Pressure dependence of superconducting and magnetic critical temperatures in the ruthenocuprates

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We study the dependence on filling and pressure of the superconducting and ferromagnetic critical temperatures of the ruthenocuprates, within the two-band model. At zero pressure, we find separate regions of coexistence of superconductivity and ferromagnetism as a function of filling, with contiguous regions merging together as the pressure increases. As a function of pressure, a stronger enhancement of the magnetic phase results in a reduced pressure effect on the superconducting critical temperature. A comparison with recent experiments on the determination of the critical temperatures as a function of the pressure is also discussed.

I. INTRODUCTION

The strong electron correlations in transition metal oxides are known to generate complex phase diagrams. Nonetheless, it was surprising to discover that one such oxide, the ruthenocuprate $RuSr_2GdCu_2O_8$ (Ru-1212), shows a low-temperature phase in which homogeneous ferromagnetism and superconductivity coexist.[1,2] This new class of materials then adds itself to the metallic ferromagnets UGe_2 (Ref. 3), $ZrZn_2$ (Ref. 4), and $URhGe$ (Ref. 5), all showing the coexistence of unconventional superconductivity and itinerant ferromagnetism at low temperature ($T \sim 1$ K) and relatively high pressure ($P \sim 1$ GPa).

The problem of the coexistence of ferromagnetism (FM) and superconductivity (SC) is puzzling due to the fact that there are at least two factors that would destroy superconductivity in a ferromagnetic medium: first, the exchange splitting lifts the energy degeneracy of the partners of a spin-up and spin-down Cooper pair; second, magnon exchange leads to repulsion for a singlet pair. Thus, the coexistence of ferromagnetic order and superconductivity in the Ru-1212 and Ru-1222 compounds raises the question of how these two antagonist states of matter can accommodate each other. Do both states coexist with no mutual interference or is there a competition between superconducting and magnetic order?

Opposite answers come from different experiments. Recent muon spin rotation experiments on Ru-1212[2] have suggested that the magnetic moments are not affected by the appearance of superconductivity below 45 K. This assumption motivated Shimahara and Hata to study the superconducting properties of a system consisting of alternating SC and FM layers in the presence of a fixed internal magnetic field, neglecting the effect of SC on FM.[6] On the other hand, experiments on chemical substitution (doping) of Ru-1212 indicate that the magnetic and superconducting critical temperatures, T_m and T_c, respectively, are affected in an opposite way with decreasing T_c and an increase of T_m from their reference values $T_c \simeq 45$ K and $T_m \simeq 132$ K in undoped Ru-1212.[7,8] These results are indicative of a strong competition between superconductivity and magnetism.

Since chemical substitution usually affects several parameters at the same time, causing changes of the microstructure of the sample, a better indication comes from the effect of hydrostatic pressure on the superconducting and magnetic phases. New experiments in hydrostatic pressure on Ru-1212[9,10] show that both T_c and T_m increase linearly with pressure P, but at different rates. This rate is distinctly larger for T_m than for the superconducting T_c, with $dT_c/dP \approx 1$ K/GPa and $dT_m/dP \approx 6.7$ K/GPa.[10] The relatively small pressure derivative dT_c/dP for the superconducting critical temperature is interpreted as an immediate consequence of a competition of ferromagnetic and superconducting phases: a stronger enhancement of the magnetic phase results in a reduced pressure effect on T_c as compared to underdoped high-T_c compounds.[10]

In this paper, we investigate the effect of hydrostatic pressure P in a phenomenological model of ferromagnetic superconductors[11] with two types of carriers pertaining to different layers and responsible for superconductivity and ferromagnetism, separately. Our main concern is the dependence of the critical temperatures T_c and T_m on pressure and filling, that could shed some light on the microscopic mechanism of the coexistence or interplay of ferromagnetism and superconductivity. The analysis follows from a detailed study of the dependence of the model parameters (hopping and exchange integrals) on pressure. The paper is organized as follows. In Sec. II we introduce the microscopic model and discuss the phase diagram and the order parameters at finite temperature. In Sec. III we give a detailed description of the dependence of the model parameters on pressure. In Sec. IV we report the numerical results for T_c and T_m. Finally, in Sec. V we present our conclusions and give directions for future work.

II. TWO-BAND MODEL

The unit cell of Ru-1212 may be described as a "double bilayer," each bilayer being composed by a CuO_2 and a RuO_2 layer, separated by an intermediate SrO layer. The two bilayer blocks are in turn separated by a Gd ion, which also serves as an inversion point for the unit cell (see, e.g., Fig. 1 in Ref. 12). As in the high-T_c cuprates, superconductivity is believed to set in within the CuO_2 layers, while ferromagnetism may be thought as mainly due to the ordering of the Ru moments in the RuO_2 layers. This has suggested that both the SC and FM phases in the ruthenocuprates are not homogeneous at the microscopic scale. In particular, the SC order parameter may develop[12] a spatial variation with nonzero total momentum as in the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO or LOFF) phase,[13,14] while recent experimental results indicate that the FM order is characterized by predominant AFM domains separated by nanoscale FM domains.[10] A separate origin of SC and FM correlations is also supported by band structure calculations,[12,15] which clearly indicate the existence of electronic subbands pertaining to the CuO_2 and to the RuO_2 layers, respectively, as well as of a hybridization term, due to the bridging apical oxygens between adjacent layers. Electronic subbands in the CuO_2 and RuO_2 layers are mainly characterized by the Cu-$3d_{x^2-y^2}$ and Ru-$4d_{xy}$ orbitals, respectively, as well as by the O-$2p_{x,y}$ orbitals.[12,15]

In order to study the coexistence of SC and FM in ferromagnetic metals, such as UGe_2 (Ref. 3), a single-band model has been originally developed within the mean-field approximation by Karchev *et al.*,[16] and then numerically discussed by Jackiewicz *et al.*[17] It has been pointed out, however, that a single band model does not produce coexistence, but rather a first order transition between phases.[18] On the other hand, coexistence of FM and SC is permitted in multiband models.[19,20]

In the case of the ruthenocuprates, a minimal model for coexisting FM and SC is then the two-band model of Cuoco *et al.*[11] There, one may additionally allow for the hybridization of the two bands pertaining to the CuO_2 and RuO_2 layers, respectively, by explicitly including an interlayer hopping term. Accordingly, we assume that the total Hamiltonian can be decomposed as

$$H_{\text{tot}} = H_{\text{SC}} + H_{\text{FM}} + H_{\text{SC-FM}}, \qquad (1)$$

with H_{SC} and H_{FM} describing the CuO_2 and RuO_2 layers, respectively, while $H_{\text{SC-FM}}$ contains both the hybridization term and exchange correlations between the two subbands. Within the mean-field approximation, the three terms read, in turn,

$$H_{\text{SC}} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} d^{\dagger}_{\mathbf{k}\sigma} d_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} [\Delta d^{\dagger}_{\mathbf{k}\uparrow} d^{\dagger}_{-\mathbf{k}\downarrow} + \text{H.c.}], \qquad (2a)$$

$$H_{\text{FM}} = \sum_{\mathbf{k}\sigma} \left(\zeta_{\mathbf{k}} + \frac{1}{2}\sigma M \right) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}, \qquad (2b)$$

$$H_{\text{SC-FM}} = \sum_{\mathbf{k}\sigma} \left[t_{\perp} (d^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \text{H.c.}) + \frac{1}{2}\sigma j_{\perp} M d^{\dagger}_{\mathbf{k}\sigma} d_{\mathbf{k}\sigma} \right]. \qquad (2c)$$

Here, $c^{\dagger}_{\mathbf{k}\sigma}$, $d^{\dagger}_{\mathbf{k}\sigma}$ [$c_{\mathbf{k}\sigma}, d_{\mathbf{k}\sigma}$] are creation (annihilation) operators for electrons, with wave number $\mathbf{k}$ and spin projection $\sigma = \pm$ or $\sigma \in \{\uparrow, \downarrow\}$ along a specified direction, in the RuO_2 (FM) and CuO_2 (SC) subbands, respectively; $\xi_{\mathbf{k}} = \epsilon^{\text{SC}}_{\mathbf{k}} - \mu$ and $\zeta_{\mathbf{k}} = \epsilon^{\text{FM}}_{\mathbf{k}} - \mu$ are the subband dispersion relations, measured with respect to the common chemical potential μ; $t_{\perp}$ is the (momentum conserving) interlayer hopping or hybridization term between the SC and FM subbands; $j_{\perp} = J_{\perp}/J_{\parallel}$ denotes the ratio of the interlayer to the in-plane exchange couplings. In Eqs. (2),

$$\Delta = g \sum_{\mathbf{k}} \langle d_{-\mathbf{k}\downarrow} d_{\mathbf{k}\uparrow} \rangle, \qquad (3a)$$

$$M = J_{\parallel} \sum_{\mathbf{k}} (\langle c^{\dagger}_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} \rangle - \langle c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}\downarrow} \rangle), \qquad (3b)$$

are the mean-field SC and FM order parameters, respectively, $\langle \cdots \rangle$ denotes a self-consistent statistical average, and $g > 0$ is the SC coupling constant, which we assume to be independent of momentum, for the sake of simplicity.

Neutron scattering experiments on the magnetic susceptibility of the ruthenocuprates[1] agree fairly well with a MF picture, thus indicating that a MF desription is adequate to describe ferromagnetism in the RuO_2 planes. In order to improve the MF approach, one should take into account the effect of spin density fluctuations via a dynamical susceptibility or vertex corrections. This improvement has not been considered in our model, where the Stoner criterion has been used in order to describe the essential aspects of magnetism.

For the band dispersions, within the rigid tight-binding approximation, we take

$$\epsilon^{\text{SC,FM}}_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y, \qquad (4)$$

where t, t' are the appropriate nearest neighbor (NN) and next-nearest neighbor (NNN) hopping amplitudes for the two layers, respectively.

Apart from a constant term, Eq. (1) can be conveniently rewritten in matrix form as

$$H_{\text{tot}} = \sum_{\mathbf{k}} B^{\dagger}_{\mathbf{k}} \hat{H} B_{\mathbf{k}}, \qquad (5)$$

where $B^{\dagger}_{\mathbf{k}} = (d^{\dagger}_{\mathbf{k}\uparrow} d_{-\mathbf{k}\downarrow} c^{\dagger}_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow})$ is a four-component spinor accounting for the two different orderings, the real symmetric matrix,

$$\hat{H} = \begin{pmatrix} \xi_{\mathbf{k}} + \frac{1}{2}j_\perp M & -\Delta & t_\perp & 0 \\ -\Delta & -\xi_{\mathbf{k}} + \frac{1}{2}j_\perp M & 0 & -t_\perp \\ t_\perp & 0 & \zeta_{\mathbf{k}} + \frac{1}{2}M & 0 \\ 0 & -t_\perp & 0 & -\zeta_{\mathbf{k}} + \frac{1}{2}M \end{pmatrix},$$

(6)

has been introduced. It is worth noting that $\hat{H}$ may be thought of as being composed of four 2×2 blocks, each diagonal block pertaining to the SC and FM subsystems, respectively. Competition between SC and FM is provided not only by the off-diagonal blocks, which only contain the interlayer hopping term $t_\perp$, of kinetic origin, but also by the magnetization-induced splitting of the SC subband, induced by the interlayer exchange coupling $J_\perp$. Inversely, the presence of superconducting correlations in the CuO_2 layers ($\Delta \neq 0$) does not explicitly enter the (2, 2) FM block, if not, e.g., through the common chemical potential μ, to be self-consistently determined as a function of the total number of electrons.

Equtation (5) can be diagonalized by means of standard techniques in terms of the four real eigenvalues $E_{\mathbf{k}\alpha}$ ($\alpha = 1, \ldots, 4$) of the band matrix, Eq. (6). The SC and FM order parameters, Δ and M, can then be derived self-consistently from Eqs. (3) as[21]

$$\Delta = \frac{g}{4N} \sum_{\mathbf{k},\alpha} \frac{\partial E_{\mathbf{k}\alpha}}{\partial \Delta} \tanh\left(\frac{\beta E_{\mathbf{k}\alpha}}{2}\right),$$

(7a)

$$M = \frac{J_\parallel}{2N} \sum_{\mathbf{k},\alpha} \frac{\partial E_{\mathbf{k}\alpha}}{\partial M} \tanh\left(\frac{\beta E_{\mathbf{k}\alpha}}{2}\right),$$

(7b)

at a fixed number of electrons N and inverse temperature $\beta = 1/k_B T$. Numerical analysis of Eqs. (7) shows[11] that the two-band model allows for the coexistence of SC and FM over a reasonable range of parameters. In Eqs. (7), the eigenenergies $E_{\mathbf{k}\alpha}$ are implicit functions of the order parameters Δ, M, via the secular equation $\det(\hat{H} - E_{\mathbf{k}\alpha}\mathbf{1}) = 0$, and their derivatives can be calculated by means of the implicit function theorem (Dini's theorem). By direct inspection of the secular equation, it can be shown that the eigenvalues $E_{\mathbf{k}\alpha}$ are even functions of Δ, while there always exist paired branches $\alpha, \bar{\alpha}$ such that $E_{\mathbf{k}\alpha}(-M) = -E_{\mathbf{k}\bar{\alpha}}(M)$. The critical temperatures T_c and T_m for the onset of SC and FM are defined as the largest temperatures for which Eqs. (7a) and (7b) have nonzero solutions Δ and M, respectively. They have been obtained by simultaneously solving Eqs. (7), linearized with respect to the appropriate order parameter.

III. PRESSURE DEPENDENCE OF THE MODEL PARAMETERS

In Eqs. (7) for the order parameters, pressure P enters through the band (t, t' in each layers, and $t_\perp$) and the cou-

pling parameters ($g, J_\parallel, J_\perp$), as well as through the doping level, here parametrized by the chemical potential μ. The phase diagram of correlated systems close to an ordering instability is usually characterized by the interplay of a pressure-induced doping variation and any other "intrinsic" pressure effect, here accounted for by the pressure dependence of all other model parameters.[22] This scenario can qualitatively explain the pressure dependence of T_c in the high-T_c cuprates,[23] in particular, also when an anisotropic doping redistribution takes place among inequivalent layers due to an applied pressure.[24] This scenario has been recently related to the proximity of an electronic topological transition, where a pressure- or strain-induced change of the topology of the Fermi surface takes place either because of a change of the electronic structure (at constant doping), or because of a doping variation (at fixed or rigid band structure, as is usually assumed).[25]

An estimate of the pressure dependence of the band parameters could, in principle, be achieved through experiments or by extensive *ab initio* calculations.[26] However, due to the limited number of experimental results on ruthenocuprates in hydrostatic pressure, in the following we will discuss a simplified scheme allowing us to describe the pressure variation of the relevant model parameters.

We will be mainly concerned with the pressure dependence of the band parameters and of the exchange integrals. Although a pressure dependence of the superconducting coupling parameter g is also to be expected on general grounds, its actual functional form would depend on the microscopic mechanism of superconductivity,[22,23] which is currently a matter of debate for the ruthenocuprates. In view of the reduced pressure effect on T_c, as compared to T_m, we will then neglect altogether the pressure dependence of g, although, as mentioned in the Introduction, the enhancement of the magnetic phase with increasing pressure could justify a reduction of $\partial T_c / \partial P$.

A. Band parameters

The relevance of the tight-binding approximation for modeling the band structure of the CuO_2 and the RuO_2 layers in both cuprate and ruthenate compounds has been reviewed by Mishonov and Penev.[26] A pressure-induced variation of the band parameters entering Eq. (4), namely the nearest-neighbor (NN) and next-nearest-neighbor (NNN) hopping amplitudes t and t', respectively, and of the interlayer hopping amplitude, $t_\perp$, entering Eq. (5), can be approximately accounted for within the extended Hückel theory.[27] In this context, such parameters can be roughly approximated by the overlap integrals between the appropriate orbitals, which are the $Cu-3d_{x^2-y^2}$ and the $O-2p_{x,y}$, for t^{SC}; the $Ru-4d_{xy}$ and the $O-2p_{x,y}$, for t^{FM}; the $O(1)-2p_x$ and $O(2)-2p_y$, for t' in both layers; and the $Ru-4d_{3z^2-r^2}$ and $O-2p_z$, for $t_\perp$. These are two-center integrals, which have been evaluated analytically in terms of the distance (and relative orientation) of the two orbital centers. At large intersite distances, the approximate behavior employed e.g., in Ref. 28 is recovered.

B. Exchange integrals

In order to calculate the dependence on hydrostatic pressure of the exchange interaction in the RuO_2 planes, $J_\parallel$, and

the interlayer exchange coupling $J_\perp$, we follow the approach of Munro[29] using the same approximation scheme and generalize it to the case of Ru-$4d_{xy}$ and Cu-$3d_{x^2-y^2}$ orbitals. In this approach the quantity $J^{-1}(dJ/dP)$ is determined within the theory of solids under hydrostatic pressure in which the application of pressure is represented in terms of the crystal compressibility and two other parameters associated with the electronic screening (Λ) and the wave-function distortion (Ω).[29] To a certain extent, therefore, these two parameters take into account for the many-body effects in an "equivalent pressure-free" model system.

The generic exchange integral at zero pressure is defined by

$$J = \int d^3\mathbf{r}_1 \, d^3\mathbf{r}_2 \, \psi_i^*(\mathbf{r}_1)\psi_j^*(\mathbf{r}_2)\frac{e^2}{r_{12}}\phi_i(\mathbf{r}_2)\phi_j(\mathbf{r}_1), \quad (8)$$

where $r_{12}=|\mathbf{r}_1-\mathbf{r}_2|$, and $\psi_i(\mathbf{r})=\psi(\mathbf{r}-\mathbf{r}_i)$ and $\phi_j(\mathbf{r})=\phi(\mathbf{r}-\mathbf{r}_j)$ are the appropriate hydrogenoid orbitals on atoms i and j, respectively. We seek for the pressure dependence of the expression (8) which is to be approximately determined as a function of Λ, Ω and the compressibility κ. To this aim, one first postulates a scaling of the charge-related coupling constants which can be written in the forms $e^2 \to \Lambda(P)e^2$ and $Z \to \Omega(P)Z/\Lambda(P)$, where Z is the effective charge number of the nuclear unit. Second, one assumes that the fractional variation of the one-electron state ψ_i and ϕ_i can be written as a function of κ, Λ, and Ω, i.e.

$$\frac{1}{\psi}\frac{\partial \psi}{\partial P} \approx f(\kappa, \Lambda, \Omega), \quad (9a)$$

$$\frac{1}{\phi}\frac{\partial \phi}{\partial P} \approx g(\kappa, \Lambda, \Omega). \quad (9b)$$

Using the fact that

$$(1/r_{12})^{-1}\frac{d(1/r_{12})}{dP} \approx \frac{1}{3}\kappa, \quad (10)$$

we can write

$$\frac{1}{J}\frac{dJ}{dP} \approx \frac{1}{3}\kappa + 2f(\kappa, \Lambda, \Omega) + 2g(\kappa, \Lambda, \Omega) + \frac{d\Lambda}{dP}$$
$$-\frac{\kappa}{3}\frac{1}{J}\int d^3\mathbf{r}_1 \, \psi^*(\mathbf{r}_1)\int d^3\mathbf{r}_2 \, \psi(\mathbf{r}_2)\frac{e^2}{r_{12}}$$
$$\times[\mathbf{r}_j \nabla \phi^*(\mathbf{r}_2 - \mathbf{r}_j) + \mathbf{r}_j \nabla \phi(\mathbf{r}_1 - \mathbf{r}_j)]. \quad (11)$$

where we have taken $\mathbf{r}_i=0$ and the last term comes from an expansion around $\mathbf{r}_j=0$. In evaluating (11), we make use of the following approximations.[29] First, it is assumed that the major contribution to the wave-function distortion comes from its radial part, $R(r)$ say, so that $\psi^{-1} \, \partial\psi/\partial P \approx R^{-1} \, \partial R/\partial P$. Second, from the same assumption it follows that

$$\mathbf{r}_j \nabla \phi \approx r_j\frac{\partial\phi}{\partial r} \approx \rho_c\frac{\partial R}{\partial\rho}, \quad (12)$$

where $\rho_c=Zc/2a_0$, c is the distance between the ions and a_0 is the Bohr radius.

In our specific case, to evaluate $J_\parallel$ we must consider the Ru $4d_{xy}$ orbitals, whose radial function, assuming a hydrogenoidlike wave function, is

$$R_{4d}(r) = \frac{1}{24\sqrt{10}}\Omega^{7/2}\left(\frac{Z}{2a_0}\right)^{3/2}e^{-\Omega\rho/2}\rho^2(6-\Omega\rho), \quad (13)$$

where $\rho=Zr/2a_0$. One thus finds

$$\frac{1}{R_{4d}}\frac{\partial R_{4d}}{\partial P} = \frac{1}{2}\left(\frac{7}{\Omega} - 2\frac{\rho}{6-\Omega\rho} - \rho\right)\frac{d\Omega}{dP}. \quad (14)$$

In this expression, one makes use of the approximation $\rho \approx \langle\rho^2\rangle_{4d}/\langle\rho\rangle_{4d}$ instead of the approximation $\rho \approx \langle\rho\rangle_{4d}$ to retain a better numerical accuracy. Using Eq. (12), we also have

$$\mathbf{r}_j \nabla \phi \approx \left(3\left\langle\frac{\rho_c}{\rho}\right\rangle_{4d} - \frac{1}{2}\rho_c\Omega - 6\left\langle\frac{\rho_c}{\rho(6-\Omega\rho)}\right\rangle_{4d}\right)R_{4d}. \quad (15)$$

Setting $f=g$ into Eq. (11) and using the relations (14) and (15), we obtain the following expression for the variation of the exchange integral $J_\parallel$ on pressure:

$$\frac{1}{J_\parallel}\frac{dJ_\parallel}{dP} \approx \frac{1}{3}\kappa\left(1 + \rho_c - 6\left\langle\frac{\rho_c}{\rho}\right\rangle_{4d} + 12\left\langle\frac{\rho_c}{\rho(6-\rho)}\right\rangle_{4d}\right)$$
$$+ \frac{d\Lambda}{dP} + 2\left(7 - \frac{\langle\rho^2\rangle_{4d}}{\langle\rho\rangle_{4d}} - 2\left\langle\frac{\rho}{6-\rho}\right\rangle_{4d}\right)\frac{d\Omega}{dP}, \quad (16)$$

where we have expanded up to the lowest contribution in Ω in the coefficients. This expression is equivalent to Eq. (10) of Munro[29] for the $3d$ orbitals.

In the evaluation of $J_\perp$ we must evaluate the exchange integral between the Cu $3d_{x^2-y^2}$ orbital (ψ) and the Ru $4d_{xy}$ orbital (ϕ). The radial function for the $3d_{x^2-y^2}$ orbital is

$$R_{3d}(r) = \frac{1}{9\sqrt{30}}\Omega^{7/2}\left(\frac{Z}{2a_0}\right)^{3/2}e^{-\Omega\rho/2}\rho^2, \quad (17)$$

so that we derive

$$\frac{1}{R_{3d}}\frac{\partial R_{3d}}{\partial P} = \frac{1}{2}\left(\frac{7}{\Omega} - \frac{\langle\rho^2\rangle_{3d}}{\langle\rho\rangle_{3d}}\right)\frac{d\Omega}{dP}. \quad (18)$$

Making use of (12) and (17), we obtain

$$\mathbf{r}_j \nabla \phi \approx \left(2\left\langle\frac{\tilde{\rho}_c}{\rho}\right\rangle_{3d} - \frac{1}{2}\tilde{\rho}_c\Omega\right)R_{3d}, \quad (19)$$

where $\tilde{\rho}_c=Z\tilde{c}/2a_0$, and $\tilde{c}$ is the distance between the Ru-Cu ions, this time. The functions f and g are now

TABLE I. Average values entering Eq. (16) and Eq. (21), as analytically evaluated by means of Eq. (13) and Eq. (17) for the radial functions.

$\langle\rho\rangle_{4d}=10.5$	$\langle\rho\rangle_{3d}=7$
$\langle\rho^2\rangle_{4d}=125.8$	$\langle\rho^2\rangle_{3d}=56$
$\langle 1/\rho\rangle_{4d}=0.125$	$\langle 1/\rho\rangle_{3d}=0.166$
$\langle\rho/6-\rho\rangle_{4d}=-1.75$	
$\langle 1/6-\rho\rangle_{4d}=-0.125$	
$\langle 1/\rho(6-\rho)\rangle_{4d}=0$	

$$f = \frac{1}{2}\left(\frac{7}{\Omega} - 2\left\langle\frac{\rho}{6-\Omega\rho}\right\rangle_{4d} - \frac{\langle\rho^2\rangle_{4d}}{\langle\rho\rangle_{4d}}\right)\frac{d\Omega}{dP},$$

$$g = \frac{1}{2}\left(\frac{7}{\Omega} - \frac{\langle\rho^2\rangle_{3d}}{\langle\rho\rangle_{3d}}\right)\frac{d\Omega}{dP}. \tag{20}$$

Using Eqs. (19) and (20) in Eq. (11), we obtain the following variation of $J_\perp$ with pressure to the lowest order in Ω:

$$\frac{1}{J_\perp}\frac{dJ_\perp}{dP} \approx \frac{1}{3}\kappa\left(1 + \tilde{\rho}_c - 4\left\langle\frac{\tilde{\rho}_c}{\rho}\right\rangle_{3d}\right) + \frac{d\Lambda}{dP}$$
$$+ \left(7 - \frac{\langle\rho^2\rangle_{4d}}{\langle\rho\rangle_{4d}} - \frac{\langle\rho^2\rangle_{3d}}{\langle\rho\rangle_{3d}} - 4\left\langle\frac{\rho}{6-\rho}\right\rangle_{4d}\right)\frac{d\Omega}{dP}. \tag{21}$$

As a first step, we assume that the contributions from $d\Omega/dP$ and $d\Lambda/dP$ in Eqs. (16) and (21) are small compared to the one from the compressibility, and neglect them altogether. In so doing, the quantities to determine in order to have the full dependence of the exchange integrals on pressure, are the compressibility κ, ρ_c, $\tilde{\rho}_c$, and all the average values that appear in Eqs. (16) and (21).

In determining ρ_c, we need to know the Ru-Ru ions distance c/a_0. The crystal structure analysis of Ru-1212[15] gives for the distance between Ru ions in the RuO layer and the apical oxygen of RuO$_6$ octahedra the value $d(\text{Ru}-\text{O}_{\text{api}})=1.912$ Å. We can then determine the Ru-Ru distance in the layer as $c=4d(\text{Ru}-\text{O}_{\text{api}})\tan(\pi/6)=4.415$ Å, or $c/a_0=7.561\,44$. Consequently, we obtain $\rho_c\simeq15.123$. From the crystal structure analysis we also know the distance between Ru and Cu ions, $d(\text{Ru}-\text{Cu})=4.102$ Å and so we obtain $\tilde{\rho}_c\simeq15.508$. All the average values that appear in Eqs. (16) and (21) have been evaluated analytically by the use of the radial functions, Eqs. (13) and (17), and their values are reported in Table I.

Finally, we need the compressibility κ. To our knowledge, no experiment has been yet performed to determine κ. We can estimate this quantity based on the pressure dependence of T_m known from experiments,[9,10] viz., $dT_m/dP=6.7$ K/GPa. Within Stoner's model of ferromagnetism, one has $k_BT_m=\pi^{-1}[6(\alpha-1)/\alpha R]^{1/2}$, where $R=(\rho'/\rho)^2-\rho''/\rho$, $\rho=\rho(\mu)$ is the density of states (DOS) at the chemical potential μ, and $\alpha=J_\parallel\rho$, $\alpha>1$ being the Stoner criterion for ferromagnetism.[30] Neglecting the pressure dependence of the DOS, one roughly finds

$$\frac{1}{T_m}\frac{\partial T_m}{\partial P} = \frac{1}{2}\frac{1}{\alpha-1}\frac{1}{J_\parallel}\frac{\partial J_\parallel}{\partial P}, \tag{22}$$

which explicitly depends on filling through α. This has to be contrasted with the relation[29]

$$\frac{1}{T_m}\frac{dT_m}{dP} = \frac{1}{J_\parallel}\frac{dJ_\parallel}{dP}, \tag{23}$$

holding within the Heisenberg model of ferromagnetism at the mean-field level. Making use of the latter, albeit filling-independent, expression and of Eq. (16), we can estimate the compressibility as $\kappa=3.4\times10^{-3}$ GPa^{-1}, which is a reasonable value, if compared to the values known for other cuprate materials with a perovskite structure.[31,32] Inserting this value back in Eqs. (16) and (21), we obtain the dependence of the exchange integrals on pressure. Comparing the relative pressure coefficients, we also obtain $(d\ln J_\parallel/dP)/(d\ln J_\perp/dP)\sim0.77$, indicating that $J_\perp$ increases faster with pressure as compared to $J_\parallel$. We would like to stress that the relation of T_m with the relevant model parameters could be different if approximations beyond the MF level are taken into account. Nevertheless, ac susceptibility and resistivity measurements on ruthenocuprates[9,10] fairly well agree with the MF picture, thus indicating that a MF desription is adequate to describe ferromagnetism in the RuO$_2$ planes.

IV. NUMERICAL RESULTS

In Fig. 1 we show our numerical results for both the superconducting critical temperatures, T_c, and the ferromagnetic critical temperature, T_m, as a function of the chemical potential μ, for 11 values of pressure $P=0-2$ GPa. Figure 2 shows the shapes of the Fermi surface relative to the RuO$_2$ layer, $\epsilon_\mathbf{k}^{\text{FM}}=\mu^*$, corresponding to the chemical potential μ^* which maximizes T_m at a given pressure. One immediately concludes that, within the present approximation, pressure has a negligible effect on the optimal filling for T_m.

At zero pressure, we take $t=0.3$ eV and $t'/t=0.45$ for both the SC and the FM bands,[12,15,33] and $t_\perp=0.05t$. The values of the coupling parameters at zero pressure have been chosen so to reproduce the observed optimal values of T_c and T_m at $P=0$. Specifically, we take $g=0.042$ eV, $J_\parallel=1.4t$, $J_\perp=0.1t$.

At zero pressure, we find three separate regions of coexistence of superconductivity and ferromagnetism, with T_m displaying three pronounced "domes" as a function of chemical potential μ. This is mainly a consequence of the Stoner criterion, which in the simplest version, i.e., neglecting interlayer exchange and in the absence of competing SC order, reads as $J_\parallel\rho>1$, so that ferromagnetism is enhanced where the DOS is largest, i.e. close to Van Hove singularities or electronic topological transitions.[25] As pressure increases, the band widens and the DOS peaks lower.[23] However, the exchange couplings $J_\parallel$ and $J_\perp$ are expected to increase, as a result of a larger overlap of the orbitals in Eq. (8), so that the Stoner criterion is satisfied over larger filling ranges. As a consequence, separate regions of coexistence of SC and FM are expected to merge, as shown in Fig. 1. As is also shown in Fig. 1, the ferromagnetic transition temperature is found to
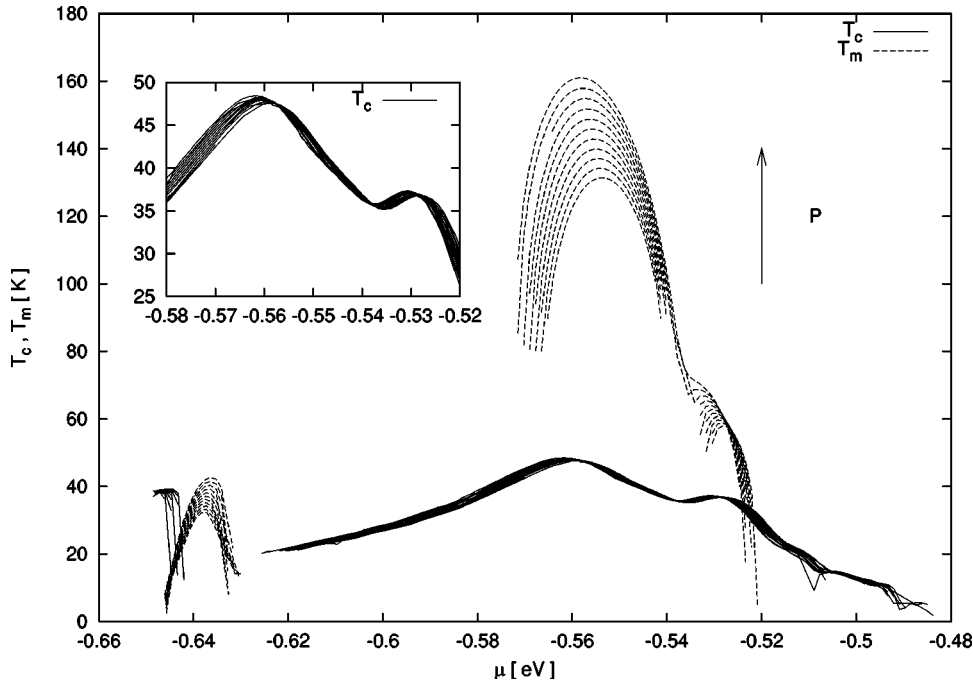
FIG. 1. Superconducting critical temperature T_c (solid lines, and inset) and ferromagnetic critical temperature T_m (dashed lines), as a function of chemical potential μ, for different pressures $P=0-2$ GPa. Lower curves correspond to lower pressures, as indicated by the arrow.

increase with pressure at a rather large rate, in good qualitative agreement with experiments. Its values go from 130 K to 160 K in the pressure range $P=0-2$ K. Thus the ferromagnetic state appears to be strongly stabilized under pressure which should have some consequences for the superconducting state.

As mentioned in Sec. III, up to now we have neglected any explicit pressure effect on the SC coupling parameter g. This is motivated by a lack of either theoretical or phenomenological input for the microscopic mechanism of superconductivity in the ruthenocuprates, which is expected to be of an unconventional nature, as is possible for the high-T_c cu-

prates. Quantitatively, this approximation should not affect our results much, in view of the small pressure effect on T_c, as compared to T_m. However, we have numerically studied the competition of SC and FM, both at zero pressure and for increasing P, by tentatively assuming a small linear dependence of g on pressure. Indeed, the effect of a competing FM phase at $P=0$ does decrease T_c, compared to the $J_\parallel=J_\perp=0$ case, as already observed by Cuoco *et al.*[11] This tendency is also confirmed at nonzero pressure.

Since we neglected any explicit dependence of the SC coupling constant g on pressure, the albeit small increase of T_c shown in the inset of Fig. 1 must be mainly attributed to the pressure-induced changes of the kinetic terms in the SC and SC+FM Hamiltonians, Eqs. (2a) and (2c), i.e., changes in the band structure. Although the fine details of the variations of T_c and T_m are related to each other in an inherently nonlinear way through Eqs. (7), one expects that a pressure-induced enhancement of the hopping parameters t, t', and $t_\perp$ results in a shift towards the band bottom of the Van Hove singularity pertaining to the SC subband, accompanied by a steepening of the DOS, which is indeed recovered in the tendency of the maxima in the T_c curves to move towards lower chemical potentials with increasing pressure (Fig. 1, inset).

V. CONCLUSIONS

We have considered the two-band model for the coexistence of superconductivity and ferromagnetism in the ruthenocuprates. We have self-consistently solved the equations for the SC (respectively, FM) critical temperature in the presence of FM (respectively, SC) order, both as a function of filling (here parametrized by the chemical potential μ), and as a function of pressure. We find separate filling ranges where the coexistence of SC and FM is allowed, merging into larger ranges, as the Stoner criterion gets more effective
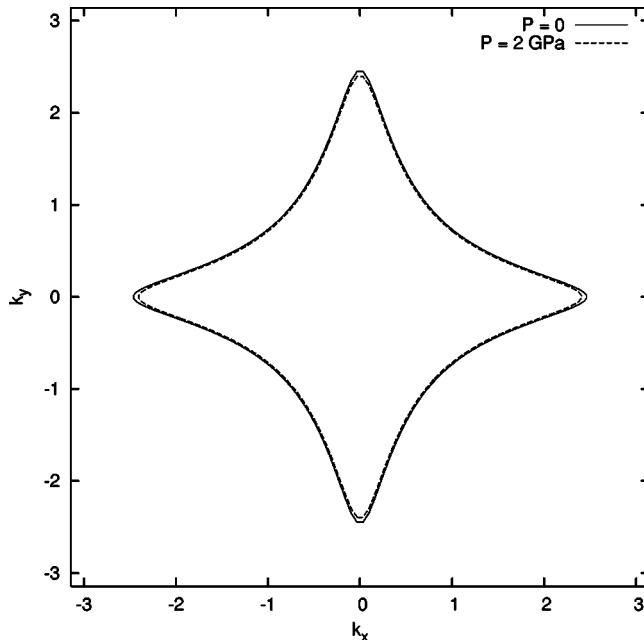

FIG. 2. Fermi lines of the RuO_2 layers corresponding to the maximum T_m in Fig. 1, for $P=0$ and $P=2$ GPa.

with increasing pressure. The ferromagnetic transition temperature is found to increase with pressure at a rate distinctly larger than that of the superconducting temperature, in good qualitative agreement with recent experiments in the ruthenocuprates. Due to the competition between superconductivity and ferromagnetism, the stronger enhancement of the magnetic phase results in a suppression of the pressure effect on T_c.

Our present model does not account for spatial variations of both order parameters, or of their symmetry in **k** space, which has been assumed to be an s wave, for the sake of simplicity. In particular, a c-axis modulation of the order parameters may be important in view of the stronger pressure dependence of the interlayer correlations. A more detailed study of the pressure dependence of the critical temperatures would require more reliable estimates of the compressibility and of the pressure dependence of the charge filling, which await more experimental work.

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