High-Tc superconductors as a New Playground for High-order Van Hove singularities and Flat-band Physics

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High- T_c superconductors as a New Playground for High-order Van Hove singularities and Flat-band Physics

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Beyond the two-dimensional (2D) saddle-point Van Hove singularities (VHSs) with logarithmic divergences in the density of states (DOS), recent studies have identified higher-order VHSs with faster-than-logarithmic divergences that can amplify electron correlation effects. Here we show that the cuprate high- T_c superconductors harbor high-order VHSs in their electronic spectra and unveil a new correlation that the cuprates with high-order VHSs display higher T_c s. Our analysis indicates that the normal and higher-order VHSs can provide a straightforward new marker for identifying propensity of a material toward the occurrence of correlated phases such as the excitonic insulators and supermetals. Our study opens up a new materials playground for exploring the interplay between high-order VHSs, superconducting transition temperatures and electron correlation effects in the cuprates and related high- T_c superconductors.

Introduction.— Many properties of materials are driven by their one-particle electronic density of states (DOS). A large DOS at the Fermi level implies that many electrons contribute to the low-energy phenomena so that many-body interactions are enhanced. In particular, extrema and saddle-points in band dispersions induce Van Hove singularities (VHSs) in the DOS [1] and the associated logarithmic divergences in two-dimensions (2D) have been a focus of interest for many years. Recent studies, however, show that 2D and 3D VHSs can be anomalously strong in some cases to yield higher-order VHSs with power-law divergences [2–5] that can further amplify many-body interaction and drive exotic correlated phenomena such as supermetals [6]. Such high-order VHSs have been reported in Moire heterostructures, slow-graphene, magic-angle twisted bilayer graphene, $\text{Sr}_3\text{Ru}_2\text{O}_7$, and other systems that host flat bands and reduced bandwidths [2, 7, 8]. Beyond classifying the DOS anomalies of higher-order VHSs, it is important to understand their complex effects to fully appreciate their general promise of driving correlated physics in materials.

The role of normal VHSs in the cuprates and the related high- T_c superconductors has been debated for decades. One of the earliest theories of cuprate superconductivity is that it is driven by a large DOS associated with the VHSs [9]. However, the connections between the cuprate superconductivity, doping, and VHSs are complex and material dependent. Thus, while in the lanthanum-based cuprates, the VHS is at the Fermi level near optimal doping, in many cuprates the VHS crosses the Fermi level well into the overdoped regime.

Over the past 35 years, evidence for what is now known as high-order VHSs has arisen in cuprates in a number of contexts. These include Andersen’s extended VHS[10] and a high-order VHS which may be associated with

pseudogap collapse [11], consistent with an earlier prediction [12]. We hope that this systematic analysis of the many ways high-order VHSs affect the cuprate phase diagram will provide guidance for their study in other materials, while shedding light on some of the many puzzles remaining in cuprates.

Here, we explore the existence of high-order VHSs in the cuprates and discuss how such VHSs can drive competing orders and other complex effects in materials. We find that VHS singularities can exist not only in the DOS or the $Q = (0, 0)$ susceptibility but also in the susceptibility at finite momenta (e.g. $Q \sim (\pi, \pi)$). These two VHSs compete with each other and undergo independent evolutions when the material is doped or its dispersion is tuned. By tuning the dispersions, one can generate flat bands with high-order VHSs that lead to frustration rather than instabilities. We also show the existence of high-order VHSs in bosonic bands and discuss that if the susceptibility is considered as a dispersion of electron-hole pair bosons, the resulting high-order bosonic VHSs would allow a straightforward identification of excitonic phases in materials. Importantly, we demonstrate a correlation between the superconducting transition temperature T_c and the strength of the associated VHS.

Beyond the cuprates, our study has important implications in several areas of high current interest as follows. (1) We show how the definition of higher-order VHSs can be extended to reveal its connection with the broad area of *flat-band* physics. (2) We demonstrate a connection between higher-order VHSs and the electronic dimensionality. (3) We show that the connection with superconductivity is indirect, implying that additional factors are involved, most likely associated with competing instabilities.

High-order VHSs— We begin by recalling that the energy dispersion in the cuprates can be approximated by

a $t - t' - t''$ model [4, 13]

$$E = -2t(c_x + c_y) - 4t'c_xc_y - 2t''(c_{2x} + c_{2y}), \quad (1)$$

where $c_{nr} = \cos(nk_r a)$, a is the lattice constant, $r = \{x, y\}$, and the hopping parameters are defined in the inset to Fig. 1(a). In this model, t sets the energy scale and thus, the evolution of energy dispersions depends on the two parameters, t'/t and t''/t which constitute the material dependence. We examine this energy dispersion considering t'/t and t''/t values relevant to cuprates and delineate high-order VHSs. It should be noted that nearly localized d - and f electrons may be sensitive to just a few hopping parameters so that similar calculations should determine the characteristic properties of high-order VHSs in many correlated materials beyond cuprates.

Figure 1(b) presents the evolution of VHS lineshapes with t' for the special value $t'' = -t'/2$ that best describes most families of cuprates [13]. The corresponding VHS peak is considered as a marker of t' which locates various cuprates along the x -axis similar to Ref. 13 where the $r \sim t'/t$ parameter correlates materials with their superconducting T_c . Such a correlation of t' with the VHS allows us to compare the strength of the VHS divergence with T_c for several families of cuprates. The vertical dotted line in Fig. 1(a) separates the VHS peaks into a logarithmic shape at small values of t' from the stronger divergence ($\sim$ power law) at large values of t' . Strikingly, this dotted line also separates cuprates with $T_c \leq 80K$ from those with $T_c > 80K$, with one exception. The Bi-cuprates are the only cuprate family in which T_c changes significantly with number of CuO_2 -layers per unit cell, even though all have similar t' -values. Hence Bi2201, with maximum T_c of 40K, ends up just on the other side of the crossover line. Note further that for bilayer cuprates, the correlation holds for the antibonding band that is closer to the Fermi level, whereas the bonding bands all have t' s that correspond to super VHSs. These results clearly suggest that high-order VHSs play a significant role in the superconductivity of the cuprates.

To further understand the evolution of VHSs, it is convenient to measure energy E from the energy of the $X = (\pi, 0)$ point, *i.e.* $E_X = 4(t' - t'')$. As seen in Fig. 1(c), there is always a VHS at E_X , which evolves from logarithmic (saddle-point) at small t' to the step at larger t' . The associated single Fermi pocket region changes into a region of Fermi surface with three pockets. The step is the point at which two pockets first appear for a given t' . The crossover occurs at a critical value t'_c where a pocket forms with the strongest VHS divergence (for that t''/t'). It has a step on the low-energy side and a power-law divergence on the high energy side. This evolution is further illustrated by replotting the data for $E > E_X$ on logarithmic scales in Fig. 1(d). There are two types of behavior, separated

by the turquoise line. For small $|t'|$ (red to turquoise curve), the divergent peak stays at E_X , evolving from logarithmic to power law. The turquoise curve has the largest, pure power-law divergence. For larger $|t'|$, all curves (black to turquoise) start off with the same power law growth at large $\delta E = E_f - E_X$, but as δE decreases, the curves gradually split off on realizing a power-law to logarithmic crossover at an energy away from E_X . Finally, we note from Fig. 1(a) that the t' of strongest VHS can be approximately determined from the dispersion, as corresponding to the flattest band near $(\pi, 0)$. Such a strong VHS corresponds to Andersen's extended VHS [10].

FIG. 1. **higher order VHSs in the cuprates ($t'' = -t'/2$).** (a) Dispersions for the five cuprates of frame (b). Inset: Definition of the hopping parameters t , t' , and t'' . (b) DOS $N(E)$ for several values of t' . As VHS moves from right to left, the white-background curves correspond to $t'/t = 0$ (red curve), -0.1 (orange), -0.2 (yellow-green), -0.25 (green), -0.258 (light blue), -0.3 (blue), -0.4 (violet), and -0.5 (black), while the colored-background curves correspond to the mono-layer cuprates as indicated in the legends with t' values from Ref. 13. Horizontal bars indicate range of VHS peak positions for 10 bilayer or trilayer cuprates[13], sorted by optimal T_c s, with red ($70K \geq T_c \geq 50K$), green ($100K \geq T_c \geq 90K$), and blue ($135K \geq T_c \geq 125K$) colors. The antibonding bands are indicated by thick bars and the bonding bands by thin bars. A clear correlation of high-order VHSs with higher superconducting T_c s is seen. (c,d) White-background data from frame (b) replotted as $E_F - E_X$, on linear (c) or logarithmic (d) scales. We consider an average DFT value of $t = -0.5$ eV for all the calculations.

VHS Dichotomy – However, our problem is far from solved. The instabilities associated with the VHSs form a Lie group which is $\text{SO}(8)$ for cuprates.[14] For our purpose, the most important subgroup is whether the instability involves intra-VHS coupling that corresponds to $q = 0$ (*i.e.*, a peak in the DOS) or inter-VHS coupling that yields a peak in the $Q = (\pi, \pi)$ susceptibility. These two unstable modes compete such that in the original Hubbard model the (π, π) instability at half-filling is a (well-known) high-order VHS with a $\ln^2$ instability which

dominates the $\ln$ DOS. Thus, focusing solely on the DOS would miss the strong antiferromagnetism of cuprates. The existence of this $\ln^2$ effect has been questioned since the Hubbard model requires extreme fine-tuning with all hopping parameters set to zero except nearest-neighbor t . However, in Section II of Supplementary Material, we display a large family of dispersions with $\ln^2$ susceptibility divergence.

Remarkably, the (π, π) VHS is completely insensitive to the Fermi surface nesting that produces structure in the DOS, only gradually crossing over from $\ln^2$ to $\ln$ as the dispersion is tuned away from the Hubbard limit by either doping or tuning hopping parameters. Hence, in general, at some hopping t'_{cross} the DOS instability will become dominant. This is accompanied by a doping x_{cross} where the dominant near- (π, π) instability crosses over to a near- Γ instability (Section I.B of Supplementary Material). We suggest that optimal superconductivity falls close to x_{cross} where superconductivity can tilt the balance between the two competing phases.

Secondary VHSs.— The above analyses do not exhaust the possibilities for high-order VHSs. When a phase transition opens a gap in the electronic spectrum, the resulting subbands each develop secondary saddle-point VHSs, with corresponding new families of higher order VHSs having properties that can be quite different from the primary VHSs discussed above. Here we provide two examples of such secondary VHSs. Firstly, let us consider the DOS in the mean-field antiferromagnetic (AFM) phase in a pure Hubbard model ($t' = t'' = 0$), where the secondary VHS displays strong frustration. Figures 2(a) and (b) show that DOS has a strong power-law divergence although it is not associated with 1D nesting. Instead, the associated dispersion is exactly balanced at a crossover from having a dispersion minimum (in the upper band) at $(\pi, 0)$ to having a local maximum, so the whole dispersion is drumhead-flat, leading to an anomalously large DOS. Notably, when t' is non-zero this evolves into a Mexican hat dispersion, with a local maximum at $(\pi, 0)$, and resulting strong frustration [15]. When the AFM gap closes with increased doping, the high-order VHS of the lower magnetic band merges into the step at the bottom of the upper magnetic band, to form the high-order VHS of the nonmagnetic band (see Ref. 15 and Fig. 17 of Ref. 12). Such a feature was recently seen experimentally [11], but the VHS interpretation was discarded because the feature was too intense to be a conventional logarithmic VHS [11, 16].

Secondly, we investigate the case of an excitonic insulator where electron and hole pockets bind together to form avoided crossings at the Fermi level. While the electron and hole pockets can have different geometries or be shifted by a fixed q , for simplicity, we consider these pockets of the same area and shape, with $q = 0$. Adding a hybridization term to such a model leads to an avoided crossing with a ‘Mexican-hat’ dis-

person (Fig. 2(c)). From Fig. 2(d) it is seen that this dispersion leads to a highly characteristic DOS in either hybridized band. The logarithmic VHSs of the original bands at ± 1.5 eV remain unchanged by hybridization whereas the band-edge VHSs split into two VHSs- a step and a power-law VHS as one moves towards the band edge. The power-law saddle points are associated with an unusual Higgs-like one-dimensionality in the bands where they are flat along the brim of the Mexican hat but form an extremum along the radial k -direction away from (π, π) . Similar avoided crossings are found in TiSe_2 [17] and often seen in the topological insulators with a band inversion [18].

FIG. 2. Emergence of secondary VHSs (a) (π, π) Antiferromagnetic Hubbard model ($t' = t'' = 0$) at half-filling with bare dispersion (red line) and gapped dispersion with mean-field gap parameter $\Delta = 0.5$ eV (blue curves). The width of the blue curve indicates spectral intensity. (b) The associated DOS. (c) Excitonic insulator model with bare dispersion (red line) and gapped dispersion with mean-field gap parameter $\Delta = 0.4$ eV (green curves) and (d) the resulting DOS. (e) Panels (b) and (d) are replotted on a $\ln$ - $\ln$ plot to show the high-order VHSs. The solid and dashed black lines provide the reference slopes of -0.54 and -1/2, respectively.

We emphasize that these VHSs can be dubbed as Overhauser VHSs [19] since his model of charge density waves involves singular interactions on a 3D spherical Fermi surface. The circular VHSs would therefore provide a realistic 2D version of this effect. In this example, a flat band leads to strong frustration which can greatly lower the transition temperature. We find in Fig. 3(e) that the secondary VHSs have distinct power laws ($p_V = 0.5, 0.54$) from the primary VHS ($p_V = 0.29$). These exceptionally strong divergences satisfy the criteria required in high-order VHSs. The secondary high-order VHSs thus can be used as a signature of excitonic instabilities in materials. This is reasonable since the optical spectra (i.e. the joint DOS) of many semiconductors and insulators are dominated by prominent VHSs and an analysis of their associated dispersion geometries would ease the identification of excitonic states [20–22].

FIG. 3. **Cuprate bosonic dispersion** ω_q . Bare dispersion (red line) and gapped dispersion with mean-field gap parameter $\Delta = 0.5$ eV (blue curves). Inset: Blowup near band minimum.

High-order VHSs in Bosonic systems.— Since VHSs are crucial in bosonic systems, one can ask the question if those VHSs can be of high-order. Here we demonstrate that the Bosonic VHSs carry features similar to the secondary VHSs discussed above. Reference 4 introduced the idea of a susceptibility density of states (SDOS) and showed its usefulness in mode-coupling theory and as a map of Fermi surface nesting. There has been recent interest in interpreting this susceptibility as a bosonic Green’s function for electron-hole pairs [23, 24]. We therefore consider $\chi_0(q, \omega) = \frac{1}{(\omega - \omega_q + i\gamma_q)} - \frac{1}{(\omega + \omega_q - i\gamma_q)}$, where ω_q is a bosonic (electron-hole) frequency and γ_q a damping rate. For $\omega \rightarrow 0$ and $\gamma_q \rightarrow 0$, $\chi_0^{-1} = -\omega_q/2$ which gives the bosonic DOS up to a factor of 2, Fig. 3. The dispersion in Fig. 3 looks unusual because the electronic susceptibility contains nonanalytic features at $T = 0$ due to Fermi surface nesting, which also show up in Kohn

anomalies of phonons [25]. Interestingly, we find that both the Mexican hat and drumhead (flat-band) dispersions exist in Bosonic systems and give rise to high-order VHSs similar to the electronic case shown in Fig. 2 or (Fig. 2 of Ref. 4).

The bosonic high-order VHSs are particularly appealing in cuprates since they make the transition from commensurate AFM to incommensurate spin-density wave (SDW) highly anomalous. At the crossover point, any signs of the electronic order are lost, leading to an emergent spin-liquid phase. Since the AFM corresponds to what one expects from a Hubbard model (insensitive to shape of the Fermi surface), while the SDW is driven by Fermi surface nesting, it is appropriate to call this a Mott-Slater transition [4], and the emergent spin-liquid phase suggests why it is so hard to explain cuprate superconductivity starting from the undoped insulator. A similar commensurate-incommensurate transition with hints of emergent spin-liquid behavior at the crossover has been observed for the 3D Hubbard model which has finite-temperature phase transitions [26].

Insight into the bosonic ring and drumhead dispersions can be gained from phononic dispersions. The electrons can be considered as moving in a quasi-static potential generated by the phonons, and a phonon soft-mode introduces a new component to the potential. The ring dispersion thus causes the electrons to move in a Mexican-hat dispersion which is a signature of the Jahn-Teller effect. For phonons, the Mexican hat dispersion is typically connected to a point of conical intersection, where several phonon modes are degenerate. This point typically lies above the brim of the Mexican hat, signaling that the high-symmetry point is unstable. Notably, the resulting strong electron-phonon coupling leads to highly exotic physics, including breakdown of the Born-Oppenheimer approximation and, possibly, time crystals [27].

Discussion.— While high-order VHSs are likely to play a prominent role in strongly-correlated materials and exotic superconductivity, a quick review of the various ways high-order VHSs arise in cuprates illustrates how complicated their role can be. There is inter-VHS nesting responsible for the strong AFM effects and Mott physics; a bosonic high-order VHS that controls the transition from commensurate (π, π) AFM to incommensurate SDW order, with emergent spin-liquid phase [4]; and a crossover at doping x_{cross} from (π, π) VHSs to Γ -centered VHSs that may be associated with the peak of the superconducting dome. For example, if high $-T_c$ superconductivity arises by tipping the balance between the competing orders, favoring the (π, π) instability, then superconductivity should be most important when the dominant instability crosses over from (π, π) to Γ . In this case, T_c should maximize near x_{cross} and decrease with larger doping. Alternatively, superconductivity could actually benefit from the proximity of the strongly correlated and frustrated Mott phase with the bad metal Slater

phase[28]. These scenarios provide a good description of the cuprates. For example, in Bi2212 T_c is maximal near x_{cross} , and $\rightarrow 0$ near x_{VHS} [29], where the pairing strength also vanishes [30].

Additional issues include understanding the dual role of a VHS, in both increasing correlations via the peak in the DOS/susceptibility, and decreasing correlations by enhancing dielectric screening, and the role of secondary VHSs in driving/suppressing further instabilities. The bosonic high-order VHSs may have important relevance to Bose metals [23] and spinon bands [24]. There is an ongoing search for exotic phase transitions that do not fit into the conventional Moriya-Hertz-Millis model of quantum criticality, particularly when nontrivial emergent excitations arise near the quantum critical point [31]. Thus, our finding that such an emergent phase can be driven by bosonic high-order VHSs may constitute the most direct evidence of the importance of high-order VHSs in correlated materials.

After years of debate on the significance of the VHSs in the cuprates, it is exciting to realize that they can be significantly more singular than previously imagined. The correlation between higher VHSs and higher superconducting T_c we delineate here shows that high-order VHSs play a crucial role in high- T_c cuprate superconductors. However, the complicated nature of this correlation can be appreciated by noting that the superconducting T_c does not usually maximize at the VHS doping x_{VHS} but at a considerably lower doping. The T_c dome is largest around the doping where magnetic order just disappears, and magnetic fluctuations are largest. It will be interesting to see if similar complex intertwined orders are associated with high-order VHSs in other materials.

We now show that high-order VHSs exist if the electronic dimensions are smaller than lattice dimensions. During the early days of many-body perturbation theory (MBPT), it was postulated that the effective electron dimensionality could be smaller than the crystal lattice dimension *i.e.* if a Fermi surface has flat parallel sections there would be good nesting, leading to quasi-1D behavior. For example, the early high- T_c superconductors such as the A15 compounds were assumed to be composed of three orthogonal interpenetrating chains of electrons [?]. The three VHSs we have discussed in the cuprates illustrate this point. While the high-order VHS of the bare dispersion remain point-like, but for the extended object with $p_V = 0.29$, the dispersion of the secondary AFM VHS is flat along an extended, curved line, with $p_V = 0.54$, and the bosonic VHS is flat over a finite area.

The above results signal a substantial extension to the definition of a higher-order VHS[3]. Recall that a 2D saddle-point VHS corresponds to a point in k space where the local dispersion has the form $ak_x^2 - bk_y^2$, leading to a logarithmic peak in the DOS while a high-order VHS was defined as a point-like object where, for example, $b \rightarrow 0$. In contrast, here we consider the possibility that

$b = 0$ over an extended line segment. This definition of high-order VHS is necessary, since the 2D materials must have a diverging VHS, and this divergence we identified is the only candidate. Such a definition can help to classify high-order VHSs in a large class of flat-band materials, which are also characterized by having dispersions with flat line- or area-segments.

One final note on the connection between the higher-order VHSs and flat bands. We have demonstrated that Higher order VHSs are surrounded by a broad wake of 'enhanced-logarithmic' VHSs, that start out with a power-law divergence before crossing over to logarithmic, as seen in Fig. 1(d). On the other hand, in the study of flat bands, there is no consensus on how flat is flat: does a material count as a flat band if there is still a small dispersion? We hypothesize that many flat band materials are associated with these enhanced-logarithmic VHSs, becoming flatter as they approach more closely to the higher-order VHSs.

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- [1] Léon Van Hove, "The occurrence of singularities in the elastic frequency distribution of a crystal," *Phys. Rev.* **89**, 1189–1193 (1953).
- [2] Noah F. Q. Yuan, Hiroki Isobe, and Liang Fu, "Magic of high-order van hove singularity," *Nature Communications* **10**, 5769 (2019).
- [3] Noah F. Q. Yuan and Liang Fu, "Classification of critical points in energy bands based on topology, scaling, and symmetry," *Phys. Rev. B* **101**, 125120 (2020).
- [4] R. S. Markiewicz, I. G. Buda, P. Mistark, C. Lane, and A. Bansil, "Entropic origin of pseudogap physics and a mott-slater transition in cuprates," *Scientific Reports* **7**, 44008 (2017).
- [5] Thiago X. R. Souza and F. Marsiglio, "The possible role of van hove singularities in the high t_c of superconducting h_3S ," *International Journal of Modern Physics B* **31**, 1745003 (2017).
- [6] Hiroki Isobe and Liang Fu, "Supermetal," *Phys. Rev. Research* **1**, 033206 (2019).
- [7] Alexander Kerelsky, Leo J. McGilly, Dante M. Kennes, Lede Xian, Matthew Yankowitz, Shaowen Chen, K. Watanabe, T. Taniguchi, James Hone, Cory Dean, Angel Rubio, and Abhay N. Pasupathy, "Maximized electron interactions at the magic angle in twisted bilayer graphene," *Nature* **572**, 95–100 (2019).
- [8] Dmitry V. Efremov, Alex Shtyk, Andreas W. Rost, Claudio Chamon, Andrew P. Mackenzie, and Joseph J. Betouras, "Multicritical fermi surface topological transitions," *Phys. Rev. Lett.* **123**, 207202 (2019).
- [9] J. E. Hirsch and D. J. Scalapino, "Enhanced superconductivity in quasi two-dimensional systems," *Phys. Rev. Lett.* **56**, 2732–2735 (1986).
- [10] O. K. Andersen, O. Jepsen, A. I. Liechtenstein, and I. I. Mazin, "Plane dimpling and saddle-point bifurcation in the band structures of optimally doped high-temperature superconductors: A tight-binding model," *Phys. Rev. B*

- [49](#), 4145–4157 (1994).
- [11] B. Michon, C. Girod, S. Badoux, J. Kačmarčík, Q. Ma, M. Dragomir, H. A. Dabkowska, B. D. Gaulin, J. S. Zhou, S. Pyon, T. Takayama, H. Takagi, S. Verret, N. Doiron-Leyraud, C. Marcenat, L. Taillefer, and T. Klein, “Thermodynamic signatures of quantum criticality in cuprate superconductors,” *Nature* **567**, 218–222 (2019).
 - [12] R. S. Markiewicz, “Mode-coupling model of mott gap collapse in the cuprates: Natural phase boundary for quantum critical points,” *Phys. Rev. B* **70**, 174518 (2004).
 - [13] E. Pavarini, I. Dasgupta, T. Saha-Dasgupta, O. Jepsen, and O. K. Andersen, “Band-structure trend in hole-doped cuprates and correlation with t_{cmax} ,” *Phys. Rev. Lett.* **87**, 047003 (2001).
 - [14] R. S. Markiewicz and M. T. Vaughn, “Classification of the van hove scenario as an SO(8) spectrum-generating algebra,” *Phys. Rev. B* **57**, R14052 (1998).
 - [15] R. S. Markiewicz, “Dispersion of ordered stripe phases in the cuprates,” *Phys. Rev. B* **62**, 1252–1269 (2000).
 - [16] M. Horio, K. Hauser, Y. Sassa, Z. Mingazheva, D. Sutter, K. Kramer, A. Cook, E. Nocerino, O. K. Forslund, O. Tjernberg, M. Kobayashi, A. Chikina, N. B. M. Schröter, J. A. Krieger, T. Schmitt, V. N. Strocov, S. Pyon, T. Takayama, H. Takagi, O. J. Lipscombe, S. M. Hayden, M. Ishikado, H. Eisaki, T. Neupert, M. Månsson, C. E. Matt, and J. Chang, “Three-dimensional fermi surface of overdoped la-based cuprates,” *Phys. Rev. Lett.* **121**, 077004 (2018).
 - [17] Bahadur Singh, Chuang-Han Hsu, Wei-Feng Tsai, Victor M. Pereira, and Hsin Lin, “Stable charge density wave phase in a $1t - \text{TiSe}_2$ monolayer,” *Phys. Rev. B* **95**, 245136 (2017).
 - [18] A. Bansil, Hsin Lin, and Tanmoy Das, “Colloquium: Topological band theory,” *Rev. Mod. Phys.* **88**, 021004 (2016).
 - [19] A. W. Overhauser, “Exchange and correlation instabilities of simple metals,” *Phys. Rev.* **167**, 691–698 (1968).
 - [20] R. S. Markiewicz and A. Bansil, “Excitonic insulators as a model of $d - d$ and mott transitions in strongly correlated materials,” *ArXiv:1708.02270* (2018).
 - [21] Liang Fu and Zhen Bi, “Excitonic density wave and spin-valley superfluid in bilayer transition metal dichalcogenide,” *ArXiv:1911.04493* (2019).
 - [22] J. C. Phillips, “Ultraviolet absorption of insulators. iii. fcc alkali halides,” *Phys. Rev.* **136**, A1705 (1964).
 - [23] D. N. Sheng, Olexei I. Motrunich, and Matthew P. A. Fisher, “Spin bose-metal phase in a spin- $\frac{1}{2}$ model with ring exchange on a two-leg triangular strip,” *Phys. Rev. B* **79**, 205112 (2009).
 - [24] Wen-Jun Hu, Yi Zhang, Andriy H. Nevidomskyy, Elbio Dagotto, Qimiao Si, and Hsin-Hua Lai, “Fractionalized excitations revealed by entanglement entropy,” *Phys. Rev. Lett.* **124**, 237201 (2020).
 - [25] R. S. Markiewicz, G. Seibold, J. Lorenzana, and A. Bansil, “Gutzwiller charge phase diagram of cuprates, including electron-phonon coupling effects,” *New Journal of Physics* **17**, 023074 (2015).
 - [26] T. Schäfer, A. A. Katanin, K. Held, and A. Toschi, “Interplay of correlations and kohn anomalies in three dimensions: Quantum criticality with a twist,” *Phys. Rev. Lett.* **119**, 046402 (2017).
 - [27] R. S. Markiewicz, “Van hove exciton-cageons and high- T_c superconductivity: Viii. solitons and nonlinear dynamics,” *Physica C: Superconductivity* **210**, 264 (1993).
 - [28] David Allender, J. W. Bray, and John Bardeen, “Theory of fluctuation superconductivity from electron-phonon interactions in pseudo-one-dimensional systems,” *Phys. Rev. B* **9**, 119–129 (1974).
 - [29] Ying Ding, Lin Zhao, Hongtao Yan, Qiang Gao, Jing Liu, Cheng Hu, Jianwei Huang, Cong Li, Yu Xu, Yongqing Cai, Hongtao Rong, Dingsong Wu, Chunyao Song, Huaxue Zhou, Xiaoli Dong, Guodong Liu, Qingyan Wang, Shenjin Zhang, Zhimin Wang, Fengfeng Zhang, Feng Yang, Qinjun Peng, Zuyan Xu, Chuangtian Chen, and X. J. Zhou, “Disappearance of superconductivity and a concomitant lifshitz transition in heavily overdoped $\text{Bi}_2\text{Sr}_2\text{CuO}_6$ superconductor revealed by angle-resolved photoemission spectroscopy,” *Chin. Phys. Lett.* **36**, 017402 (2019).
 - [30] J. G. Storey, J. L. Tallon, and G. V. M. Williams, “Saddle-point van hove singularity and the phase diagram of high- T_c cuprates,” *Phys. Rev. B* **76**, 174522 (2007).
 - [31] Subir Sachdev, “Quantum criticality: Competing ground states in low dimensions,” *Science* **288**, 475 (2000).

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AUTHOR CONTRIBUTIONS

R.S.M., B.S., C.L., and A.B. all contributed to the research reported in this study and the writing of the manuscript.

ADDITIONAL INFORMATION

The authors declare no competing financial interests.

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