

Vestigial Van Hove Singularity and Higher-Temperature Superconducting Phase Induced by Perpendicular Uniaxial Pressures in Quasi-Two-Dimensional Superconductors

Hiroshi Shimahara

Graduate School of Advanced Science and Engineering, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

(Received July 6, 2020)

We examine quasi-two-dimensional superconductors near half-filling under uniaxial pressures perpendicular to conductive layers (hereafter called perpendicular pressures). It is a natural conjecture that the perpendicular pressure decreases the transition temperature T_c because it increases the interlayer electron hopping energy t_z , which weakens the logarithmic enhancement in the density of states due to the two-dimensional Van Hove singularity. It is shown that, contrary to this conjecture, the perpendicular pressure can significantly enhance T_c in systems off half-filling before it decreases T_c , and the strength of the enhancement significantly depends on the pairing symmetry. When the indices d, d', cz, and sz are defined for the basis functions $\gamma_d \propto \cos k_x - \cos k_y$, $\gamma_{d'} \propto \sin k_x \sin k_y$, $\gamma_{cz} \propto \cos k_z$, and $\gamma_{sz} \propto \sin k_z$, respectively, it is shown that for s-, d-, cz-, and cz-d-wave pairing, T_c steeply increases with increasing t_z near a cusp at a certain value of t_z . On the other hand, for p-, cz-p-, sz-p-, and d'-wave pairing, T_c is almost unaffected by t_z . For sz- and sz-d-wave pairing, T_c exhibits a broad and weak peak. Here, for example, the cz-d-wave state is an interlayer spin-singlet d-wave state with an order parameter proportional to $\gamma_{cz}\gamma_d$. The enhancement in T_c is the largest for this state and the second largest for the d-wave pairing and interlayer spin-singlet (cz-wave) pairing. These results may explain recent observations in Sr_2RuO_4 under perpendicular pressures. A comparison between the theoretical and experimental results indicates that the p-, cz-p-, and sz-p-wave states, including chiral states, and the d'-wave state are the most likely candidates for the intrinsic 1.5-K phase, and the d-, cz-d-, and cz-wave states are the most likely candidates for the 3-K phase induced by the perpendicular pressure. The cz-p- and sz-p-wave states are interlayer spin-triplet and interlayer spin-singlet p-wave states with horizontal line nodes, respectively.

Introduction — It has been frequently pointed out that the logarithmic Van Hove singularity in the density of states can enhance the superconducting transition temperature T_c in quasi-two-dimensional systems near half-filling.^{1–5)} Despite the long history of research on this mechanism, the effect of interlayer electron motion on this mechanism has not been frequently examined, probably because the interlayer hopping energy t_z increases the dimensions of the system and removes the logarithmic singularity;⁵⁾ hence, t_z seems to decrease T_c . In this study, however, we illustrate that t_z can significantly enhance the density of states and T_c .

The effect of t_z on superconductivity might have been observed recently in a real material. The compound Sr_2RuO_4 is a quasi-two-dimensional superconductor with tetragonal symmetry,^{6,7)} and its pairing symmetry has been under debate since the discovery of superconductivity in this compound.^{6–8)} To clarify the pairing symmetry, the application of uniaxial pressures in various directions can be a useful tool.^{9–13)} Hicks et al. examined shifts of T_c due to symmetry-breaking in-plane strains⁹⁾ and found that a $[1, 0, 0]$ strain significantly enhances T_c . They argued that the orthorhombic distortion enhances the density of states owing to the Van Hove singularity,³⁾ and this can be the origin of the enhancement in T_c .⁹⁾ Although this phenomenon under an in-plane pressure is not directly related to the effect of t_z that we examine below, it suggests that the Van Hove singularity can enhance T_c by an appreciable amount in this compound. Before their study, Kittaka et al. examined Sr_2RuO_4 under uniaxial pressures in the $[0, 0, 1]$ direction, which is perpendicular to conductive layers (hereafter called perpendicular pressures).¹⁰⁾ Their study suggests that a perpendicular pressure induces

superconductivity with an onset T_c above 3 K, while interestingly, the transition to the intrinsic superconducting phase remains with its transition temperature $T_c \approx 1.5$ K appearing to be unaffected. In contrast to the in-plane strains, the distortion in this direction does not change the symmetry of the system and weakens the enhancement in the density of states due to the Van Hove singularity. Nevertheless, the observed phenomena can be explained by a scenario based on a vestigial Van Hove singularity, which will be explained below.

The tetragonal quasi-two-dimensional system can be modeled by the one-particle electron energy

$$\epsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}_{\parallel}}^{\parallel} - 2t_z \cos k_z, \quad (1)$$

where $\epsilon_{\mathbf{k}_{\parallel}}^{\parallel} = -2t(\cos k_x + \cos k_y)$ with $\mathbf{k}_{\parallel} = (k_x, k_y)$ and the lattice constants a , b , and c have been absorbed into the definitions of the momentum components k_x , k_y , and k_z , respectively. When $t_z = 0$, the saddle points of $\epsilon_{\mathbf{k}_{\parallel}}^{\parallel}$ at $\mathbf{k}_{\parallel} = (\pm\pi, 0)$ and $(0, \pm\pi)$ give rise to the Van Hove singularity. A perpendicular pressure increases t_z and removes the singularity. We denote the electron density per site and the chemical potential as n and μ , respectively. When we apply the theory to Sr_2RuO_4 , the dispersion in Eq. (1) is a simplified model; however, the model near half-filling can simulate the physical situation of the γ band in this compound, in which the Fermi surface is near the saddle points.⁹⁾ We use units in which $\hbar = k_B = t = 1$.

Density of states — The mechanism by which t_z enhances the density of states can be interpreted as follows. The density of states defined by

$$\rho(\epsilon) = \frac{1}{N} \sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}})$$

is expressed as

$$\rho(\epsilon) = \int_{-\pi}^{\pi} \frac{dk_z}{2\pi} \rho_{\parallel}(\epsilon + 2t_z \cos k_z) \quad (2)$$

with

$$\rho_{\parallel}(\epsilon) \equiv \int \frac{d^2k}{(2\pi)^2} \delta(\epsilon - \epsilon_{\mathbf{k}}^{\parallel})$$

being the density of states of the square lattice system.¹⁴⁾ Here, N denotes the number of sites. $\rho_{\parallel}(\epsilon)$ diverges logarithmically at $\epsilon = 0$, and $\rho_{\parallel} \approx (2\pi^2 t)^{-1} \ln(16t/|\epsilon|)$ for $|\epsilon| \ll t$. When $t_z \neq 0$, the integration over k_z in Eq. (2) removes this divergence, and when t_z increases, the peak height $\rho(0)$ decreases, as expected; however, because $\int \rho(\epsilon) d\epsilon = 1$ is a constant, the suppression of the peak height leads to an increase in $\rho(\epsilon)$ in some other regions of ϵ . It is evident from Eq. (2) that when $|\mu| \leq 2t_z$, the contribution to $\rho(\mu)$ from the electron states near $k_z = \pm \arccos(-\mu/2t_z)$ is large because of the logarithmic enhancement in ρ_{\parallel} . It is verified that $\partial\rho/\partial\epsilon = 0$ for $|\epsilon| \leq 2t_z$, which implies that the top of the vestigial peak is a plateau.

Figure 1 illustrates how the perpendicular pressure enhances the density of states $\rho(\mu)$ at the Fermi level when the system is nearly half-filled. The curves show $\rho(\epsilon)$, and the thin vertical lines indicate $\epsilon = \mu$ for $n = 0.9$. The logarithmic singularity in $\rho(\epsilon)$ disappears for any finite t_z , and a plateau appears.⁵⁾ The density of states at the Fermi level $\rho(\mu)$ increases as t_z increases from 0 when the system is not half-filled. For example, $\rho(\mu) \approx 0.231$ for $t_z = 0.05$, whereas $\rho(\mu) \approx 0.257$ for $t_z = 0.1$, as shown by the red dashed and black solid curves, respectively. When t_z increases further, $\rho(\mu)$ decreases. For example, $\rho(\mu) \approx 0.202$ for $t_z = 0.3$. In s-wave superconductors, the increase and decrease in $\rho(\mu)$ immediately result in an increase and a decrease in T_c , respectively.

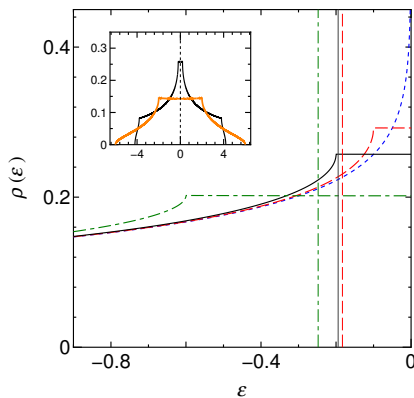


Fig. 1. (Color online) Densities of states and the Fermi levels. The curves and thin vertical lines show $\rho(\epsilon)$ and $\epsilon = \mu$, respectively, the intersections of which yield $\rho(\mu)$ for various values of t_z . The red dashed, black solid, and green dot-dashed curves and lines show the results for $t_z = 0.05, 0.1$, and 0.3 , respectively. The blue short-dashed curve shows $\rho(\epsilon)$ for $t_z = 0$. The inset shows overall profiles of $\rho(\epsilon)$. The orange thick solid curve shows $\rho(\epsilon)$ for $t_z = 1$.

Superconductivity — In anisotropic superconductors, T_c is a function of an effective density of states, in which the momentum dependence of the order parameter is incorporated.

The pairing interaction is expanded as

$$V_{\mathbf{k}\mathbf{k}'} = - \sum_{\alpha} \bar{g}_{\alpha} \gamma_{\alpha}(\mathbf{k}) \gamma_{\alpha}(\mathbf{k}'), \quad (3)$$

where α is the index of the basis function and \bar{g}_{α} is the coupling constant for the α -wave state. The functions $\gamma_{\alpha}(\mathbf{k})$ are orthonormal bases,³⁾ which satisfy

$$\frac{1}{N} \sum_{\mathbf{k}} \gamma_{\alpha}(\mathbf{k}) \gamma_{\alpha'}(\mathbf{k}) = \delta_{\alpha\alpha'}.$$

The pressure affects the values of \bar{g}_{α} ; however, we leave the effect of the change in \bar{g}_{α} for future research and focus on the effect of the change in the density of states.

The order parameter is expanded as

$$\Delta_{\mathbf{k}} = \sum_{\alpha} \Delta_{\alpha} \gamma_{\alpha}(\mathbf{k}),$$

and the linearized gap equations are

$$\Delta_{\alpha} = \frac{\bar{g}_{\alpha}}{N} \sum_{\mathbf{k}} \sum_{\alpha'} \gamma_{\alpha}(\mathbf{k}) W(\xi_{\mathbf{k}}) \gamma_{\alpha'}(\mathbf{k}) \Delta_{\alpha'},$$

where $W(\xi_{\mathbf{k}}) = \tanh(\beta \xi_{\mathbf{k}}/2)/2\xi_{\mathbf{k}}$. Because of the symmetry of the system, these equations are decoupled into subsets by the pairing symmetries. When the pairing state is not a mixed-symmetry state, the order parameter $\Delta_{\mathbf{k}}$ is a linear combination of basis functions with the same symmetry, which is expressed as

$$\Delta_{\mathbf{k}} = \sum_{\alpha \in S_{\lambda}} \Delta_{\alpha} \gamma_{\alpha}(\mathbf{k}), \quad (4)$$

where S_{λ} is a set of α values such that all γ_{α} have the same symmetry λ . As a consequence of the superposition, the order parameter of the most stable state is localized near the Fermi surface in momentum space,¹⁵⁾ reflecting the range of interaction of the order of v_F/ω_c , which is much larger than the lattice constants, where v_F denotes the Fermi velocity. In this paper, we simplify the problem by retaining a single principal basis function γ_{α} for each pairing symmetry and restrict the range of interaction by introducing the cutoff energy ω_c instead of superposing many basis functions to localize $\Delta_{\mathbf{k}}$ near the Fermi surface. Hence, we retain a single α in the summations in Eqs. (3) and (4) and replace $\gamma_{\alpha}(\mathbf{k})$ with $C \theta(\omega_c - |\xi_{\mathbf{k}}|) \gamma_{\alpha}(\mathbf{k})$, where C is a normalization constant and $\xi_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} - \mu$. The equation for T_c is

$$1 = \frac{\bar{g}_{\alpha}}{N} \sum_{\mathbf{k}} W(\xi_{\mathbf{k}}) \theta(\omega_c - |\xi_{\mathbf{k}}|) [\gamma_{\alpha}(\mathbf{k})]^2,$$

and when $\omega_c \ll t$, we obtain

$$T_c = \frac{2e^{\gamma}}{\pi} \omega_c e^{-1/\lambda_{\alpha}}, \quad (5)$$

where $\lambda_{\alpha} = g_{\alpha} \rho_{\alpha}(\mu)$, $g_{\alpha} \equiv \bar{g}_{\alpha} C^2$, and $\gamma = 0.57721 \dots$ is the Euler's constant. Here, $\rho_{\alpha}(\epsilon)$ is the effective density of states for α -wave pairing, which is expressed as

$$\rho_{\alpha}(\epsilon) \equiv \int \frac{d^3k}{(2\pi)^3} \delta(\epsilon - \epsilon_{\mathbf{k}}) [\gamma_{\alpha}(\mathbf{k})]^2.$$

We adopt $\gamma_{p_x}(\mathbf{k}) = \sqrt{2} \sin k_x$ and $\gamma_{p_y}(\mathbf{k}) = \sqrt{2} \sin k_y$ as the principal basis functions of the p_x - and p_y -wave states, respectively. These states are degenerate in the tetragonal system, and they and any superposition of them, for example, the chi-

ral $p_x \pm ip_y$ wave states, have the same transition temperature. Hence, as far as T_c is concerned, we simply call them the p-wave states. Among them, the one with the lowest free energy occurs below T_c , and presumably, the chiral states have the lowest free energy because they are full-gap states. We adopt $\gamma_s = 1$ and $\gamma_d = \cos k_x - \cos k_y$, respectively, as the principal bases of the s- and d-wave states. For the d_{xy} -wave state, we adopt $\gamma_{d_{xy}} = 2 \sin k_x \sin k_y$. We also examine interlayer pairing between adjacent layers,¹⁶⁾ for which the order parameter has a factor $\cos k_z$ or $\sin k_z$. Hence, the resultant order parameter is a product of $\cos k_z$ or $\sin k_z$ and an in-plane basis, such as γ_s , γ_p , and γ_d . For example, when the latter is the s-wave function, i.e., $\hat{\gamma}_s = 1$, the principal bases are

$$\gamma_{cz}(\mathbf{k}) = \sqrt{2} \cos k_z, \quad \gamma_{sz}(\mathbf{k}) = \sqrt{2} \sin k_z,$$

where we defined the indices cz and sz for $\cos k_z$ and $\sin k_z$, respectively. The cz-wave state is a spin singlet, whereas the sz-wave state is a spin triplet. For the d- or p-wave in-plane states, the principal bases are

$$\gamma_{cz-d} = \gamma_{cz}\gamma_d, \quad \gamma_{sz-d} = \gamma_{sz}\gamma_d,$$

$$\gamma_{cz-p} = \gamma_{cz}\gamma_p, \quad \gamma_{sz-p} = \gamma_{sz}\gamma_p.$$

The cz-d- and sz-p-wave states are spin singlets, whereas the sz-d- and cz-p-wave states are spin triplets.

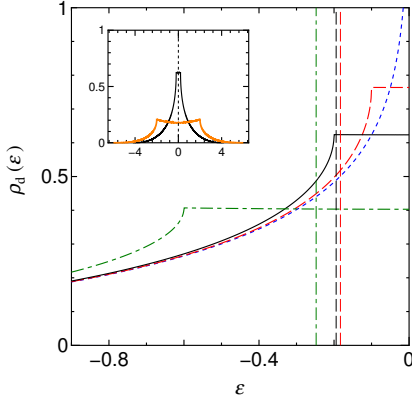


Fig. 2. (Color online) Effective density of states $\rho_d(\epsilon)$ for the d-wave pairing with $\Delta_{\mathbf{k}} \propto \cos k_x - \cos k_y$. The legend of this figure is the same as that of Fig. 1.

Figure 2 shows that the effective density of states $\rho_d(\mu)$ at the Fermi level is enhanced by the same mechanism as that for $\rho(\mu)$, and the enhancement in $\rho_d(\mu)$ is much larger than that in $\rho_s(\mu) = \rho(\mu)$ because $[\gamma_d(\mathbf{k})]^2$ is large near the saddle points at $(k_x, k_y) = (\pm\pi, 0)$ and $(0, \pm\pi)$. This example illustrates that the enhancement effect of the present mechanism significantly depends on the pairing symmetry. For a comparison between different pairing symmetries, we evaluate T_c under the condition that the values of T_c at $t_z = 0$ are equated. For explicit evaluations, we adopt specific values $n = 0.9$ and $\omega_c = 300$ K and assume that $T_c \approx 1.5$ K at $t_z = 0$.¹⁷⁾

The results are shown in Fig. 3, and it is found that the enhancement in T_c is the largest and the next largest for the cz-d-wave state and the d- and cz-wave states, respectively. For these three states and s-wave states, T_c increases steeply near a cusp at a certain value of t_z . For the interlayer sz- and sz-d-

wave states, T_c exhibits a broad peak. For p-, sz-p-, cz-p-, and d_{xy} -wave states, T_c changes little when t_z increases. (Strictly speaking, T_c decreases slightly as shown in Fig. 4.) This originates from the fact that the order parameters of these states vanish at the saddle points of $\epsilon_{\mathbf{k}_{\parallel}}^{\parallel}$ because of the in-plane bases proportional to $\sin k_x$, $\sin k_y$, or $\sin k_x + i \sin k_y$. Note that this result holds for any p-wave states because every term of the order parameters of the p-wave states is proportional to one of $\sin(mk_x)$ and $\sin(mk_y)$ with $m = 1, 2, \dots$, which vanish at the saddle points $(k_x, k_y) = (\pm\pi, 0)$ and $(0, \pm\pi)$.

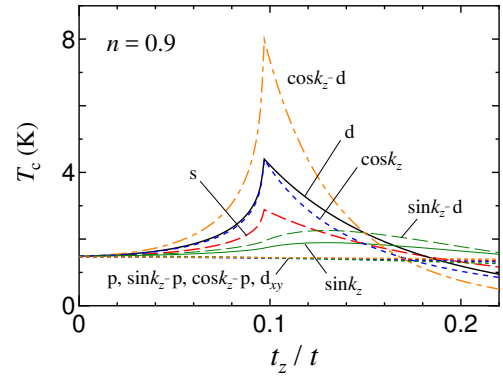


Fig. 3. (Color online) Transition temperatures for various pairing symmetries when $T_c \approx 1.5$ K at $t_z = 0$.¹⁷⁾ The black solid and red dashed curves present the results for the d- and s-wave states, respectively. The red, blue, orange, and green thick dotted curves present the results for the p-, cz-p-, sz-p-, and d_{xy} -wave states, respectively. Most parts of the dotted curves overlap. The blue short-dashed and orange dot-dashed curves present the results for the cz- and cz-d-wave states, respectively. The green thin solid and dashed curves present the results for the sz-s- and sz-d-wave states, respectively.

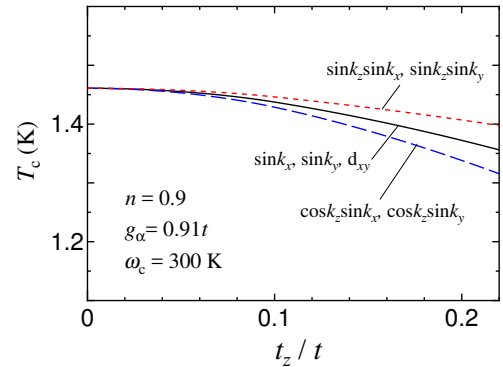


Fig. 4. (Color online) Transition temperatures when $n = 0.9$, $\omega_c = 300$ K, and $g_{\alpha} = 0.91t$ for $\alpha = p, cz-p, sz-p$, and d_{xy} .

Ruthenate superconductors — The present model seems to explain some of the experimental observations in Sr_2RuO_4 . In the experimental result,¹⁰⁾ the transition temperature of the intrinsic state is not changed by a perpendicular pressure. The theoretical result shown in Figs. 3 and 4 indicates that this can be explained if the intrinsic state is one of the p-, sz-p-, cz-p-, and d_{xy} -wave states. The sz- and sz-d-wave states are the second-most likely candidates because their T_c values weakly depend on t_z in the theoretical result. Table I lists

the order-parameter structures and properties of some of the most likely candidates for the intrinsic states. Among them, only the sz-p and cz-p states exhibit horizontal line nodes, which are suggested by the field-angle-dependent specific-heat measurement.¹⁸⁾ In particular, in the spin-triplet state $[cz-(p_x + ip_y)]\hat{d}$ and the spin-singlet state $sz-(p_x + ip_y)$, the time-reversal symmetry (TRS) is broken, which is suggested by muon spin relaxation (μ SR),¹⁹⁾ where \hat{d} denotes the d-vector and $\hat{d} \equiv \hat{d}/|\hat{d}|$. Over twenty years, it had been considered that the absence of the Knight shift²⁰⁾ supports equal-spin states; however, recently, a pronounced drop of ^{17}O NMR Knight shift in the superconducting state was reported.^{21,22)} This implies that the intrinsic state is an antiparallel spin state or at least contains a component of antiparallel spin states, where the spin quantization axis is taken in the direction parallel to the magnetic field. The temperature dependence of the upper critical field seems to support antiparallel spin states.^{8,23)}

Table I. Examples of candidates for the intrinsic state that is unaffected by the perpendicular pressure. \hat{x} , \hat{y} , and \hat{z} denote the unit vectors in the x -, y -, and z -directions in the d-vector space, respectively. For the other unlisted candidates, such as the states with $p_x\hat{y} \pm p_y\hat{x}$, $p_x\hat{z}$, and $(p_x \pm p_y)\hat{d}$, the properties of the nodes and TRS can easily be found from tables in previous studies, for example, in Ref. 7. The only difference is the possibility of the factors $\cos k_z$ and $\sin k_z$, which add horizontal line nodes to the order parameter.

Structure of the order parameter	Spin	Line nodes	TRS
$p_x\hat{x} \pm p_y\hat{y}$	triplet	none	unbroken
$cz-(p_x\hat{x} \pm p_y\hat{y})$	triplet	horizontal	unbroken
$p_x\hat{y} \pm ip_y\hat{x}$	triplet	none	broken
$cz-(p_x\hat{x} \pm ip_y\hat{y})$	triplet	horizontal	broken
$(p_x + ip_y)\hat{d}$	triplet	none	broken
$[cz-(p_x + ip_y)]\hat{d}$	triplet	horizontal	broken
$sz-(p_x + ip_y)$	singlet	horizontal	broken
d_{xy}	singlet	vertical	unbroken

The observed 3-K phase in Sr_2RuO_4 cannot be among p-, sz-p-, cz-p-, and d_{xy} -wave pairing in the present Van Hove scenario, because their transition temperatures are almost unaffected by $t_z \neq 0$. If any one of them is the 3-K phase, T_c must be approximately 3 K for any smaller t_z , which is inconsistent with the experimental fact. Moreover, for the s-, sz-, and sz-d-wave states, the enhancement of T_c is too weak to be the 3-K phase. In contrast, the transition temperatures of the cz-d-, d-, and cz-wave states are significantly enhanced by $t_z \neq 0$, as shown in Fig. 3, and hence, these states are most likely the 3-K phase. All of these states are spin-singlet states.

Figure 5 depicts the Van Hove scenario for Sr_2RuO_4 under perpendicular pressures. Since the transition temperature given in Eq. (5) is the instability temperature of the normal state, only the highest one is realized at each t_z . Therefore, the candidates for the intrinsic phase are the p-, cz-p-, and sz-p-wave states, and the candidates for the higher-temperature phase are the d-, cz-, and cz-d-wave states. Figures 5 (a) and (b) present the results of two examples of combinations of the intrinsic and higher-temperature phases, i.e., the p- and d-wave states and the sz-p- and cz-d-wave states, respectively. In both cases, because the higher-temperature phases (d- and cz-d-wave states) have more nodes than the intrinsic phases (chiral p- and chiral sz-p-wave states, respectively), the transitions presented by the dotted curves must be com-

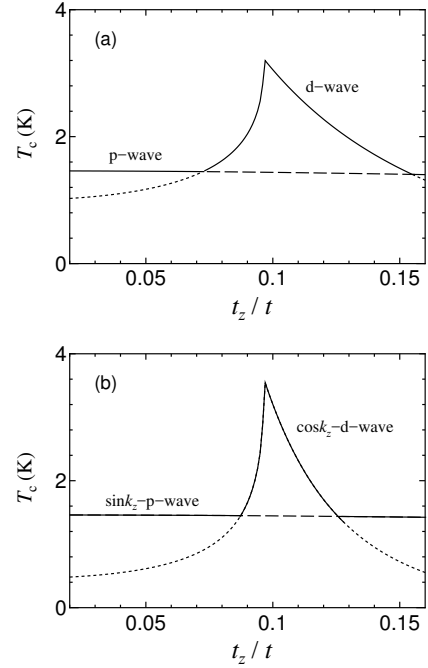


Fig. 5. Transition temperatures when $n = 0.9$ and $\omega_c = 300$ K. (a) When p-wave and d-wave pairing interactions coexist. $g_p = 0.91t$ and $g_d = 0.34t$ are assumed. (b) When sz-p-wave and cz-d-wave pairing interactions coexist. $g_{sz-p} = 0.91t$ and $g_{cz-d} = 0.30t$ are assumed.

pletely suppressed, whereas the dashed curves might survive as approximate transition temperatures to mixed states or approximate first-order transition temperatures to the low-temperature phases.

Conclusion — In conclusion, it was shown that the superconducting transition temperature can be strongly enhanced by uniaxial pressures perpendicular to the most conductive layers in quasi-two-dimensional superconductors off half-filling because of a vestigial Van Hove singularity. We examined this effect for various types of pairing states including those induced by interlayer pairing. Among them, the enhancement is the largest for the interlayer d-wave state with $\Delta_{\mathbf{k}} \propto \cos k_z(\cos k_x - \cos k_y)$, and it is also large for the d-wave state with $\Delta_{\mathbf{k}} \propto \cos k_x - \cos k_y$. In contrast, this effect does not exist for the interlayer and intralayer p-wave states, because $\sin(mk_x)$ and $\sin(mk_y)$ vanish at $(k_x, k_y) = (\pm\pi, 0)$ and $(0, \pm\pi)$. These behaviors are consistent with experimental observations in Sr_2RuO_4 under perpendicular pressures,¹⁰⁾ if we assume that the higher-temperature phase is one of the intralayer and interlayer spin-singlet d- and s-wave states and the intrinsic 1.5-K phase is one of the intralayer and interlayer p-wave states. The interlayer p-wave states can be either spin-singlet or spin-triplet states depending on the factors $\cos k_z$ and $\sin k_z$, respectively.

As future studies, the structures of the mixed states below the second (lower) transition temperature when the 3-K phase occurs and the superconductivity under uniaxial pressures in the other directions will be examined in separate papers. For a close comparison with the observed facts in Sr_2RuO_4 , details of the Fermi-surface structures of all α , β , and γ bands may need to be incorporated.

- 1) J.E. Hirsch and D.J. Scalapino, Phys. Rev. Lett. **56**, 2732 (1986).
- 2) R.S. Markiewicz, J. Phys. Chem. Solids **58**, 1179 (1997), and references therein.
- 3) H. Shimahara and S. Takada, Jpn. J. Appl. Phys. **26**, L1674 (1987), and references therein.
- 4) H. Shimahara and S. Takada, J. Phys. Soc. Jpn. **57**, 1044 (1988).
- 5) R.S. Markiewicz, Physica C **177**, 171 (1991).
- 6) Y. Maeno, H. Hashimoto, K. Yoshida, S. Nishizaki, T. Fujita, J.G. Bednorz, and F. Lichtenberg, Nature (London) **372**, 532 (1994).
- 7) A.P. Mackenzie and Y. Maeno, Rev. Mod. Phys. **75**, 657 (2003), and references therein.
- 8) Y. Maeno, S. Kittaka, T. Nomura, S. Yonezawa, and K. Ishida, J. Phys. Soc. Jpn. **81**, 011009 (2012).
- 9) C.W. Hicks, D.O. Brodsky, E.A. Yelland, A.S. Gibbs, J.A.N. Bruin, M.E. Barber, S.D. Eddins, K. Nishimura, S. Yonezawa, Y. Maeno, and A.P. Mackenzie, Science **344**, 283 (2014).
- 10) S. Kittaka, H. Taniguchi, S. Yonezawa, H. Yaguchi, and Y. Maeno, Phys. Rev. B **81**, 180510(R) (2010).
- 11) H. Taniguchi, S. Kittaka, S. Yonezawa, H. Yaguchi, and Y. Maeno, J. Phys.: Conf. Ser. **391**, 012108 (2012).
- 12) H. Taniguchi, K. Nishimura, S.K. Goh, S. Yonezawa, and Y. Maeno, J. Phys. Soc. Jpn. **84**, 014707 (2015).
- 13) Y. Imai and M. Sigrist, J. Phys. Soc. Jpn. **89**, 014702 (2020).
- 14) Expressions for $\rho_{||}$ are presented in previous papers, such as Refs. 3 and 4.
- 15) An example in which a linear combination of basis functions is localized near the Fermi surface for the most stable state is presented in Ref. 24.
- 16) Y. Hasegawa, K. Machida, and M. Ozaki, J. Phys. Soc. Jpn. **69**, 336 (2000).
- 17) We assume the coupling constant of the principal basis γ_α so that $T_c \approx 1.5$ K at $t_z = 0$: $g_\alpha = 0.81t$ if α is s, sz, or cz; $g_\alpha = 0.365t$ if α is d, sz-d, or cz-d; $g_\alpha = 0.91t$ if α is p; and $g_\alpha = 0.69t$ if α is d_{xy} .
- 18) S. Kittaka, S. Nakamura, T. Sakakibara, N. Kikugawa, T. Terashima, S. Uji, D.A. Sokolov, A.P. Mackenzie, K. Irie, Y. Tsutsumi, K. Suzuki, and K. Machida, J. Phys. Soc. Jpn. **87**, 093703 (2018).
- 19) G.M. Luke, Y. Fudamoto, K.M. Kojima, M.I. Larkin, J. Merrin, B. Nachumi, Y.J. Uemura, Y. Maeno, Z.Q. Mao, Y. Mori, H. Nakamura, and M. Sigrist, Nature (London) **394**, 558 (1998).
- 20) K. Ishida, H. Mukuda, Y. Kitaoka, K. Asayama, Z.Q. Mao, Y. Mori, and Y. Maeno, Nature (London) **396**, 658 (1998).
- 21) A. Pustogow, Y. Luo, A. Chronister, Y.-S. Su, D.A. Sokolov, F. Jerzenbeck, A.P. Mackenzie, C.W. Hicks, N. Kikugawa, S. Raghu, E.D. Bauer, and S.E. Brown, Nature **574**, 72 (2019).
- 22) K. Ishida, M. Manago, K. Kinjo, and Y. Maeno, J. Phys. Soc. Jpn. **89**, 034712 (2020).
- 23) K. Machida and M. Ichioka, Phys. Rev. B **77**, 184515 (2008).
- 24) H. Shimahara, J. Phys. Soc. Jpn. **58**, 1735 (1989).