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 $d, d', cz, sz$ and $sz$ are defined for the basis functions $\gamma_d \propto \cos k_x - \cos k_z$, $\gamma_{d'} \propto \sin k_x \sin k_z$, $\gamma_{cz} \propto \cos k_z$, 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$_2$RuO$_4$ 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.

\[ \epsilon_k = \epsilon^\parallel_{k_0} - 2t_z \cos k_z, \]

where $\epsilon^\parallel_{k_0} = -2\mu (\cos k_x + \cos k_y)$ with $k_0 = (k_x, k_y)$ 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 $\epsilon^\parallel_{k_0}$ at $k_0 = (\pm \pi, 0)$ 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 $\mu$, respectively. When we apply the theory to Sr$_2$RuO$_4$, the dispersion in Eq. (1) is a simplified model; however, the model near half-filling can simulate the physical situation of the $\gamma$ band in this compound, in which the Fermi surface is near the saddle points. 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
black solid curves, respectively. When \( \rho_s \) describes a superconducting state, the increase and decrease in \( \rho \) is evident from Eq. (2) when \( |\mu| \leq 2t_c \), the contribution to \( \rho(\mu) \) from the electron states near \( k_c = \pm \arccos(-\mu/2t_c) \) is large because of the logarithmic enhancement in \( \rho(\mu) \). It is verified that \( \partial \rho/\partial \epsilon = 0 \) for \( |\epsilon| \leq 2t_c \), 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 \( t_c \), and a plateau appears.

The density of states at the Fermi level \( \rho(\mu) \) increases as \( t_c \) increases from 0 when the system is not half-filled. For example, \( \rho(\mu) \approx 0.231 \) for \( t_c = 0.05 \), whereas \( \rho(\mu) \approx 0.257 \) for \( t_c = 0.1 \), as shown by the red dashed and black solid curves, respectively. When \( t_c \) increases further, \( \rho(\mu) \) decreases. For example, \( \rho(\mu) \approx 0.202 \) for \( t_c = 0.3 \). In \( s \)-wave superconductors, the increase and decrease in \( \rho(\mu) \) immediately result in an increase and a decrease in \( T_c \), respectively.

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

\[
V_{kk'} = -\sum_\alpha \tilde{g}_\alpha \gamma_\alpha(k) \gamma_\alpha(k'),
\]

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

\[
\sum_k \gamma_\alpha(k) \gamma_{\alpha'}(k) = \delta_{\alpha\alpha'}.
\]

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

The order parameter is expanded as

\[
\Delta_k = \sum_\alpha \Delta_\alpha \gamma_\alpha(k),
\]

and the linearized gap equations are

\[
\Delta_\alpha = \frac{g_\alpha}{N} \sum_k \sum_{\alpha'} \gamma_\alpha(k) W(\xi_k) \gamma_{\alpha'}(k) \Delta_{\alpha'},
\]

where \( W(\xi_k) = \tanh(\beta \xi_k/2)/2\xi_k \). 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 \( \Delta_k \) is a linear combination of basis functions with the same symmetry, which is expressed as

\[
\Delta_k = \sum_{\alpha \in S_{\lambda}} \Delta_\alpha \gamma_\alpha(k),
\]

where \( S_{\lambda} \) is a set of \( \alpha \) values such that all \( \gamma_\alpha \) have the same symmetry \( \lambda \). As a consequence of the superposition, the order parameter of the most stable state is localized near the Fermi surface in momentum space, reflecting the range of interaction of the order of \( v_F/\omega_c \), 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 \( \gamma_\alpha \) and restrict the range of interaction by introducing the cutoff energy \( \omega_c \) instead of superposing many basis functions to localize \( \Delta_k \) near the Fermi surface. Hence, we retain a single \( \alpha \) in the summations in Eqs. (3) and (4) and replace \( \gamma_\alpha(k) \) with \( C \theta(\omega_c - |\xi_k|) \gamma_\alpha(k) \), where \( C \) is a normalization constant and \( \xi_k \equiv \epsilon_k - \mu \). The equation for \( T_c \) is

\[
1 = \frac{g_\alpha}{N} \sum_k W(\xi_k) \theta(\omega_c - |\xi_k|) |\gamma_\alpha(k)|^2.
\]
and when $\omega_c \ll t$, we obtain

$$T_c = \frac{2e^\pi}{\pi^2} \omega_c e^{-1/\lambda_c},$$

(5)

where $\lambda_c = g_a \rho_0(\mu)$, $g_a \equiv \frac{\pi^2}{4} g_0^2$, and $\gamma = 0.57721 \ldots$ is the Euler’s constant. Here, $\rho_0(\epsilon)$ is the effective density of states for $\alpha$-wave pairing, which is expressed as

$$\rho_0(\epsilon) \equiv \int \frac{d^3k}{(2\pi)^3} \delta(\epsilon - \epsilon_k) |\gamma_\alpha(k)|^2.$$ We adopt $\gamma_p = \sqrt{2} \sin k_x$ and $\gamma_d = \sqrt{2} \sin k_y$, as the principal bases 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 chiral state, 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 $\gamma_x = 1$ and $\gamma_y = \cos k_x - \cos k_y$, respectively, as the principal bases of the $s$- and $d$-wave states. For the $d$-wave state, we adopt $\gamma_{dd} = 2 \sin k_x \sin k_y$. We also examine interlayer pairing between adjacent layers [16], for which the order parameter has a factor $\cos k_x$ or $\sin k_x$. Hence, the resultant order parameter is a product of $\cos k_x$ or $\sin k_x$ and an in-plane basis, such as $\gamma_x$, $\gamma_y$, and $\gamma_i$. For example, when the latter is the $s$-wave function, i.e., $\gamma_i = 1$, the principal bases are

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

where we defined the indices $cz$ and $sz$ for $\cos k_x$ and $\sin k_x$, 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.

Figure 2 shows that the effective density of states $\rho_0(\mu)$ at the Fermi level is enhanced by the same mechanism as that for $\rho(\mu)$, and the enhancement in $\rho_0(\mu)$ is much larger than that in $\rho(\mu) = \rho(\mu)$ because $|\gamma(\mu)|^2$ 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 $t_c = 0$ 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 $t_c = 0$.

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 $t_c$. For the interlayer $sz$- and $sz$-$d$-wave states, $T_c$ exhibits a broad peak. For $p$-, $sz$-$p$-, $cz$-$p$-, and $d$-$d$-wave states, $T_c$ changes little when $t_c$ 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 $k_x, sin k_x$, 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 $\sin(k_m)$ and $\sin(m\pi)$ with $m = 1, 2, \ldots$, which vanish at the saddle points $(k_x, k_y) = (\pm \pi, 0)$ and $(0, \pm \pi)$.

**Ruthenate superconductors** — The present model seems to explain some of the experimental observations in Sr$_2$RuO$_4$. 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-wave states. The sz- and sz-d-wave states are the second-most likely candidates because their $T_c$ values weakly depend on $t_c$ 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$_y$)]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 ($\mu$SR) [19], where $d$ denotes the d-vector and $\hat{d} \equiv d/|d|$. The absence of the Knight shift [20] and the behaviors of the upper critical field [8,21] seem to contradict each other because they support equal-spin states and antiparallel spin states (for example, the cz-p- and sz-p-wave states in the present candidates), respectively.

| 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 |
| $p_y \hat{y} \pm p_x \hat{x}$ | triplet | none | broken |
| $cz-(p_x \hat{x} \pm p_y \hat{y})$ | 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 |
| $d_{1v}$ | singlet | vertical | unbroken |

The observed 3-K phase in Sr$_2$RuO$_4$ cannot be among $p$-, sz-$p$-, cz-$p$-, and d-wave states. The structure of these phases is almost unaffected by $t_c \neq 0$. If any one of them is the 3-K phase, $T_c$ must be approximately 3 K for any smaller $t_c$, 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 $t_c \neq 0$, as shown in Fig. 4 and hence, these states are most likely the 3-K phase. All of these states are spin-singlet states.

![FIG. 4: (Color online) Transition temperatures when $n = 0.9$, $\omega_k = 300$ K, and $g_\alpha = 0.91t$ for $a = p$, cz-p, sz-p, and $d_{1v}$.](image)

![FIG. 5: Transition temperatures when $n = 0.9$ and $\omega_k = 300$ 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.](image)
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 \( \Delta_k \propto \cos k_x \cos k_y \), and it is also large for the d-wave state with \( \Delta_k \propto \cos k_x - \cos k_y \). 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 \( \text{Sr}_2\text{RuO}_4 \) 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 \( \text{Sr}_2\text{RuO}_4 \), details of the Fermi-surface structures of all \( \alpha, \beta, \) and \( \gamma \) bands may need to be incorporated.

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