Formation of Molecular-Orbital Bands in a Twisted Hubbard Tube: Implications for Unconventional Superconductivity in K$_2$Cr$_3$As$_3$

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We study a twisted Hubbard tube modeling the [CrAs]$_∞$ structure of quasi-one-dimensional superconductors A$_2$Cr$_3$As$_3$ (A=K, Rb, Cs). Thirty molecular-orbital bands emerging from the quasi-degenerate atomic orbitals are exactly solved. An effective Hamiltonian is derived for a region where three partially-filled bands intersect the Fermi energy. The deduced local interactions among these active bands show a significant reduction compared to the original atomic interactions. The resulting three-channel Luttinger liquid shows various interaction-induced instabilities including two kinds of spin-triplet superconducting instabilities due to gapless spin excitations, with one of them being superseded by the spin-density-wave phase in the intermediate Hund’s coupling regime. The implications of these results for the alkali chromium arsenides are discussed.

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Introduction. Recently, the alkali chromium arsenides A$_2$Cr$_3$As$_3$ (A=K,Rb,Cs) have been found as a new family of inorganic quasi-one dimensional (Q1D) superconductors with strong electron correlations.$^{1,2}$ They show almost linear resistivity from $T_c$ to room temperature and large upper critical fields far beyond the Pauli limit. The basic building block of these compounds is the chromium arsenide cluster, [CrAs]$_6$, consisting of two conjugated triangular complexes [CrAs]$_3$ as shown schematically in Fig.1(a). These clusters are then alternatively aligned along the c-axis forming a [CrAs]$_∞$ double-wall nanotube, and intercalated by A$^+$ cations within the ab-plane forming a hexagonal lattice. The first principle calculations based on density functional theory (DFT)$^{4,5}$ predict a three-dimensional (3D) Fermi surface (FS) sheet ($γ$-band) and two Q1D FS sheets ($α$- and $β$-bands), essentially contributed from the Cr 3$d$ electrons. The immediate NMR experiment$^{6}$ has revealed a power law behavior of the spin-lattice relaxation rate, manifesting the 1D Luttinger liquid feature above $T_c$. The penetration depth measurement$^{7}$, together with the previous experiments$^{4,6}$, has evidenced a line nodal feature of the pairing state below $T_c$.

However, due to the existing 3D $γ$-band$^{6,7}$, whether the superconductivity is solely originated from the Q1D structure of A$_2$Cr$_3$As$_3$ is uncertain. Under ambient pressure, $T_c$ decreases from 6.1 K, to 4.8 K and 2.2 K for A=K, Rb, and Cs, respectively$^{1,2}$, indicating that increasing the distance between [CrAs]$_∞$ tubes may suppress the superconductivity. In fact the nearly isotropic 3D bulk CrAs compound was found to be superconducting with $T_c ∼ 2.2$ K under pressure of $∼ 0.7$ GPa$^{8,9}$. The nodal feature, if exists, seems more natural for 2D or 3D FS’s. Interestingly, Zhou et al pointed out that a $f$-wave pairing state could arise from the 3D band with a line nodes at small on-site Coulomb interaction and moderate Hund’s coupling, while a fully gapped $p$-wave pairing state could dominate at the Q1D band.$^{10}$ It has been proposed that such triplet superconductivity, with some variations in spatial symmetry, can be driven by the ferromagnetic fluctuations within the sublattice of Cr atoms.$^{10}$

In order to further understand the formation of low energy bands and clarify the distinct influences of the 3D band and the Q1D bands on superconductivity, it is particularly important to understand the electronic property of a single fundamental [CrAs]$_∞$ tube. In this paper, we model this system by a twisted Hubbard lattice composed of in-plane triangular complexes coupled along the c-axis with the gliding reflection symmetry as shown in Fig.1(b).$^{12}$ In each unit cell there are two Cr-triangles, conjugated to each other forming a buckled Cr hexagon as shown Fig.1(a). The influence of the As 4$p$ orbitals can be effectively accounted for the indirect hopping of Cr-3$d$ electrons. So in general the model

![Fig. 1: (Color online) (a) A CrAs molecular in the ab plane. The solid (dotted) circles connected by the solid (dotted) lines represent the Cr atoms in the first (second) triangle in a unit cell. The isolated outer solid (dotted) circles represent the As atoms in the corresponding planes. (b) A Q1D CrAs tube. $t^{(i)}$ ($i = 1 \sim 4$) represent the four kinds of n.n. hopping parameters. The blue (green) filled circles represent the Cr atoms in each triangles. The As atoms are not shown.]
involves all five Cr-3d atomic orbitals (AOs) or totally thirty energy bands. In the realistic case, fortunately, only three partially-filled bands are enough to capture the low energy excitations.\textsuperscript{13} We will explicitly show how these bands come from the molecular orbitals (MOs) of [CrAs]\textsubscript{6}.\textsuperscript{10} Our purpose is then to understand their cooperative low temperature physics. The proposed effective model is of interest in its own right as we shall explore in the following.

Model Hamiltonian. The Hubbard model for a single [CrAs]\textsubscript{∞} tube is expressed as

\[
H = H_0 + H_{\text{int}},
\]

\[
H_0 = - \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle \sigma \sigma'} t(\mathbf{r}, \mathbf{r}') d_{\sigma}^{\dagger}(\mathbf{r}) d_{\sigma'}(\mathbf{r}'),
\]

\[
H_{\text{int}} = U \sum_{\mathbf{r}, \mathbf{r}' \neq \mathbf{r}'} n_{\uparrow}(\mathbf{r}) n_{\uparrow}(\mathbf{r}') - J_H \sum_{\mathbf{r}, \mathbf{r}' \neq \mathbf{r}'} S_{\mathbf{r}}^{(m)} S_{\mathbf{r}'}^{(m')} - J_p \sum_{\mathbf{r}, \mathbf{r}' \neq \mathbf{r}'} d_{\uparrow}^{\dagger}(\mathbf{r}) d_{\downarrow}(\mathbf{r}) d_{\downarrow}^{\dagger}(\mathbf{r}) d_{\uparrow}(\mathbf{r}').
\]

Where, $H_0$ represents the non-interacting part consisting of the tight-binding kinetic energy and the crystalline electric field (CEF) splitting, $d_{\sigma}^{\dagger}(\mathbf{r})$ the annihilation operators of Cr 3d electrons at the site $\mathbf{r}$ with angular momentum $m = 0, \pm 1, \pm 2$, spin $\sigma = \uparrow, \downarrow$, $n_{\sigma}^{(m)}$ and $S_{\mathbf{r}}^{(m)}$ are the corresponding density and spin operators. The two twisted Cr triangles could have different $E_{\text{trm}} = E_{\text{tr}}^{(1)}$, $E_{\text{tr}}^{(2)}$, accountable for possible occupation difference $H_{\text{int}}$ represents the local interactions including the intraorbital Coulomb interaction $U$, the interorbital Coulomb interaction $U'$, the Hund’s coupling $J_H$, and the pair-hopping $J_p$, respectively.

There are four kinds of adjacent intraorbital hoppings $t_{m,m'}^{(i)} \equiv t_{m,m'}^{(i)} (i = 1 \sim 4)$, corresponding to the nearest neighbor (n.n.) sites (1) in the first triangle, (2) in the second triangle, (3) between the two intracell triangles, and (4) between the two intercell triangles, respectively, as illustrated in Fig.II(b). Due to the metallic bonding among Cr atoms, the direct orbitals mixings among $m = 0$, $m = \pm 1$, and $m = \pm 2$ are relatively small, and the indirect hybridization is mainly bridged by the As 4p orbitals. So it is legitimate to consider a simpler situation for the adjacent interorbital hopping: $t_{m,m'}^{(i)} = \eta_{m,m'}^{(i)} \delta_{m,m'}$ for $m \neq m'$, with $|\eta| < 1$. In this situation, the atomic orbitals are quasi-degenerate as the only non-vanishing mix terms between the $m = \pm 1$ or $m = \pm 2$ orbitals are isotropic in space. Finally, we also include the next n.n. intraorbital hopping $t_{m,m}^{(i)}$ along the tube direction.

Molecular-orbital bands. Denoting each site by $\mathbf{r} = (n, a, \xi)$, with $a = 1, 2, 3$ being the site location in the first ($\xi = 1$) or second ($\xi = 2$) triangles in the $n$-th unit cell. It is convenient to introduce a base $d_{n}^{(m)} = (d^{(m)}(n,1), d^{(m)}(n,1,2), c^{(m)}(n,1), c^{(m)}(n,2,1), c^{(m)}(n,2,2), c^{(m)}(n,3,1), c^{(m)}(n,3,2))^{T}$ for electrons of the atomic $m$-orbital in the $n$-th unit cell (the spin index $\sigma$ is implied). For $m = 0$, this base accommodates a representation for the in-plane $C_3$ rotational symmetry, leading to six MOs corresponding to $E, E', A', A''$ states, respectively. For $m = \pm 1, \pm 2$, because of orbital mixing, we need to introduce a set of new base $d^{(m)}_{\uparrow \downarrow} = \frac{1}{\sqrt{2}}[d^{(m)}_{n \uparrow} \pm d^{(m)}_{n \downarrow}]$. Thus for a single [CrAs]\textsubscript{6} cluster and in the absence of the CEF effect, we have totally thirty MOs defined by $C_{\tau}^{(\alpha)} = (Q_{0} \otimes \hat{R}) d_{\tau}$ for $\tau = 0$ (denoting $d^{(0)}_{\uparrow \downarrow} \equiv d^{(0)}_{n \uparrow \downarrow}$), $\pm 1$ and $\pm 2$, respectively, with

\[
\hat{R} = \frac{1}{\sqrt{3}} \left[ \begin{array}{ccc} 1 & 1 & 1 \\ 1 & \omega & \omega^{-1} \\ \omega^{-1} & \omega & 1 \end{array} \right], Q_{0} = \frac{1}{\sqrt{2}} \left[ \begin{array}{cc} 1 & -1 \\ 1 & 1 \end{array} \right].
\]

Where, $\omega = e^{i\phi}$ ($\phi = 2\pi/3$), $\hat{R}$ acts on the internal degrees of freedom in a triangle ($a = 1, 2, 3$), and $Q_{0}$ on the triangle sublattices ($\xi = 1, 2$).

It is straightforward to show that when the triangles are coupled along the $c$-axis via the intercell hopping, the MO base in the Bloch form $C_{\tau}^{(\alpha)} = \left( c_{\tau}^{(1)}, c_{\tau}^{(1)}, c_{\tau}^{(2)}, c_{\tau}^{(2)}, c_{\tau}^{(2)}, c_{\tau}^{(2)} \right)^{T}$ is a natural base diagonalizing the tight-binding Hamiltonian (even in the presence of the CEF). This can be implemented by using a boost

\[
Q_{0} \rightarrow Q_{3}^{(\alpha)}(k) = \left( \begin{array}{cc} \cos \alpha_{(1)} & \sin \alpha_{(1)} e^{-i\vartheta_{c}} \\ \sin \alpha_{(2)} e^{i\vartheta_{c}} & \cos \alpha_{(2)} \end{array} \right).
\]

All the thirty MO bands can be then obtained as

\[
E^{(\gamma)}_{\tau \xi}(\mathbf{k}) = -\frac{\lambda^{(\gamma)}_{\tau \xi}}{2} \left[ \begin{array}{cc} (e^{(\gamma)}_{(1)} + e^{(\gamma)}_{(2)}) & (1 - \xi)\sqrt{(e^{(\gamma)}_{(1)} - e^{(\gamma)}_{(2)})^{2} + 4\rho_{\tau}^{2}} \end{array} \right],
\]

with $k$ the crystal momentum along the tube direction, $\lambda^{(\gamma)}_{\tau \xi} = [1 + \text{sign}(\gamma)|\eta|] \lambda_{\tau}$, $\lambda_{1} = 2$ and $\lambda_{2} = \lambda_{3} = -1$ being the eigenvalues of $\hat{R}$. Other parameters are defined by $\tan \theta_{\tau \sigma} = \frac{(\ell_{\gamma} \sin k)}{i(\ell_{\gamma} \cos k)}$, $\cos \alpha_{\tau \xi} = \frac{1}{\sqrt{1 + (\Delta_{\tau \xi}^{(\gamma)})^{2}}}$,

\[
\Delta_{\tau \xi}^{(\gamma)} = \frac{E^{(\gamma)}_{\tau \xi} - E^{(\gamma)}_{\tau \xi}}{\rho_{\tau} \rho_{\tau}}, \quad \frac{E^{(\gamma)}_{\tau \xi}}{\rho_{\tau} \rho_{\tau}} = \frac{\rho_{\tau}}{\sqrt{(\ell_{\gamma}^{(3)} - i \ell_{\gamma}^{(4)})^{2} + 4\ell_{\gamma}^{(3)} \ell_{\gamma}^{(4)} \cos k}}, \quad \text{and} \quad \mu \text{ the chemical potential}.
\]

Due to the CEF effect, $E^{(\xi)}_{m = \pm 1}$ are relatively larger than $E^{(\xi)}_{m = 0, \pm 2}$ as revealed by the DFT calculations.\textsuperscript{25} So we fit the DFT band structure along the $\Gamma \rightarrow A$ direction using the MO bands within $\tau = 0, \tau = \pm 2$. Notice that the three partially-filled energy bands, i.e., the 3D $\gamma$-band characterized mainly by the $d_{z^2}$ orbital ($m = 0$), the Q1D $\alpha$- and $\beta$-bands characterized mainly by the $d_{xy}$ and $d_{x^2-y^2}$ orbitals ($|m| = 2$), are all hole-like near the
\(\gamma\)-point and electron-like near the \(A\)-point. Therefore, the \(\gamma\) band corresponds to the singlet MO band labeled by \((\tau = 0, a = 1, \xi = 1)\). The \(\alpha\)-and \(\beta\)-bands, which are slightly higher than the \(\gamma\)-band at the \(\Gamma\)-point and degenerate along the whole \(\Gamma \rightarrow A\) direction, correspond to the doublet MO bands labeled by \((\tau = 2, a = 2, \xi = 2)\) and \((\tau = 2, a = 3, \xi = 2)\), respectively. The best fitting using \(E_n^{(0)}, E_n^{(+2)} = E_n^{(2)}\) are shown in Fig.2.\(^{13}\)

For simplicity, from now on, we shall use the band subscript \(\nu\) \((=1,2,3)\) to account for the three MO bands intersecting the Fermi energy. In our solution, these active MO bands fall into \(A'\) \((\text{with } \lambda_1 = 2)\) and \(E'\) \((\text{with } \lambda_2 = \lambda_3 = -1)\) representations of the \(D_{3h}\) group. Hence they are associated with phases \(\phi_{\nu} = 0, 2\pi/3, -2\pi/3\), or assigned chirality \(\theta_{\nu} = 0, 1, \text{ and } -1\), respectively. In the full 1D Brillouin zone, there are three pairs of Fermi points \((k_{F_1}, -k_{F_2})\), satisfying 0 < \(k_{F_1} < k_{F_2} = k_{F_3} < \pi\) as schematically shown in Fig.3. By integrating out all other inactive bands, we obtain the effective theory describing the low energy property of the active bands:

\[ H_{\text{eff}} = \sum_{k\nu,\sigma} E_\nu(k) \hat{n}_{k\nu\sigma} + \sum_n H_{\text{int}}^{(n)} \tag{7} \]

Where, \(\hat{n}_{k\nu\sigma} = c_{k\nu\sigma}^\dagger c_{k\nu\sigma}\) is the density operator of electrons in the \(n\)-th MO band, \(H_{\text{int}}^{(n)}\) the residual short-range interactions in the MOs in the unit cell, given by

\[ H_{\text{int}}^{(n)} = \sum_\nu \bar{U}_\nu \hat{n}_{\nu\uparrow}(n) \hat{n}_{\nu\uparrow}(n) + \sum_{\nu \neq \nu', \sigma'\sigma} \bar{U}_{\nu \nu'} \hat{n}_{\nu\sigma}(n) \hat{n}_{\nu'\sigma'}(n) \]

\[ - \sum_{\nu \neq \nu'} \bar{J}_{\nu \nu'} \hat{\mathbf{S}}_{\nu}(n) \cdot \hat{\mathbf{S}}_{\nu'}(n) \]  

\[ + \bar{J}_{23} \left[ c_{\uparrow}(n)c_{\downarrow}(n)c_{\downarrow}(n)c_{\uparrow}(n) \right] + (2 \leftrightarrow 3) + \text{h.c.} \tag{8} \]

In this expression, the electron annihilation operator in the \(n\)-th unit cell are defined by the Fourier transformation \(c_{\nu\sigma}(n) = \frac{1}{\sqrt{v_{\text{cell}}} \sum_{k} e^{i k n c_{\nu\sigma}} (\text{with } c_{0} \text{ being the lattice spacing}). Notice that only those terms preserving the neutrality condition \(\sum_\nu \theta_{\nu} = 0\) could survive. As the short-range interactions are mainly due to the slowly-varying part, the matrix \(\bar{Q}_0\) is used in deducing Eq.(8), obtaining the following interaction parameters:

\[ \bar{U}_{\nu} = U/6 \text{ for } \nu = 1, 2, 3; \bar{U}_{12} = \bar{U}_{13} = U'/12 - J_H/24; \]

\[ \bar{U}_{23} = (U + U' + J_H + J_p)/48; \bar{J}_{12} = \bar{J}_{13} = J_H/6; \]

\[ \bar{J}_{23} = (U + U' + J_H + J_p)/12; \text{ and } \bar{J}_{123} = J_p/6. \]

The last term in Eq.(8) is due to the pair-hopping term in Eq.(3). The influence of inactive bands is mainly accounted to the renormalized tight-binding parameters.

In Fig.3, the three partially filled bands are shown with three pairs of Fermi points. Notice that the bands \(\nu = 2, 3\) are degenerated.
is neglected as in the doped case here. The intra-
mover forward scattering term $g_{\nu}^{(4)}$ only renormalizes the Fermi velocities and does not influence the nature of superconductivity we concern, and henceforth we assume the Fermi velocities being the same. The one-loop renormalization group (RG) equations for these $g_{\nu}^{(j)}$ are of common type, resembling to those for 3-leg Hubbard ladders\textsuperscript{16,17} or a variant of carbon nanotubes\textsuperscript{18-20}. The instabilities of these RG equations are classified routinely: (i) the intraband instabilities as those developed in the single-channel Luttinger liquid, and (ii) the interband instabilities as those developed in the two-channel band Luttinger liquid.\textsuperscript{21} This suggests the validity of conventional bosonization approach based on the spin-charge separation, where various ordering instabilities can be determined by the Luttinger parameters. The new ingredients in the present problem are the peculiar symmetry surviving in the active MO bands and their dependence on the local electron interactions.

The right- and left-moving fields are then expressed in terms of the charge fields ($\phi_{\nu,c}$, $\theta_{\nu,c}$) and the spin fields ($\phi_{\nu,s}$, $\theta_{\nu,s}$) (for each $\nu = 1, 2, 3$) by

$$
R_{\nu,\sigma}(z) = \frac{F_{R,\nu}\sigma}{\sqrt{2\pi c} e^{i\pi/2(\tilde{\theta}_{\nu,c} + \sigma\tilde{\phi}_{\nu,c} - \tilde{\phi}_{\nu,c} - \tilde{\phi}_{\nu,c})}},
$$

$$
L_{\nu,\sigma}(z) = \frac{F_{L,\nu}\sigma}{\sqrt{2\pi c} e^{i\pi/2(\tilde{\theta}_{\nu,c} + \sigma\tilde{\phi}_{\nu,c} + \tilde{\phi}_{\nu,c} + \sigma\tilde{\phi}_{\nu,c})}}. \tag{14}
$$



The Klein factors $F_{R,\nu}\sigma$ and $F_{L,\nu}\sigma$ ensure the fermionic statistics between the right and left moving fermions. Next, in order to diagonalize the kinetic part, we need to introduce a set of new base

$$
\tilde{\phi}_{\nu,1} = \eta_{\gamma,+} \left( \frac{-b_{\gamma} + \sqrt{8a_{\gamma}^2 + b_{\gamma}^2}}{2a_{\gamma}} \phi_{\gamma,1} + \phi_{\gamma,2} + \phi_{\gamma,3} \right),
$$

$$
\tilde{\phi}_{\nu,2} = \eta_{\gamma,-} \left( \frac{-b_{\gamma} - \sqrt{8a_{\gamma}^2 + b_{\gamma}^2}}{2a_{\gamma}} \phi_{\gamma,1} + \phi_{\gamma,2} + \phi_{\gamma,3} \right),
$$

$$
\tilde{\phi}_{\nu,3} = \frac{1}{\sqrt{2}} (-\phi_{\gamma,2} + \phi_{\gamma,3}), \tag{15}
$$

where $\gamma = s, c$ and $\eta_{\gamma,\pm} = \left( \frac{8a_{\gamma}^2 + b_{\gamma}^2 \pm \sqrt{8a_{\gamma}^2 + b_{\gamma}^2}}{2a_{\gamma}} \right)^{-\frac{1}{2}}$ are the normalization constants, $a_c = \frac{4\gamma}{\pi}$, $b_c = \frac{2\gamma}{\pi}$, $a_s = \frac{-2\gamma}{\pi}$, $b_s = \frac{-2\gamma}{\pi}$. Similar relationship applies to the fields $\theta_{\nu,c}$ and $\theta_{\nu,c}$. Hence, we arrive at the following three-channel Tomonaga-Luttinger liquid Hamiltonian

$$
\tilde{H}_0 = \int dz \sum_{\nu=1,2,3,\gamma=s,c} \left[ \frac{v_F}{2} (\nabla\tilde{\theta}_{\nu,\gamma})^2 + \gamma_{\nu,\nu}(\nabla\tilde{\phi}_{\nu,\gamma})^2 \right]. \tag{16}
$$

where, $\gamma_{\nu,\nu} = t_s + \frac{1}{2} b_{\gamma} - (-1)^{\nu} \frac{\sqrt{8a_{\gamma}^2 + b_{\gamma}^2}}{2a_{\gamma}}$ for $\nu = 1, 2$, and $\gamma_{\nu,3} = t_c - b_{\gamma}$, $t_c = \frac{v_F}{2} + \frac{\tilde{\theta}_{\nu}}{2\pi}, t_s = \frac{v_F}{2} - \frac{\tilde{\theta}_{\nu}}{2\pi}$. Therefore, the Luttinger parameters are obtained explicitly by

$$
K_{c,1} = \frac{1 + \frac{U}{4\pi v_F} + \frac{1}{\pi v_F} \sqrt{8 \left( \frac{U}{6} - \frac{2J_H}{12} \right)^2 + \left( \frac{U}{12} \right)^2}}{\sqrt{2}},
$$

$$
K_{s,1} = \frac{1 - \frac{U}{4\pi v_F} + \frac{1}{\pi v_F} \sqrt{8 \left( \frac{U}{6} - \frac{2J_H}{12} \right)^2 + \left( \frac{U}{12} \right)^2}}{\sqrt{2}},
$$

$$
K_{c,2} = \frac{1 - \frac{U}{4\pi v_F} - \frac{1}{\pi v_F} \sqrt{8 \left( \frac{U}{6} + \frac{2J_H}{12} \right)^2 + \left( \frac{U}{12} \right)^2}}{\sqrt{2}},
$$

$$
K_{s,2} = \frac{1 - \frac{U}{4\pi v_F} - \frac{1}{\pi v_F} \sqrt{8 \left( \frac{U}{6} + \frac{2J_H}{12} \right)^2 + \left( \frac{U}{12} \right)^2}}{\sqrt{2}},
$$

$$
K_{c,3} = 1, K_{s,3} = 1.
$$

Here, we have adopted the conventional relations $J_p = J_H$ and $U' = U - 2J_H$ reflecting the rotational symmetry of the original AOs.\textsuperscript{22}

Now since $U > 0$ and $J_H > 0$, one can find that: (i) $K_{c,1} < 1$ in the entire region and $K_{s,1} < 1$ only when $U < J_H$; (ii) $K_{c,2} < 1$ in the region $0.2U < J_H < 0.6U$ and $K_{s,2} > 1$ in the entire region; (iii) $K_{c,3} = K_{s,3} = 1$. Specifically, in the physically relevant regime, $U > J_H$, the spin excitations are always gapless, so $K_{s,i}$ could be fixed to unit due to the spin-SU(2) symmetry. Because $K_{c,1} < 1$, the channel-"1" is in the spin-density-wave (SDW) phase.\textsuperscript{14,15} The channel-"3" involves the anti-bonding of the two degenerate MO bands $\nu = 2, 3$ as shown in Eq.(15). Both spin and charge excitations are critical. Due to the absence of spin gap, the dominating superconducting instability is the interband spin triplet pairing, driven by the interband scattering between the two Q1D $\alpha$- and $\beta$-bands.

The most intriguing case is the channel-"2", whose property depends on the ratio $J_H/U$. We plot the phase diagram determined by the Luttinger parameters in this channel in Fig.\textsuperscript{4} interestingly, this channel corresponds to the anti-bonding state involving all three MO bands as shown in Eq.(15). Meanwhile, $K_{c,2} > 1$ in the intermediate regime where $K_{c,2} < 1$, the SDW instability dominates. It should be noticed that in either cases where the interband triplet superconducting instabilities dominate, the spin-singlet superconducting instability is the sub-dominating instability.\textsuperscript{15} It is also understood

![FIG. 4: (Color online) Luttinger parameters for the channel-"2": $K_{c,2} > 1$ everywhere, and $K_{c,2} < 1$ only in the intermediate regime between the lines $J_H = 0.2U$ and $J_H = 0.6U$.](image-url)
that various interaction-induced cosine terms, which is neglected in the Hamiltonian Eq.(16), could influence the ordering patterns and this will be explored elsewhere.

Summary and discussions. We have derived a mapping from the local AO's to the MO bands in an orbital quasi-degenerate Hubbard tube. This allows to understand the formation of the three active bands in the K$_2$Cr$_3$As$_3$ compound. It also differentiates the dependence of residual MO interactions on the original local AO interactions. Using the bosonization method and assuming the spin-charge separation, we find that the spin excitations are always gapless as long as $U > J_H$. There are two kinds of spin-triplet superconducting pairing instabilities, the one involves the Q1D $\alpha$- and $\beta$-bands, another involves all three bands. We also found that there is an intermediate regime $0.2 < J_H/U < 0.6$ where the SDW phase emerges.

So far most of available experiments seem consistent with the Q1D Luttinger liquid scenario, except for the possible line nodal structure in the superconducting gap as the Luttinger liquid involves only isolated Fermi points. The line nodal feature is likely associated with the 3D $\gamma$-band. It is puzzling how a 3D superconducting pairing state could emerge out from the normal state of essentially Q1D Luttinger liquid characteristic.

Our present result provides a plausible answer to this question. On one hand, one of the three active bands, corresponding to $\nu = 1$ or the original AO with $m = 0$, evolves with the intertube hopping and crossovers to the 3D $\gamma$-band (as indicated by the DFT calculations) which could lead to the line nodal feature. On the other hand, the interband triplet superconducting pairing instability in the channel-"2" discussed here is driven not only by the $\gamma$-band, but also by the $(\alpha, \beta)$-bands. The latter two bands could remain Q1D because the intertube hopping among the atomic orbitals with $m = \pm 2$ is sufficiently small. In realistic situations, slight mixing between $m = 0$ and $m = \pm 2$ exists but the formation of the MO bands with the specific symmetry is robust. Therefore, the spin-triplet pairing instability in the channel-"2" could lead to a triplet pairing state consisting of both the 3D and Q1D bands. This exotic possibility makes the superconductivity in K$_2$Cr$_3$As$_3$ quite distinct to other known candidates of spin-triplet superconductors.

Finally, the recent pressure experiments on K$_2$Cr$_3$As$_3$ indicate the suppression effect of $T_c$ with decreasing intertube distance, opposite to the tendency revealed in the compounds A$_2$Cr$_3$As$_3$ with A=K, Rb, and Cs under ambient pressure. In particular, the reported hydrostatic and uniaxial pressure studies suggest that the optimal lattice exists already in the pristine regular [CrAs]$_6$ cluster under ambient pressure. The Q1D superconducting instability discussed here is sensitive to the regularity of the Cr-triangles and the uniform orbital mixing bridged by As-$4p$ orbitals, seemingly consistent with these observations. We hope that further experimental and theoretical studies can clarify the Q1D to 3D crossover in this class of materials.

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On the other hand, their explicit values are not important here because only symmetry property and local interactions are crucial as could be seen later.

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