phi_{j_{1}}(\tau,\mathbf{r}_{1},\mathbf{r}_{2}) \right\}, \end{split}$$

$$(7)$$

where  $\tau_{\pm} = \frac{1}{2}(\tau_x \pm \tau_y)$  are the Pauli matrices.

In order to study the fluctuations of the order-parameter phase and to map the corresponding superconducting effective action on the quasi-2D XY model, it is convenient to make decomposition of  $\psi_{\sigma,j}(\tau, \mathbf{r}) \ \psi^{\dagger}_{\sigma,j}(\tau, \mathbf{r})$  on their modulus  $\chi_{\sigma,j}(\tau, \mathbf{r})$  and phase  $\theta_j(\tau, \mathbf{r})$ , which as is shown below is proportional to the order-parameter phase:

$$\psi_{\sigma,j}(\tau,\mathbf{r}) = \chi_{\sigma,j}(\tau,\mathbf{r})e^{i\theta_j(\tau,\mathbf{r})/2},$$
  
$$\psi_{\sigma,j}^{\dagger}(\tau,\mathbf{r}) = \chi_{\sigma,j}^{\dagger}(\tau,\mathbf{r})e^{-i\theta_j(\tau,\mathbf{r})/2}.$$

In this case the Nambu operators are

$$\Psi_{j}(\tau, \mathbf{r}) = e^{i\tau_{z}\theta_{j}(\tau, \mathbf{r})/2} \Upsilon_{j}(\tau, \mathbf{r}),$$
  

$$\Psi_{j}^{\dagger}(\tau, \mathbf{r}) = \Upsilon_{j}^{\dagger}(\tau, \mathbf{r}) e^{-i\tau_{z}\theta_{j}(\tau, \mathbf{r})/2},$$
(8)

where  $\Upsilon_j(\tau, \mathbf{r})$  and  $\Upsilon_j^{\dagger}(\tau, \mathbf{r})$  are "neutral" Nambu spinor operators:

$$\Upsilon_{j}(\tau,\mathbf{r}) = \begin{bmatrix} \chi_{j\uparrow}(\tau,\mathbf{r}) \\ \chi_{j\downarrow}^{\dagger}(\tau,\mathbf{r}) \end{bmatrix}, \quad \Upsilon_{j}^{\dagger}(\tau,\mathbf{r}) = [\chi_{j\uparrow}^{\dagger}(\tau,\mathbf{r}),\chi_{j\downarrow}(\tau,\mathbf{r})].$$

The order parameter can be expressed as

$$\phi_j(\tau, \mathbf{r}_1, \mathbf{r}_2) = \Delta(\tau, \mathbf{r}_1, \mathbf{r}_2) e^{i\theta_j(\tau, \mathbf{r}_1, \mathbf{r}_2)}$$
  
$$\phi_j^{\dagger}(\tau, \mathbf{r}_1, \mathbf{r}_2) = \Delta(\tau, \mathbf{r}_1, \mathbf{r}_2) e^{-i\theta_j(\tau, \mathbf{r}_1, \mathbf{r}_2)},$$

where we assume that the modulus of the order parameter  $\Delta(\tau, \mathbf{r}_1, \mathbf{r}_2)$  does not depend on the layer index. It is also natural to assume that

$$\phi_i(\tau, \mathbf{r}_1, \mathbf{r}_2) \simeq \Delta(\tau, \mathbf{r}) e^{i\theta_j(\tau, \mathbf{R})},\tag{9}$$

where  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$  and  $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$  are the relative and center-of-mass coordinates, correspondingly.<sup>27,21</sup> The relation (9) means that the dynamics of the Cooper pairs is described by the order-parameter modulus, the symmetry of

which depends, generally speaking, on the relative pair coordinate. The motion of the superconducting condensate is described by the order-parameter phase, which changes slowly with the distance and can be described by the centerof-mass coordinate. In this case it is easy to obtain

$$\phi_{j}^{\dagger}(\tau,\mathbf{r}_{1},\mathbf{r}_{2})\Psi_{j}^{\dagger}(\tau,\mathbf{r}_{1})\tau_{-}\Psi_{j}(\tau,\mathbf{r}_{2})$$

$$+\Psi_{j}^{\dagger}(\tau,\mathbf{r}_{1})\tau_{+}\Psi_{j}(\tau,\mathbf{r}_{2})\phi_{j}(\tau,\mathbf{r}_{1},\mathbf{r}_{2})$$

$$\simeq\Delta(\tau,\mathbf{r})Y_{j}^{\dagger}(\tau,\mathbf{r}_{1})\tau_{x}Y_{j}(\tau,\mathbf{r}_{2}).$$
(10)

Substituting Eqs. (8)-(10) into the expression for the partition function (6) it is easy to get

$$Z = \int \Delta D \Delta D \,\theta e^{-\beta \Omega(\Delta,\theta)}$$

where the thermodynamic potential is

$$\beta\Omega(\Delta,\theta) = \int_0^\beta d\tau \int d^2 r \frac{N\Delta(\tau,\mathbf{r})^2}{V(\mathbf{r})} - \operatorname{Tr} \ln G^{-1},$$

where N is number of the layers. The Nambu spinor Green function G can be expressed as

$$G^{-1} = \mathcal{G}^{-1} - \Sigma,$$

where  $\mathcal{G}^{-1}$  is a part of the inverse Green's function which does not depend on the order-parameter phase:

$$\begin{aligned} \mathcal{G}_{j_1 j_2}^{-1}(\tau_1, \tau_2, \mathbf{r}_1, \mathbf{r}_2) &= \langle \tau_1, \mathbf{r}_1, j_1 | \mathcal{G}^{-1} | \tau_2, \mathbf{r}_2, j_2 \rangle \\ &= \delta_{j_1 j_2} \delta(\mathbf{r}_1 - \mathbf{r}_2) \, \delta(\tau_1 - \tau_2) \\ &\times \left[ -\partial_{\tau_1} - \tau_z \left( -\frac{\boldsymbol{\nabla}_{\mathbf{r}_1}^2}{2m} + 2t - \mu \right) \right] \\ &- \delta_{j_2, j_1 \pm 1} \delta(\mathbf{r}_1 - \mathbf{r}_2) \, \delta(\tau_1 - \tau_2) \tau_z t_z \\ &+ \delta_{j_1 j_2} \tau_x \Delta(\tau_1 - \tau_2, \mathbf{r}_1 - \mathbf{r}_2). \end{aligned}$$

The self-energy  $\Sigma$  is the sum of the parts which come from the in-plane and interplane order-parameter phase interactions  $\Sigma^{\parallel}$  and  $\Sigma^{\perp}$ , respectively,

$$\Sigma = \Sigma^{\parallel} + \Sigma^{\perp},$$

where

$$\begin{split} \boldsymbol{\Sigma}_{j_1 j_2}^{\parallel}(\boldsymbol{\tau}_1, \boldsymbol{\tau}_2, \mathbf{r}_1, \mathbf{r}_2) \\ &= \langle \boldsymbol{\tau}_1, \mathbf{r}_1, j_1 | \boldsymbol{\Sigma}^{\parallel} | \boldsymbol{\tau}_2, \mathbf{r}_2, j_2 \rangle \\ &= \delta_{j_1 j_2} \delta(\mathbf{r}_1 - \mathbf{r}_2) \, \delta(\boldsymbol{\tau}_1 - \boldsymbol{\tau}_2) \\ &\times \left\{ \frac{i \boldsymbol{\tau}_z}{2} \partial_{\boldsymbol{\tau}_1} \theta_{j_1}(\boldsymbol{\tau}_1, \mathbf{r}_1) - \frac{i}{4m} \boldsymbol{\nabla}_{\mathbf{r}_1}^2 \theta_{j_1}(\boldsymbol{\tau}_1, \mathbf{r}_1) \right. \\ &+ \frac{\boldsymbol{\tau}_z}{8m} [ \boldsymbol{\nabla}_{\mathbf{r}_1} \theta_{j_1}(\boldsymbol{\tau}_1, \mathbf{r}_1) ]^2 - \frac{i}{2m} \boldsymbol{\nabla}_{\mathbf{r}_1} \theta_{j_1}(\boldsymbol{\tau}_1, \mathbf{r}_1) \boldsymbol{\nabla}_{\mathbf{r}_1} \right] \end{split}$$

$$\begin{split} \Sigma_{j_{1}j_{2}}^{\perp}(\tau_{1},\tau_{2},\mathbf{r}_{1},\mathbf{r}_{2}) \\ &= \langle \tau_{1},\mathbf{r}_{1},j_{1} | \Sigma^{\perp} | \tau_{2},\mathbf{r}_{2},j_{2} \rangle \\ &= -\delta_{j_{2},j_{1}\pm 1} \delta(\mathbf{r}_{1}-\mathbf{r}_{2}) \,\delta(\tau_{1}-\tau_{2}) \\ &\times \tau_{z}t_{z}(1-\exp\{-i\tau_{z}[\theta_{j_{1}}(\tau_{1},\mathbf{r}_{1})-\theta_{j_{2}}(\tau_{2},\mathbf{r}_{2}).]\}). \end{split}$$

The potential term of the thermodynamic potential is

$$\beta\Omega_{pot}(\Delta) = \int_0^\beta d\tau \int d^2 r \frac{N\Delta(\tau, \mathbf{r})^2}{V(\mathbf{r})} - \operatorname{Tr} \ln \mathcal{G}^{-1}$$

and the kinetic term can be expanded in powers of the selfenergy  $\Sigma$ :

$$\beta\Omega_{kin}(\Delta,\theta) = \operatorname{Tr}\sum_{n=1}^{\infty} \frac{1}{n} (\mathcal{G}\Sigma)^n.$$
(11)

# **III. THE BKT TRANSITION IN THE 2D CASE**

Let us begin with the case in which there is no interplane coupling:  $t_z=0$ . In this case the behavior in each plane is independent and the system undergoes the BKT transition. Let us assume that the order-parameter phase fluctuations are small. In this case to get the thermodynamic potential up to the second order in  $\nabla \theta$  we neglect all the terms in Eq. (20), except n=1,2. Also we neglect the time dependence of  $\theta$ and the second derivative  $\nabla^2 \theta$ . The effective potential in this case has the following structure (see, for example Ref. 8):

$$\Omega(\Delta,\theta) = \Omega_{pot}(\Delta) + \frac{J_{\parallel}}{2} \int d^2 r (\nabla \theta)^2, \qquad (12)$$

where

$$J_{\parallel} = \int \frac{d^2 k dk_z}{(2\pi)^3} \left\{ \frac{n_f(\mathbf{k})}{4m} - \frac{1}{16m^2} \frac{1}{T} \frac{\mathbf{k}^2}{\cosh^2[\sqrt{\xi(\mathbf{k})^2 + \Delta(\mathbf{k})^2}/2T]} \right\}, \quad (13)$$

and the momentum distribution function  $n_f(\mathbf{k})$  is

$$n_f(\mathbf{k}) = 1 - \tanh\left[\frac{\sqrt{\xi(\mathbf{k})^2 + \Delta(\mathbf{k})^2}}{2T}\right] \frac{\xi(\mathbf{k})}{\sqrt{\xi(\mathbf{k})^2 + \Delta(\mathbf{k})^2}}.$$
(14)

The free fermion spectrum  $\xi(\mathbf{k})$  in Eqs. (13) and (14) is defined by Eq. (2) at  $t_z = 0$ , in this case.

The minimization of the effective potential (12) at  $\nabla \theta$ = 0 with respect to the superconducting order parameter  $\Delta(\mathbf{k})$  leads to the standard gap equation

$$\Delta(\mathbf{p}) = \int \frac{d^2 k dk_z}{(2\pi)^3} \frac{\Delta(\mathbf{k})}{2\sqrt{\xi(\mathbf{k})^2 + \Delta(\mathbf{k})^2}} \tanh\left[\frac{\sqrt{\xi(\mathbf{k})^2 + \Delta(\mathbf{k})^2}}{2T}\right] \times V(\mathbf{p}, \mathbf{k}).$$
(15)

and

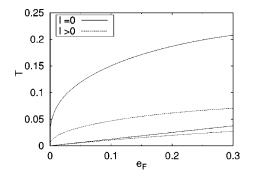


FIG. 1. Phase diagram of the 2D system in different pairing channels for the coupling parameter G=1. The solid lines are  $T_{\Delta}$  (the upper curve) and  $T_{BKT}$  for the *s*-wave pairing channel. The dashed lines are the corresponding curves for the case  $l \neq 0$ . Here and below all quantities are normalized on the 2D free-electron bandwidth *W*.

The minimization of the effective potential at  $\nabla \theta = 0$  with respect to the chemical potential  $\delta \Omega_{pot} / \delta \mu = -\upsilon n_f$  ( $\upsilon$  is the volume of the system) gives the equation which connects  $\mu$ and the particle density  $n_f$  in the system, or the 2D Fermi energy  $e_F = \pi n_f / m$ :

$$n_f = \int \frac{d^2 k dk_z}{(2\pi)^3} n_f(\mathbf{k}), \qquad (16)$$

where the momentum distribution function  $n_f(\mathbf{k})$  is defined in Eq. (14).

To search for the solutions with different angular momenta l of the pairs, we assume that the interaction potential has the following form:

$$V(\mathbf{p}, \mathbf{k}) = V \cos(l\varphi_{\mathbf{p}}) \cos(l\varphi_{\mathbf{k}}). \tag{17}$$

Below we use the dimensionless coupling parameter  $G = mV/(2\pi)$  for the numerical calculations.

In the case of the interaction (17) the gap depends only on the momentum direction

$$\Delta(\mathbf{p}) = \Delta_l \cos(l\varphi_{\mathbf{p}}),$$

where  $\Delta_l$  is the amplitude of the superconducting gap in the case of the pair angular momentum equal to l. The solution of the gap equation together with that of the number equation at  $\Delta_l = 0$  give the critical temperature of the mean-field superconducting transition  $T_{\Delta} \equiv T_c^{MF}$  on the charge-carrier density  $n_f$ . The solution of the equation

$$T = \frac{\pi}{2} J_{\parallel}(\Delta_l, \mu, T) \tag{18}$$

together with those of the gap equation and the number equation give the dependence of the critical temperature of the BKT transition on the charge-carrier density  $n_f$ . Equation (18) is obtained by mapping Eq. (12) on the corresponding thermodynamic potential of the 2D spin XY model.

As it follows from the system of Eqs. (15), (16), and (18), the solution for  $T_{\Delta}$  and  $T_{BKT}$  do not depend on l when  $l \neq 0$  for the case of the simple interaction potential (17). This

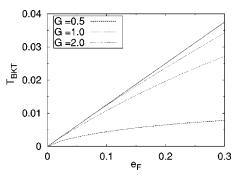


FIG. 2. The doping dependence of  $T_{BKT}$  at  $l \neq 0$  and different coupling parameters: G=0.5 (dash-dotted line), G=1.0 (dotted line), and G=2.0 (dashed line). The solid line is the function  $T_{BKT}=e_F/8$ .

follows from the fact that the *l* dependence of the integral is only as  $\cos^2(l\varphi)$  and from the identity

$$\int_0^{2\pi} \frac{d\varphi}{(2\pi)} F[\cos^2(l\varphi)] = \int_0^{2\pi} \frac{d\varphi}{(2\pi)} F[\cos^2(\varphi)],$$

where  $F[\cos^2(l\varphi)]$  is an arbitrary function without singularities, and *l* is an arbitrary nonzero integer number. Therefore it is necessary to analyze the solutions with l=0 and l=1.

The phase diagram of the system in the 2D case is presented in Fig. 1. The temperature  $T_{\Delta}$  is much higher in the *s* channel. However,  $T_{BKT} \simeq e_F/8$  in both channels at a small carrier density. This result can be easily obtained analytically from Eqs. (13) and (18).

The doping dependence of  $T_{BKT}$  in the cases of l=0 and  $l\neq 0$  is presented in Figs. 2 and 3, correspondingly. The relation  $T_{BKT} \simeq e_F/8$  holds up to higher values of the carrier density in the *s* channel at a fixed value of coupling. This means that the local pairs are bound tighter in this case.

## IV. TRANSITION IN THE CASE OF COUPLED LAYERS

Let us consider a system of coupled layers. The selfenergy, proportional to the interlayer coupling, can be written as

$$\Sigma^{\perp} = t_z \tau_z \Sigma_1^{\perp} + t_z \Sigma_2^{\perp},$$

where

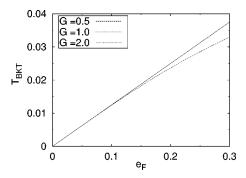


FIG. 3. The same as in Fig. 2 for the case l=0. The lines for G=1.0 and for G=2.0 practically coincide with  $T_{BKT}=e_F/8$ .

$$\begin{split} \Sigma_{1j_{1}j_{2}}^{\perp}(\tau_{1},\tau_{2},\mathbf{r}_{1},\mathbf{r}_{2}) &= \langle \tau_{1},\mathbf{r}_{1},j_{1}|\Sigma_{1}^{\perp}|\tau_{2},\mathbf{r}_{2},j_{2} \rangle \\ &= -\delta_{j_{2},j_{1}\pm1}\delta(\mathbf{r}_{1}-\mathbf{r}_{2})\,\delta(\tau_{1}-\tau_{2}) \\ &\times \cos[\,\theta_{j_{1}}(\tau_{1},\mathbf{r}_{1})-\theta_{j_{2}}(\tau_{2},\mathbf{r}_{2})], \end{split}$$

$$\begin{split} \Sigma_{2j_{1}j_{2}}^{\perp}(\tau_{1},\tau_{2},\mathbf{r}_{1},\mathbf{r}_{2}) &= \langle \tau_{1},\mathbf{r}_{1},j_{1}|\Sigma_{2}^{\perp}|\tau_{2},\mathbf{r}_{2},j_{2} \rangle \\ &= \delta_{j_{2},j_{1}\pm1}\delta(\mathbf{r}_{1}-\mathbf{r}_{2})\,\delta(\tau_{1}-\tau_{2}) \\ &\times \sin[\,\theta_{j_{1}}(\tau_{1},\mathbf{r}_{1})-\theta_{j_{2}}(\tau_{2},\mathbf{r}_{2})]. \end{split}$$

Similarly to the 2D case, we assume that the phase of the order parameter changes slowly in the interlayer direction. Therefore, the thermodynamic potential can be calculated up to second order in  $(\theta_i - \theta_{i \pm 1})$ :

$$\Omega_{kin}^{\perp} = t_z T \operatorname{Tr}(\mathcal{G}\tau_z \Sigma_1^{\perp}) + \frac{t_z^2}{2} T \operatorname{Tr}(\mathcal{G}\Sigma_2^{\perp} \mathcal{G}\Sigma_2^{\perp}).$$
(19)

The terms proportional to  $\Sigma^{\parallel}\Sigma^{\perp}$  and  $\Sigma_1^{\perp}\Sigma_2^{\perp}$  are zero due to reflection symmetry in the *z* direction.

To map the system on the quasi-2D XY model with nearest-neighbor interaction we need to obtain

$$\Omega_{kin} = \frac{J_{\parallel}}{2} \sum_{j} \int d^2 r (\boldsymbol{\nabla} \theta_j)^2 + J_z \sum_{j} [1 - \cos(\theta_j - \theta_{j-1})].$$
(20)

This dependence comes from the first term in Eq. (19). The second term in Eq. (19) is proportional to  $\sin(\theta_j - \theta_{j\pm 1})\sin(\theta_j - \theta_{j\pm 1})$ , which is equivalent to the XY model with next-nearest-neighbor and next-next-nearest-neighbor interactions. Therefore we neglect this term since it is of a higher order  $(\sim t_z^2)$  on the interlayer hopping with respect to the first term (which is  $\sim t_z$ ). However, if the coupling  $t_z$  is not small this term can lead to important physical consequences (see, for example, an analysis for the 2D case<sup>28</sup>). Thus, the parameter  $J_z$  is

$$J_z = t_z \int \frac{d^2 k dk_z}{(2\pi)^3} n_f(\mathbf{k}) \cos(ak_z).$$
(21)

Now we have obtained the kinetic part of the thermodynamic potential  $\Omega_{kin}$  in the case of the slowly fluctuating phase of the order parameter. This function is given by Eq. (20), where the parameters  $J_{\parallel}$  and  $J_z$  are given by Eqs. (13) and (21). Similarly to Eq. (21), an additional integration over  $k_z$  must be performed in Eq. (13).

The effective action (19) was studied in Refs. 22–25 in the case in which the parameters  $J_{\parallel}$  and  $J_z$  where considered independent of the fermion Hamiltonian parameters. It was shown<sup>23</sup> that there is only one phase transition in such a system at  $T_c$ , which is bigger than the temperature of the BKT transition in the case of noncoupled layers  $T_{BKT}$  $= (\pi/2)J_{\parallel}$ . In the case of small coupling  $T_c \approx T_{BKT}$  and when  $t_z$  is increasing to the interplane hopping value,  $T_c$  is approaching the value  $T_{BKT} = 4\pi J_{\parallel} \approx 8T_{BKT} = T_f$  of the fluxon transition, when interlayer order starts to take place. More precisely, the following expression for the effective free energy was considered:

$$\mathcal{F} = \frac{1}{8\pi} \int d^2 r dz \Biggl\{ (\nabla \times \mathbf{A})^2 + \frac{1}{\lambda_e} \sum_j \left[ \frac{\phi_0}{2\pi} \nabla \theta_j(\mathbf{r}) - \mathbf{A}(\mathbf{r}, z) \right]^2 \delta(z - jd) \Biggr\} \\ - \frac{J_z}{\xi_0^2} \int d^2 r \cos \Biggl[ \theta_j(\mathbf{r}) - \theta_{j-1}(\mathbf{r}) - \frac{2\pi}{\phi_0} \int_{(j-1)d}^{jd} A_z(\mathbf{r}, z') dz' \Biggr] \\ - E_c \sum_{j \in \mathbf{r}} s_j^2(\mathbf{r}),$$
(22)

where  $\mathbf{A}(\mathbf{r},z)$  is the vector potential,  $\phi_0 = hc/2e$  is the flux quantum,  $E_c$  is the loss of the condensation energy in a volume  $\xi_0^2 d$ ,  $\xi_0$  is the in-plane correlation length,  $d_0$  is the thickness of each layer, and  $d(>d_0)$  is the interlayer distance. The field  $s_j(\mathbf{r})$  describes vorticity of the lattice,  $s_j(\mathbf{r}) = 1$  if the vortex is present at the point, and  $s_j(\mathbf{r}) = 0$ , otherwise. The length scale  $\lambda_e$  is connected with the London in-plane penetration length  $\lambda_L$  as  $\lambda_e = \lambda_L^2/d_0$ . It was shown by a renormalization-group study<sup>24,25</sup> that in a physical case  $\lambda_e \gg d_0$  the self-consistent equation that describes the dependence of the critical temperature  $T_c$  on the free-energy parameters (22) has the form

$$T_{c} \simeq \frac{\tau [E_{c} + (\tau/8) \ln(T_{c}/J_{z})]}{E_{c} + \tau \ln(T_{c}/J_{z})},$$
(23)

where  $\tau = \phi_0^2 / 4\pi e^2$  is connected with the BKT transition temperature as  $\tau = 8T_{BKT}$ .

The comparison of expressions (22) and (20), gives the next self-consistent equation for the critical temperature  $T_c$ , which follows from Eq. (23):

$$T_{c} \approx 4 \pi J_{\parallel} \frac{E_{c} + (\pi J_{\parallel}/2) \ln(T_{c}/J_{z})}{E_{c} + (4 \pi J_{\parallel}) \ln(T_{c}/J_{z})},$$
(24)

where the in-plane correlation length  $\xi_0$  is absorbed in the parameter  $J_z$  [i.e.,  $t_z(a/\xi_0)^2 \rightarrow t_z$ ]. The parameter  $E_c$  actually should be renormalized by including the influence of the interlayer coupling on the vortex system.<sup>25</sup> It is considered here as a model parameter, which should be found experimentally, in particular, its doping dependence should be taken into account. For calculation we use the value  $E_c = 0.01W$  (for estimation of  $E_c$  based on an amplitude-dependent Ginzburg-Landau theory, see, for example, Ref. 29).

It is interesting to note that in the limit of very small carrier densities, when  $J_{\parallel} \simeq e_F \rightarrow 0$ , the analytical solution for  $T_c$  can be obtained to be  $T_c \simeq 4 \pi J_{\parallel} \simeq e_F$ . This is different from the one-layer case when  $T_c = T_{BKT} \simeq e_F/8$ , independently of the pair angular momentum *l*. However, the region of extremely low carrier densities is not interesting from a physical point of view.

To find the critical temperature  $T_c$  one needs to solve the system of Eqs. (15), (16), and (24) with functions

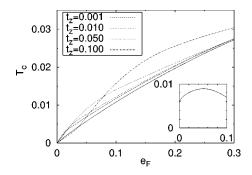


FIG. 4. The doping dependence of  $T_c$  of the layered system in the case  $l \neq 0$  at different values of interlayer hopping and  $G = 1.0, E_c = 0.01$ . The solid line is the corresponding 2D temperature  $T_{BKT}$ . The inset is the interlayer hopping dependence of  $T_c$  at G = 1 and  $e_F = 0.05$ .

 $J_{\parallel}(\mu, T, \Delta(T))$  and  $J_{z}(\mu, T, \Delta(T))$  defined in Eqs. (13) and (21). The numerical solutions show that  $T_{c} < T_{BKT}$  at small carrier densities in the case of large values of interlayer hopping  $t_{z}$  and not very strong coupling G (Fig. 4). This means that the dependence of the parameters  $J_{\parallel}$  and  $J_{\perp}$  on coupling, carrier density, and temperature leads to the nontrivial relation between  $T_{c}$  and the 2D critical temperature  $T_{BKT}$  at some values of model parameters, different from  $T_{c} > T_{BKT}$ , as was predicted for the case of fixed  $J_{\parallel}$  and  $J_{\perp}$ .

In general,  $T_c$  grows with interlayer coupling  $t_z$  (Figs. 4 and 5). However, in the case of small carrier density the critical temperature decreases with  $t_z$  growth when  $l \neq 0$  (in Fig. 4, in the l=0 case, this effect takes place at smaller coupling G). This can be explained as a consequence of the fact that the density of states on the Fermi level  $\rho(e_F)$  at small carrier densities decreases when system tends to become three dimensional with  $t_z$  growth  $[\rho(e_F) \approx \sqrt{e_F}$  in the 3D case and  $\rho(e_F) = \text{const in the 2D case}]$ . On the other hand, the role of the term  $\sim t_z^2$  must be studied, in addition, at rather large values of  $t_z$ , when interlayer hopping becomes of order of intralayer hopping, i.e.,  $t_z \approx 0.1W$  (see Ref. 28 again).

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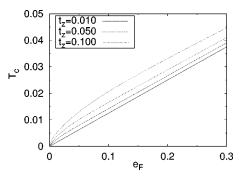


FIG. 5. The same as in Fig. 4 for the case l=0.

# **V. CONCLUSIONS**

To summarize, the doping dependence of the superconducting critical temperature of layered superconductors on the charge-carrier density has been studied in cases of different angular momenta of the pairs l, coupling, and interlayer hopping. It has been shown that the critical temperature  $T_c$  is smaller then the 2D critical temperature  $T_{BKT}$  at some values of the model parameters, contrary to that of the XY model with the parameters  $J_{\parallel}$  and  $J_{\perp}$  which do not depend on carrier density  $n_f$ , interparticle coupling V, and the temperature of the system T. In particular, at small carrier densities  $T_c \neq e_F/8$ , contrary to the dependence of  $T_{BKT}$  in the 2D case. The critical temperature  $T_c$  grows with  $t_z$ , except in the case of nonzero angular momentum of the pairs at small carrier densities.

At the same time some questions remained unresolved. In particular, the behavior of the system when interlayer coupling  $t_z$  is not very small has to be studied and the doping dependence of the vortex condensation energy should be taken into account. These problems are scheduled to be studied in the future.

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