Orbital entanglement mechanism of superconductivity in strontium titanate

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We show that the bottom of the conduction band in SrTiO₃ is formed by the Kramers doublet of states with finite angular momentum involving a spin-orbit-coupled superposition of all three t₂g orbitals of Ti. Analysis of electron correlations based on the Hubbard model shows that superconductivity may be mediated by the orbital entanglement of electrons due to the Mott-Hubbard’s coupling between t₂g orbitals. The proposed mechanism is likely relevant to other multiband superconductors.

Introduction. Strontium titanate SrTiO₃ (STO) exhibits unique and puzzling electronic and structural properties that have motivated its extensive studies over the last 50 years [1–3]. The dielectric constant of STO is anomalously large and almost diverges at low temperature without the onset of ferroelectricity, in a manner consistent with quantum paraelectricity [4]. Ferroelectricity in STO can be stabilized by strain or interfacial effects in thin films [5, 7]. Electron-doped STO also exhibits superconductivity (sc) at remarkably low carrier concentrations of 10¹⁷ cm⁻³, corresponding to the Fermi energy of only 1 meV [5, 8]. Experiments suggest s-wave symmetry of the sc order parameter [9, 10]. Furthermore, the existence of quantum paraelectricity in STO is conducive of the conventional phonon mechanism of sc. However, sc in STO cannot be explained by the conventional Bardeen-Cooper-Schrieffer (BCS) or Migdal-Eliashberg theories relying on the electron-electron attraction mediated by the retarded lattice response to electron motion [11, 12], since the Fermi energy in STO is comparable to or smaller than the energy of phonons mediating sc [13–14].

The dome-like dependence of the critical temperature Tc on doping in STO is similar to that of high-temperature superconductors, albeit with a small maximum Tc = 0.4 K [15, 16]. Furthermore, tunneling measurements provide evidence for multi-band sc, similar to pnictides and some other unconventional superconductors [17]. A variety of models were developed to explain sc in STO, including long-range electron-phonon interaction [18], soft bosonic modes [19], intervalley phonons [20] and quantum paraelectric fluctuations [21, 22], but its mechanism remains debated. In particular, it remains contentious whether the ferroelectric distortions enhance sc in STO [23, 24] or suppress it [19, 26, 27].

Here, we utilize the tight-binding approximation to analyze the spin and orbital properties of the conduction band in STO. In the limit of negligible spin-orbit coupling (SOC), electrons residing in one of the three t₂g orbitals of Ti are confined to hop within one of the three orthogonal planes. Their orbital state is conserved due to the orbital selectivity of hopping, resulting in the formation of three highly anisotropic conduction sub-bands. SOC becomes dominant near the bottom of the conduction band, in the cubic phase mixing all three of the t₂g sub-bands into a Kramers doublet with the maximum total angular momentum j = 5/2. We utilize the Hubbard model to demonstrate a possible sc mechanism arising due to the entanglement akin to antiferromagnetic (AF) Mott correlations, but involving instead the spin-orbit-coupled pseudo-spin. sc in this state is a consequence of the phase twist of entangled electrons with unquenched orbital momentum, qualitatively different from BCS.

Conduction band without SOC. We now show that in the limit of negligible spin-orbit coupling (SOC), the conduction band of STO is characterized by highly anisotropic orbitally-selective transport properties. While the bandstructure of STO has been extensively studied [28–32], we are not aware of prior studies of the relation between the orbital states of electrons and their band properties revealed by our analysis.

STO is a semiconductor with indirect bandgap of 3.25 eV. At room temperature, it has a cubic perovskite structure, with octahedral coordination of Ti formed by six nearest-neighbor oxygens aligned with the principal crystal axes, Fig. 1(a). Antiferrodistortive rotations of the TiO₆ octahedra below 105 K result in small distortions of the octahedral environment of Ti [33]. These distortions reduce the orbital selectivity of hopping, which is not expected to qualitatively change the mechanism of sc discussed below.

The conduction band of STO is dominated by the hopping between t₂g orbitals of Ti and p-orbitals of its nearest-neighbor oxygens characterized by the matrix elements tᵢⱼν = ⟨dᵢ|V''|pᵢ⟩ [24]. Here, index i enumerates the nearest-neighbor oxygens, dᵢ is one of the three t₂g orbital wavefunctions of Ti forming a pseudo-vector...
function of the Ti orbital of Ti and the \( p \) \( \pi \)-orbitals, and \( V' \) is the perturbation of the atomic potential resulting in orbital hybridization. The effects of SOC are separately analyzed below.

We now show that hopping is described by a single orbitally-selective matrix element. Consider the \( d_{yz} \) orbital of Ti and the \( p_{z} \) orbital of the neighboring oxygen on the \( x \)-axis, Fig. [1(b)]. The dependence of the wavefunction \( \psi_{ij} \) on the axial angle \( \theta_{x} \) for rotations around the \( x \)-axis, measured starting from the y-axis in the positive \( z \)-direction, is \( \sin(2\theta_{x}) \). Meanwhile, for the \( p_{z} \) orbital of oxygen on the \( x \)-axis, this dependence is \( \sin(\theta_{y}) \). In the cubic phase, the potential \( V' \) is axially symmetric. In the cylindrical coordinate system \( (x, \rho_{x}, \theta_{x}) \) aligned with the \( x \)-axis, the corresponding matrix element is

\[
t_{1,3}^{1} = \int f(x, \rho_{x}) \sin(\theta_{x}) \sin(2\theta_{x}) d\theta_{x} = 0,
\]

where \( f(x, \rho_{x}) \) is a function of radial and axial coordinates.

This conclusion also follows from the observation that each lobe of the \( p_{z} \) orbital overlaps with both the positive and the negative lobes of the \( d_{yz} \) orbital, Fig. [1(b)]. Hopping between the \( d_{yz} \) orbital and the \( p_{z} \) orbital of the oxygen on the \( z \)-axis is also prohibited by symmetry. The only symmetry-allowed matrix element involving the \( d_{yz} \) orbital, \( t_{2,3}^{1} \), corresponds to hopping to the \( p_{z} \) orbital of nearest-neighbor oxygens on the \( y \)-axis, since both orbitals are described by the same dependence \( \cos(\theta_{y}) \) on the rotation angle around the \( y \)-axis. By the cubic symmetry of STO, the only finite matrix element involving the \( d_{yz} \) orbital is \( t_{1,3}^{2} = t_{2,3}^{1} = 0 \), which corresponds to hopping along the \( z \)-axis. Hopping between \( d_{yz} \) and the \( p_{z} \) orbitals is prohibited by symmetry in all directions, Fig. [1(c)].

We conclude that an electron in the \( d_{yz} \) orbital of Ti can hop only onto the \( p_{z} \) orbital of the two nearest-neighbor oxygens on the \( y \)-axis or the \( p_{y} \) orbital of the two nearest-neighbor oxygens on the \( z \)-axis. By the same symmetry arguments, it can then hop from oxygen only onto the \( d_{yz} \) orbital of the nearest-neighbor Ti along the corresponding Ti-O-Ti chain [see Fig. [1(b)]]. Thus, electrons initially in the \( d_{yz} \) orbital propagate only in the \( yz \) plane while retaining their orbital state.

Since oxygen merely mediates orbital-selective hopping between Ti atoms, hereinafter we consider only the state projections on the Ti \( t_{2g} \) orbitals. Orbital-state-preserving hopping between the \( d_{yz} \) orbital of Ti and its four nearest Ti neighbors in the \( yz \) plane is described by a single hopping parameter \( t \), which is negative since \( d_{yz} \) is antisymmetric with respect to both the \( y \)- and the \( z \)-axes [see Fig. [1(b)]. By symmetry, the hopping of electrons in the \( d_{xz} \) and \( d_{xy} \) orbitals occurs only within the \( xz \) and \( xy \) planes, respectively. The corresponding Hubbard Hamiltonian is

\[
\hat{H}_{\text{hop}} = \sum_{\bar{n},l,s} \epsilon_{0} \hat{c}_{\bar{n},l,s}^\dagger \hat{c}_{\bar{n},l,s} + t(1 - \delta_{l,t}) \hat{c}_{\bar{n},l,s}^\dagger \hat{c}_{\bar{n}+1,l,s} + h.c.,
\]

where \( \epsilon_{0} \) is the level energy, \( \hat{c}_{\bar{n},l,s}^\dagger \) is the electron creation operator on site \( \bar{n} \) in orbital \( d_{\bar{n},l,s} \) with projection \( s = \pm 1/2 \) of spin on the \( z \)-axis, \( \epsilon_{0} \hat{c}_{\bar{n},l,s} \hat{c}_{\bar{n},l,s}^\dagger \) is a second-neighbor hopping term.

The single-particle eigenstates are Bloch waves

\[
\psi_{\bar{k},l,s} = \frac{1}{\sqrt{N}} \sum_{k} e^{i\bar{k}\cdot\bar{n}} \hat{c}_{\bar{n},l,s}^\dagger |0\rangle = \hat{c}_{\bar{k},l,s}^\dagger |0\rangle
\]

formed from the orbitals \( d_{l} \), with dispersion \( E_{l} = \epsilon_{0} + 2t \sum_{l} \cos(k_{l} \alpha) \). Here, \( \alpha \) is the lattice constant and \( N \) is the total number of sites. We choose \( \epsilon_{0} = -4t \) so that \( H_{\text{hop}} \) is the kinetic energy. Below, we discuss other plane wave solutions whose \( k \)-dependence is the same as Eq. [2], but the spin-orbital structure of the atomic states will be different.

In the discussed approximation, the \( l^{th} \) sub-band is non-dispersive in the \( t^{th} \) direction and is parabolic at small \( k \) in the other two directions. The Fermi surface consists of three cylinders aligned with the reciprocal axes and spanning the Brillouin zone, Fig. [2(b)]. This bandstructure is in overall correspondence with ab initio calculations, which predict a highly anisotropic star-shaped Fermi surface stretched along the principal axes [31]. To the best of our knowledge, the orbitally-selective origin of this anisotropy has not been explored.

**SOC effects.** SOC contributes to the band structure via band velocity and the atomic spin-orbit interaction [35]. The velocities near the bottom of the conduction band are small, so at light doping the latter is dominant. The atomic SOC Hamiltonian is \( \hat{H}_{\text{SO}} = -\gamma \sigma^{i} \cdot \lambda \), where \( \lambda \approx 18 \) meV for STO, \( \hat{L} \) and \( \hat{\sigma} \) are the orbital and spin angular momentum in units of Planck’s constant. The SOC Hamiltonian on the \( t_{2g} \) subspace is \( \hat{H}_{\text{SO}} = i\gamma \lambda /2 \sum_{l,l',s,s'} \epsilon_{l,l'} \sigma^{l} \hat{c}_{l,l',s}^\dagger \hat{c}_{l',l,s} \), where \( \sigma^{l} \) is the \( l^{th} \) Pauli matrix and \( \epsilon_{l,l'} \) is the Levi-Civita symbol.

General solution for \( \hat{H} = \hat{H}_{\text{hop}} + \hat{H}_{\text{SO}} \) at arbitrary \( \vec{k} \) is precluded by the anisotropy of hopping. For \( \vec{k} \) along \( k_{z} \), the \( d_{1} \) and \( d_{2} \) sub-bands are degenerate, and split
from the $d_3$ sub-band by $\Delta E \approx t a^2 k^2$. According to the perturbation theory, their mixing with the $d_3$ sub-band is negligible at $k \gg a^{-1}/\sqrt{\lambda/L}$. The eigenstates of $\hat{H}$ on the $d_1$, $d_2$ orbital subspace are Bloch waves with the atomic orbital structure $d_{\pm} = (d_1 \pm i d_2)/\sqrt{2}$ characterized by definite orbital moment projections $M = \pm 1$ on the z-axis, resulting in the splitting of the $d_1$, $d_2$ band into a two-fold degenerate $j = 1/2$ sub-band $d_+ \uparrow, d_− \downarrow$, and $j = 3/2$ sub-band $d_- \uparrow, d_+ \downarrow$ split by $\lambda$. Here, the up/down arrows denote the spin direction.

At $k = 0$, the kinetic energy vanishes and $\hat{H}$ can be diagonalized. The ground state is split by SOC into a Kramers doublet with the atomic spin-orbital structure $\psi_1 = (d_1 \uparrow + i d_2 \uparrow - d_3 \downarrow)/\sqrt{3}$, $\psi_2 = (d_1 \downarrow - i d_2 \downarrow - d_3 \uparrow)/\sqrt{3}$ with $j = 5/2$ and energy $-\lambda$, and a four-fold degenerate state with structure $d_+ \downarrow, d_- \uparrow, (d_1 \uparrow + i d_2 \uparrow + 2 d_3 \downarrow)/\sqrt{6}, (d_1 \downarrow - i d_2 \downarrow + 2 d_3 \uparrow)/\sqrt{6}$ with $j = 1/2$ and energy $\lambda/2$.

We use perturbation theory to analyze the effects of hopping. At $k \ll a^{-1}/\sqrt{\lambda/L}$, hopping-induced mixing between the lowest-energy doublet $\psi_1, \psi_1$ and the $j = 1/2$ quadruplet is negligible. The hopping term is diagonal on the subspace of plane waves $\psi_{k, \sigma}$ formed from the atomic states $\psi_{\sigma}$, where $\sigma = 1, 2$ is pseudo-spin. The dispersion $E(k) \approx \frac{1}{2}(ka)^2 - \lambda$ is isotropic, with effective mass $m^* = 3\hbar^2/4ta^2$. The degeneracy of the two subbands is protected by a combination of time reversal and spatial inversion symmetries [36], preserved by the antiferromagnetic transition but lifted by the ferroelectric distortions at large doping.

For $k$ along $k_z$, $\psi_1, \psi_2$ become mixed by hopping with other spin-orbital states at $k \approx a^{-1}/\sqrt{\lambda/L}$, evolving at large $k$ into $d_3 \uparrow, d_3 \downarrow$ [Fig. 2(b)]. Meanwhile, the four-fold degenerate $j = 1/2$ state evolves into two $d_3$ subbands discussed above in the large-$k$ limit. By symmetry, the dependences are similar for other principal directions.

Possible sc mechanism due to orbital entanglement. We now show that electron interaction can result in success mediated by the entanglement of unquenched orbital states involved in $\psi_1, \psi_2$. We analyze Coulomb interactions using the Mott-Hund’s interaction Hamiltonian [37]

$$\hat{H}_{\text{int}} = \sum U \hat{n}_{\alpha, l, \uparrow} \hat{n}_{\alpha, l, \downarrow} + (U - 2J) \hat{n}_{\alpha, l, \uparrow} \hat{n}_{\alpha, l, \downarrow} + (U - 3J) \hat{n}_{\alpha, l, \uparrow} \hat{n}_{\alpha, l, \downarrow}, \quad (3)$$

The first term is the Mott’s energy of electrons with opposite spins on the same orbital, the other two represent the Hund’s energy of electrons on different orbitals, with common notations for the coefficients [38, 39].

We estimate that at doping levels relevant to SC in STO, only the small-momentum part of the lowest subband is occupied [see Fig. 2(a)]. In the basis of $\psi_1, \psi_2$, the interaction Hamiltonian Eq. (3) is

$$\hat{H}_{\text{int}} = \sum_{\alpha} \hat{c}^+_\alpha \uparrow \hat{c}^+_\alpha \downarrow \hat{c}^-_{\alpha, 2} \hat{c}^-_{\alpha, 2} \hat{c}^-_{\alpha, 1}, \quad (4)$$

where $V = U - 16J/9 > 0$ and $\hat{c}^\dagger_{\alpha, \sigma}$ is the annihilation operator of electron in the state $\psi_{\alpha, \sigma}$ with pseudo-spin $\sigma = 1, 2$ labeling $\psi_1, \psi_2$. Equation (4) is similar to the Mott's energy, with spin replaced by the pseudo-spin $\sigma$.

We now show that the competition between the kinetic energy and interaction results in a pseudo-spin single-like state akin to the spin-singlet in the Mott state [40], but with an additional gauge symmetry that leads to sc. For just two electrons in the conduction band, the kinetic energy is minimized in the Bloch state with momentum $k = 0$. According to the Pauli principle, they occupy both states $\psi_1$ and $\psi_2$, so the interaction energy is $E_{\text{int}} = V$. Their interaction energy is minimized by localizing on different sites, but kinetic energy is then increased by $\sim t$.

Kinetic energy is dominant in metals, stabilizing Bloch waves. Dominant interaction leads to the localized Mott state. In STO, these energies are comparable [41]. Consider two electrons that form Gaussian wavepackets of width $\Delta x$ on a chain of length $L$, Fig. 3(a). The interaction energy $E_{\text{int}}$ is minimized when the wavepackets are separated by the maximum distance $d = L/2$ (for periodic boundary conditions) and are narrow, while kinetic energy $E_{\text{hop}}$ is minimized for plane waves with opposite pseudo-spins, so that they occupy the same $k = 0$ state. In the limit $\Delta x \gg L, \psi_{1, 2}(x) \approx b(1 - [(x ± L/4)^2]/4\Delta x^2)$ with normalization $b = 1/\sqrt{L(1 - TL^2/192\Delta x^2)}$, giving $E_{\text{hop}} \approx h^2/2m^*\Delta x^2$, $E_{\text{int}} \approx V(1 - L^2/24\Delta x^2)$. The requirement for the minimum of the total energy at finite $\Delta x$ gives the condition $V > 12h^2/m^*L^2$ for the Bloch state instability with respect to the polaronic-like localization. The 3d generalization $V > 3h^2n^{2/3}/m^*$ is always satisfied at sufficiently small electron density $n$.

The above results do not depend on the specific choice of orthogonal orbitals. Such correlated states can then be described by the two-electron wavefunction

$$\Psi = \sum_{n_1, n_2} f(n_1, n_2)(\alpha \hat{c}^+_\alpha \downarrow \hat{c}^+_\alpha \uparrow + \beta \hat{c}^+_\alpha \downarrow \hat{c}^+_\alpha \uparrow)|0\rangle, \quad (5)$$

where $|\alpha|^2 + |\beta|^2 = 1$, $n_1, n_2$ are site indices, and $f(n_1, n_2)$ is the product of Gaussian distributions describing the two wavepackets.

The orbital state of an additional, third, electron is
frustrated unless $|\alpha|^2 + |\beta|^2 = 1$, in which case its pseudo-spin can become entangled with the first two electrons to minimize their same-orbital spatial overlap. Thus, many-electron interactions stabilize an orbitally entangled singlet-like ground state of the form

$$\Psi = \sum_{n_1, n_2} \frac{f(n_1, n_2)}{\sqrt{2}} (\hat{c}_{n_1, 1} \hat{c}_{n_2, 1}^+ + e^{i\phi} \hat{c}_{n_1, 2} \hat{c}_{n_2, 2}^+) |0\rangle,$$

where $\phi$ is a gauge parameter absent for a true spin-singlet because of the Pauli principle. Translational invariance is captured by the momentum representation

$$\Psi = \sum_k g(\sqrt{2k}\Delta) (e^{ikd_x} \hat{c}_{k, 1}^+ \hat{c}_{-k, 2} + e^{i(\phi - kd_x)} \hat{c}_{k, 1} \hat{c}_{-k, 2}^+) |0\rangle,$$

where $g(x)$ is the Gaussian function with unit width, and $d$ is the distance between the paired electrons. This equation can be generalized to 3d using $d = n^{-1/3}$. In the mean-field approach, condensation of the effectively bound electron pairs can be described by the anomalous correlator $\Delta = \langle \sum_k g(\sqrt{2k}\Delta) (e^{ikd_x} \hat{c}_{k, 1}^+ \hat{c}_{-k, 2} + e^{i(\phi - kd_x)} \hat{c}_{k, 1} \hat{c}_{-k, 2}^+) \rangle$, with the condensate amplitude determined, e.g. by minimizing the energy of the correlated state $|11\rangle$. We leave such analyses to future studies.

We now show that orbital entanglement described by Eq. (6) leads to sc. Consider the 1d wavefunction Eq. (6) with the phase varying along the x-axis, e.g. $\phi \approx \Delta \phi (n_1 + n_2)$ with small $\Delta \phi$. A phase gradient results in the particle velocity $\hat{v} = i[\hat{H}, \hat{x}] / \hbar$, where $\hat{x} = \sum n \hat{c}_{n, \sigma}^+ \hat{c}_{n, \sigma}$ is the coordinate operator. For the hopping Hamiltonian Eq. (1), the corresponding operator for the particle flux between sites $n$ and $n + 1$ is

$$\hat{j}_{n, n+1} = i \sum_k (\hat{c}_{k, 1}^+ \hat{c}_{n+1, 1} - \text{h.c.}) / \hbar.$$ Applying it to the state Eq. (6) with position-dependent $\phi$, we obtain

$$\langle \hat{j}_{n, n+1} \rangle = \langle f(n, n+1) - f(n+1, n) \rangle \Delta \phi / 3 \hbar.$$ This current is a consequence of the chiral contribution of the orbital $d_2$ to the states $\hat{\psi}_1$, such that the current $j_2$ carried by its contribution to $\hat{\psi}_1$ is the same as the current carried by its contribution to $\hat{\psi}_2$. In contrast, the currents $j_3$ carried by $d_3$ are opposite, canceling each other, Fig. 3(b).

The presented sc mechanism, qualitatively different from BCS, is mediated by a combination of unquenched orbital moments in a Kramers doublet and orbital selectivity of hopping. Entanglement converts the circulating orbital currents into a macroscopic charge current. A similar mechanism was recently conjectured for the $d_{x^2-y^2}$ and $d_{xy}$ orbitals in cuprates [12], suggesting that it may be general to multiband sc. We note that because of the coupling between spin and orbital states, spin is not a good quantum number, so the order parameter cannot be characterized by the usual spin-singlet or triplet symmetry of BCS [13, 44].

Our first central result, the highly orbitally- and direction-selective electron hopping, may provide insight into the properties of high-mobility electron gas at the STO/LaAlO$_3$ interfaces [45], where symmetry lowering at the interface is expected to suppress the spin-orbit mixing of the conduction band bottom, resulting in reduced electron scattering due to the selection rules imposed by the orbital moment conservation.

Our second central result is that at sufficiently small carrier densities, electron interactions result in a polaronic-like state supporting sc via entanglement of unquenched orbital moments. In principle, the coupling strength of the proposed mechanism is sufficient to account for the observed dome-like dependence of $T_c$ on electron concentration $n$ [36]. The sc Fermi surface instability requires $n < n_c = (V m^* / 3h^2)^{3/2}$. sc is observed in STO for doping up to $n_c \approx 3 \times 10^{20}$ cm$^{-3}$ [47], providing a lower-bound estimate for $V \gtrsim 0.1$ eV, consistent with the typical values of Mott-Hund’s energy [37].

The proposed mechanism may be complementary to the electron interactions mediated by incipient ferroelectric distortions discussed as the possible mechanism of sc in STO [21, 35], but not considered in our analysis. Interplay between different sc mechanisms may explain the plateau of $T_c$ at $n = 10^{18} - 10^{19}$ cm$^{-3}$ distinguishing STO from other unconventional superconductors [27]. In this context, we note that lowering of the spatial symmetry can quench the orbital moments of the Kramers doublet, consistent with the observed correlation between the hardening of ferroelectric distortions and sc suppression [19, 26, 27]. On the other hand, symmetry lowering can prevent orbital moment quenching due to hybridization between the Kramers doublet and other orbital states at large $k$ [see Fig. 1(b)], enhancing sc in strained STO at large doping [23, 24]. The latter mechanism may also explain the enhancement of sc in thin STO films [49]. Finally, both antiferroelectric and ferroelectric distortions decrease the orbital selectivity of electron hopping, suppressing orbital entanglement.

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LJ17592 (Physical Review Letters)
Orbital entanglement mechanism of superconductivity in cuprates
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