

# Charge Density Wave and Magnetism in Kagome Superconductors

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## Abstract

In this study, we systematically investigate the regulatory effects of electronic correlations on multiple ordered states in kagome superconductors based on the single-orbital extended Hubbard model. Our results demonstrate that the intersite Coulomb interaction  $V$  serves as a key factor driving the formation of charge density wave (CDW): The CDW phase emerges as the thermodynamically stable ground state when  $V$  exceeds a critical threshold ( $\sim 0.6$  eV). In contrast, the on-site Coulomb interaction  $U$  suppresses CDW formation, revealing a clear competitive interplay between  $U$  and  $V$ . Furthermore, a sufficiently strong on-site Coulomb interaction  $U$  ( $U \geq 6$  eV) induces a stable intertwined charge-spin density wave (SCDW) coexisting with the CDW background, while the intersite Coulomb interaction  $V$  tends to suppress magnetic order. This study elucidates the interplay and competition mechanisms between charge order and spin order in kagome lattice systems, providing a theoretical foundation for the tunability of quantum states in this material family.

## Keywords

Kagome Superconductors, Intersite Coulomb Interaction, On-Site Coulomb Interaction, Charge Density Waves, Spin Density Wave

## 1. Introduction

Recently, kagome superconductors have attracted extensive attention in Kagome superconducting materials have attracted significant attention in the field of condensed matter physics due to their unique Kagome lattice structure, which induces a wealth of novel physical properties and quantum states, such as quantum spin liquids, topological states, charge density waves, and spin density waves [1]-[4]. These materials provide an ideal platform for exploring the coupling and competition of various quantum ordered states.

The vanadium-based Kagome superconductor  $AV_3Sb_5$  ( $A = K, Rb, Cs$ ) exhibits a  $2 \times 2$  CDW at low temperatures, which breaks the rotational symmetry and induces an electronic nematic phase [5]-[7]. This system lacks long-range static magnetic order under ambient pressure [8] [9], characterized primarily by the coupling of pure charge order and nematic order. In contrast, the magnetic Kagome metal FeGe demonstrates strong coupling behavior between charge density waves and spin density waves (SDW) [10]-[12], with these two types of quantum orders coexisting and their microscopic phase transition mechanisms differing significantly from those in the vanadium-based systems [13] [14]. The newly synthesized chromium-based Kagome material  $CsCr_3Sb_5$  further broadens the research landscape of Kagome superconductors, presenting a unique intertwined ordered state of CDW and SDW at 55 K [15].

In the Kagome lattice, geometric frustration leads to a complex interplay and close correlation between electronic nematic phases and charge density waves. Although existing theories have investigated the dynamics of charge density waves and spin density waves [16]-[20], a universal physical picture for the coupling mechanisms between charge and spin order in different Kagome material systems remains elusive. Moreover, the regulatory patterns of various Coulomb interaction parameters on these ordered states have yet to be fully revealed.

In this study, we employ the single-orbital extended Hubbard model to systematically explore how electronic correlations modulate diverse ordered phases of Kagome superconductors. Our calculations identify that the intersite Coulomb potential  $V$  is crucial for forming charge-density-wave (CDW): The CDW phase emerges as the thermodynamically stable ground state when  $V$  exceeds a critical threshold ( $\sim 0.6$  eV). Conversely, the on-site Coulomb interaction  $U$  suppresses CDW formation, revealing a clear competitive interplay between  $U$  and  $V$ . Furthermore, at sufficiently large on-site Coulomb interaction ( $U \geq 6$  eV), an intertwined charge-spin density wave (SCDW) emerges atop the CDW parent phase, while the intersite Coulomb interaction  $V$  tends to suppress magnetic order formation.

## 2. Model

We only considered the vanadium atoms on the kagome lattice, each unit cell contains three vanadium atoms. Accordingly, we construct a single-orbital extended Hubbard model:

$$H = \sum_{ij,\alpha\beta,\sigma} t_{ij}^{\alpha\beta} c_{i\alpha\sigma}^\dagger c_{j\beta\sigma} + U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + V_1 \sum_{\langle ij \rangle} n_i n_j + V_2 \sum_{\langle\langle ij \rangle\rangle} n_i n_j \quad (1)$$

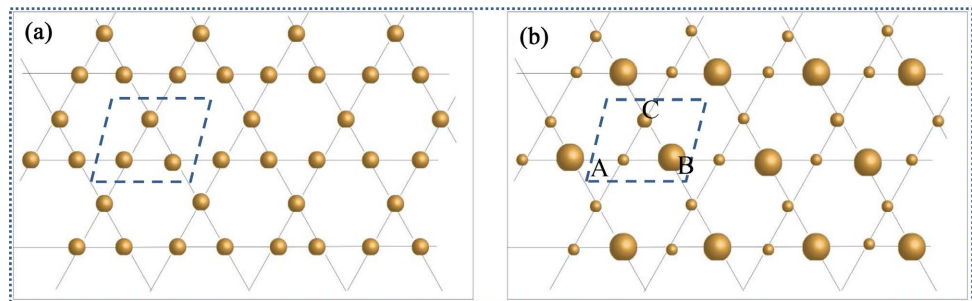
here,  $U$  denotes the on-site Coulomb interaction, while  $V_1$  and  $V_2$  respectively represent the nearest-neighbor Coulomb interaction and the next-nearest-neighbor Coulomb interaction. In conventional Hubbard model studies, the intersite Coulomb interaction  $V$  was frequently neglected under the assumption that its magnitude is negligible compared to the onsite Coulomb interaction. However, recent investigations have underscored the pivotal role of  $V$  in various quantum

materials, particularly in iron-based superconductors, where it has been shown to drive phenomena such as nematicity and CDW. Motivated by these findings, we explicitly incorporate  $V$  into the study of bilayer nickelates to explore the complex spin-charge intertwined phases discussed above.

The mean-field wave functions,  $|\Psi_{MF}\rangle$ , serve as ground states for the mean-field Hamiltonians corresponding to both the CDW and magnetic phases:

$$H_{MF} = H_0 + \sum_i \Delta_{CDW} e^{iR_i Q_{CDW}} n_i + \sum_{i\alpha\sigma} \sigma \left[ \Delta_M(\alpha) e^{iR_i Q_M} \right] n_{i\alpha\sigma} \quad (2)$$

here,  $\Delta_{CDW}$  and  $\Delta_M$  denote the order parameters for the charge density wave (CDW) and magnetic order, respectively. The mean-field Hamiltonian thus includes the CDW order parameter  $\Delta_{CDW}$  and the magnetic order parameter  $\Delta_M$ , by which various ordered phases can be characterized. **Figure 1(a)** is obtained when both  $\Delta_{CDW}$  and  $\Delta_M$  are set to zero, while **Figure 1(b)** results from optimizing only the  $\Delta_{CDW}$  parameter. Due to geometric frustration inherent in the kagome lattice, the electronic nematic phase and charge density waves exhibit a tightly intertwined and mutually influential relationship. Specifically, asymmetric electron occupancy among the three inequivalent lattice sites—where the electron density on one site markedly differs from that on the other two—triggers the spontaneous formation of a charge density wave (*i.e.*, electronic nematic phase) characterized by a specific spatial periodicity.



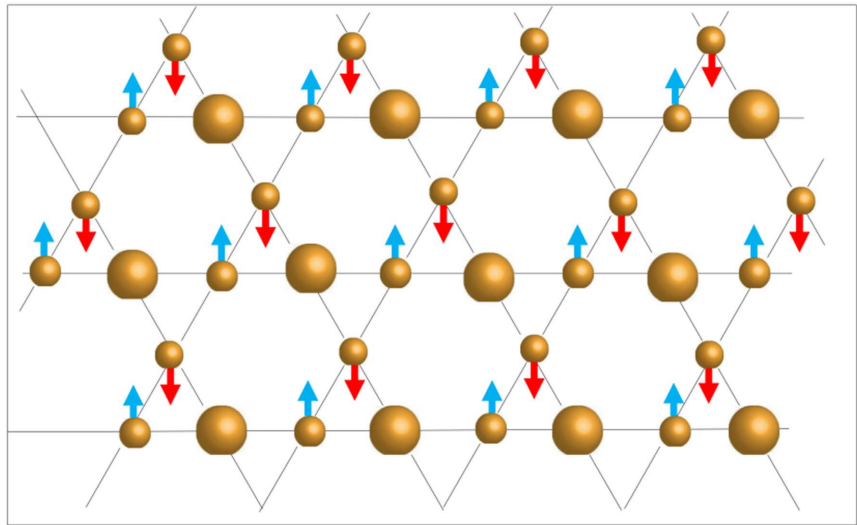
**Figure 1.** Schematic illustration of charge density waves in vanadium-based Kagome superconductors: (a) Uniform phase without charge modulation. (b) charge density wave (electronic nematic). The size of the spheres represents the magnitude of the electron density.

For SCDW, we simultaneously optimize  $\Delta_{CDW}$  and  $\Delta_M$ . The schematic configuration of the constructed SCDW phase is presented in **Figure 2**. Based on the charge modulation of the charge density wave, the spins display a periodic antiferromagnetic ordering: along a certain lattice direction, spins alternate between up and down, forming a striped antiferromagnetic configuration, leading to a spin-charge intertwined order (SCDW). This magnetic structure features the coupling of both antiferromagnetism and charge modulation.

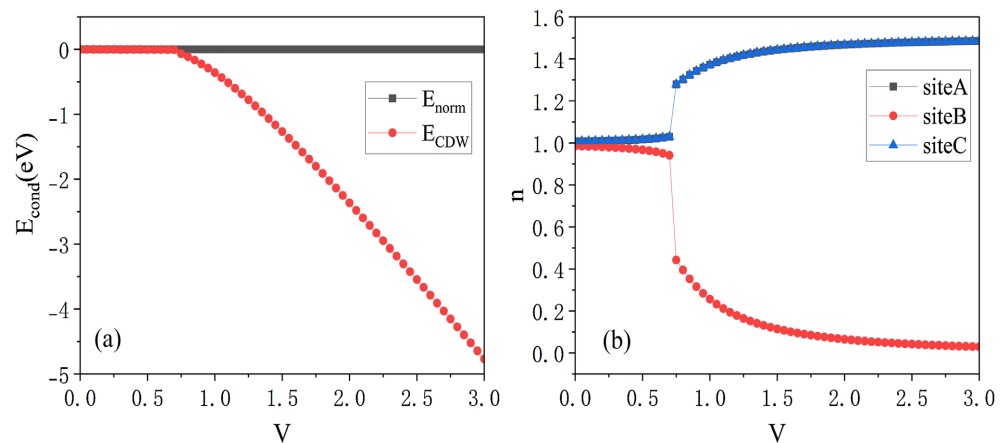
### 3. Charge Density Wave

Firstly, setting  $t = U = 1$  eV,  $V_1 = V_2 = V$ , we obtain the condensation energy  $E_{cond}$  for the CDW phase and the uniform phase as well as the electron density

$n$ , as shown in **Figure 3**. In this paper, the condensation energy refers to the energy gain of the ordered phase relative to the disordered phase.



**Figure 2.** the configurations of intertwined spin-charge density wave state in Kagome superconductors (SCDW).

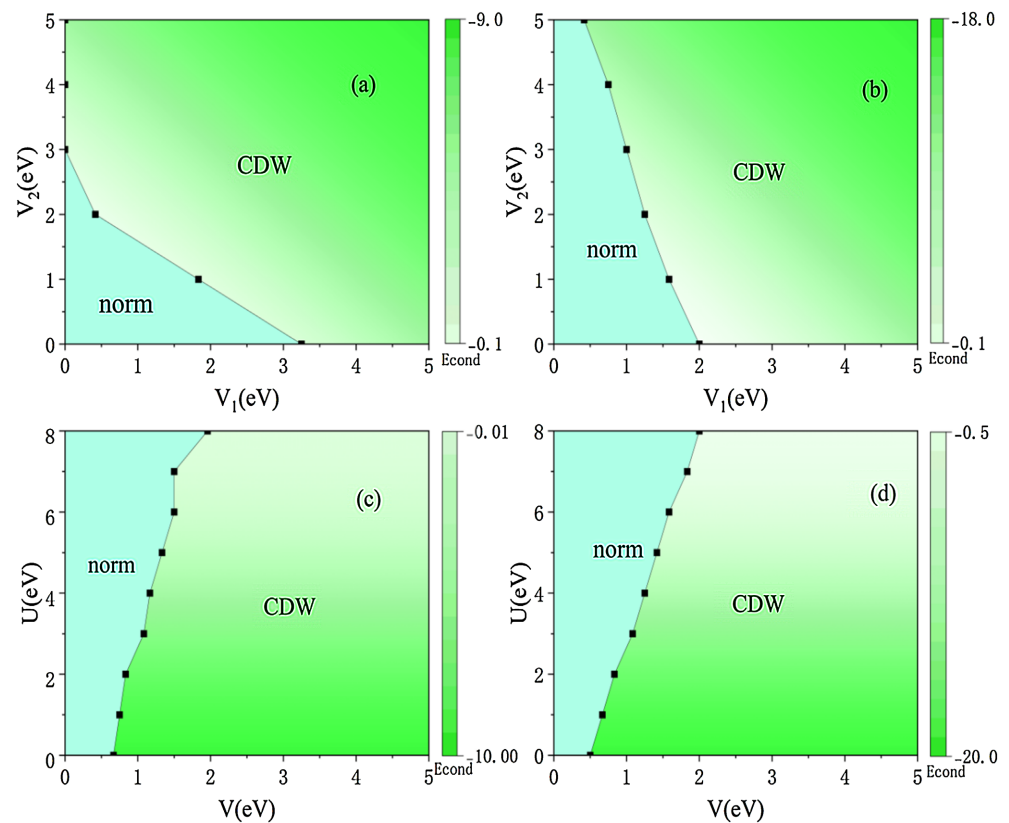


**Figure 3.** Results changing with  $V$ , where  $t = U = 1.0$  eV: (a) Comparison of the energies of the uniform phase  $E_{\text{norm}}$  and the CDW phase  $E_{\text{CDW}}$ . (b) Electron density  $n$  at the sites A, B and C in the CDW phase, as shown in **Figure 1(b)**.

In **Figure 3(a)**, the condensation energies of CDW and uniform phases are nearly equal at small  $V$ , indicating that the system remains uniformly distributed. When  $V$  exceeds 0.6 eV, the condensation energy of CDW becomes lower than that of the uniform phase, the energy difference increases monotonically with  $V$ , indicating that the charge density wave phase is energetically favored over the uniform phase. **Figure 3(b)** shows calculated electron densities  $n$  at sites A, B and C. For  $V > 0.6$  eV, the electron density on site B differs obviously from sites A and C. This proves an electronic nematic phase exists in Kagome superconductors. The system reduces total energy by forming CDW, namely the electronic nematic phase. Note that the threshold  $V > 0.6$  eV is model-dependent.

In **Figure 4**, we investigate the effects of the intersite Coulomb interaction  $V$  and the on-site Coulomb interaction  $U$  on the charge density wave. **Figure 4(a)** and **Figure 4(b)** show that, for different filling fractions, the nearest-neighbor Coulomb interaction  $V_1$  and the next-nearest-neighbor Coulomb interaction  $V_2$  favor a phase transition from the uniform state to the CDW state. As  $V_1$  and  $V_2$  increase, the condensation energy of the CDW state gradually decreases, rendering the CDW state more stable relative to the uniform phase. This behavior indicates that an enhancement of the intersite Coulomb interactions promotes the formation of the CDW state. The above trend suggests that the intersite Coulomb repulsion  $V$  is a key factor driving the system into the CDW phase in kagome superconductors.

As shown in **Figure 4(c)** and **Figure 4(d)**, setting  $V_1 = V_2 = V$ , the critical  $V$  required for the transition from the uniform phase to the CDW phase grows with increasing  $U$ . This trend reveals that enhancing the on-site Coulomb interaction  $U$  suppresses the formation and stability of the CDW phase.

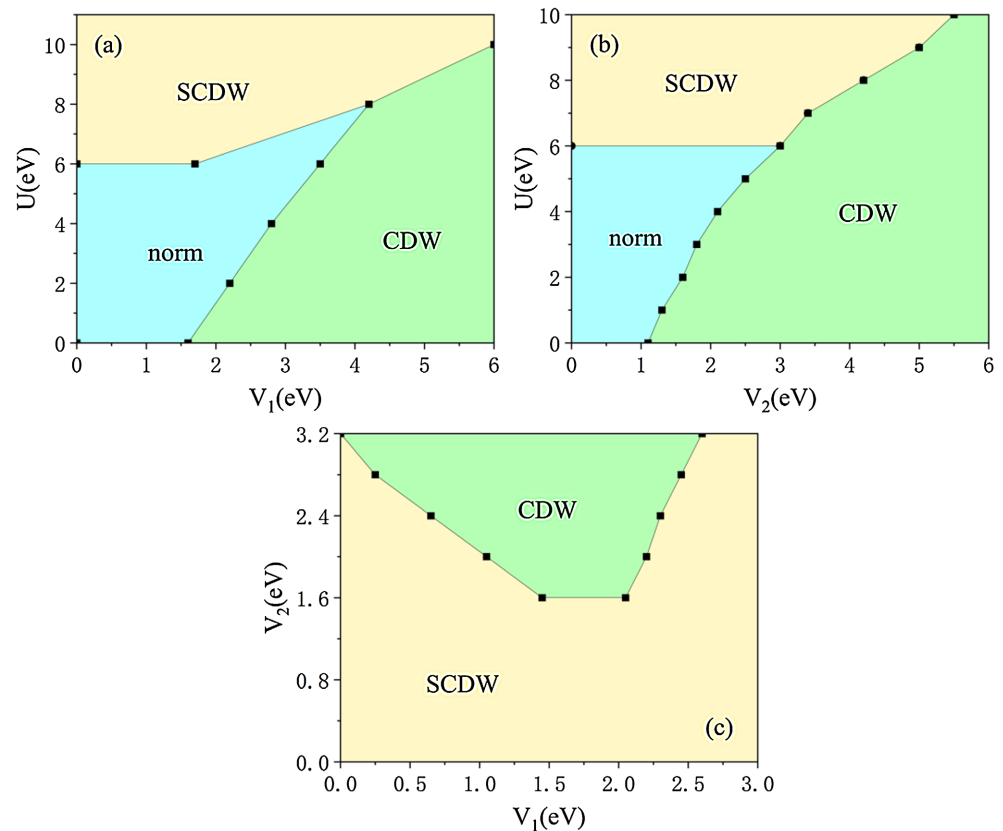


**Figure 4.** Phase diagram at specific fillings: (a), (b)  $U = 5\text{eV}$ ,  $V_1$  versus  $V_2$  plot at filling 1/2 and 2/3. (c), (d)  $U$  versus  $V_1 = V_2$  phase diagram at filling 1/2 and 2/3. the blue region corresponds to the uniform phase, and the green region indicates the CDW phase. The intensity of the green color scales with the condensation energy.

#### 4. The Intertwined Spin-Charge Density Wave

In this section, we set the filling at 1/2. Setting  $V_2 = 0$ , the phase diagram of the

on-site Coulomb interaction  $U$  versus the nearest-neighbor Coulomb interaction  $V_1$  is obtained, as shown in **Figure 5(a)**. It is found that when the on-site Coulomb interaction  $U$  dominates, the system undergoes a transition from the uniform phase to the intertwined spin-charge order (SCDW) phase. The SCDW phase begins to emerge at  $U=6$  eV. As  $U$  further increases, the region of the SCDW phase gradually expands and becomes stabilized. This result demonstrates the existence of the SCDW phase in kagome superconductors, and indicates that the on-site Coulomb interaction  $U$  is a crucial factor in driving and stabilizing the intertwined spin-charge order. When the nearest-neighbor Coulomb interaction  $V_1$  dominates, the system undergoes a transition from the uniform phase to the charge density wave (CDW) phase, and the CDW phase tends to be stabilized. In this regime, no SCDW phase appears, indicating that an enhancement of  $V_1$  is unfavorable for the formation of magnetic order.



**Figure 5.** phase diagram: (a) The  $U$ -  $V_1$  phase diagram for  $V_2 = 0$ ; (b) The  $U$ -  $V_2$  phase diagram for  $V_1 = 0$ ; (c) The  $V_1$ -  $V_2$  phase diagram for  $U = 6$  eV. The blue region corresponds to the uniform phase, the green region indicates the CDW phase and the yellow region indicates the SCDW phase.

Setting  $V_1 = 0$ , the phase diagram of the on-site Coulomb interaction  $U$  versus the next-nearest-neighbor Coulomb interaction  $V_2$  is obtained, as shown in **Figure 5(b)**. The phase diagrams in **Figure 5(a)** and **Figure 5(b)** are qualitatively similar, indicating that  $V_1$  and  $V_2$  play equivalent roles in regulating the SCDW phase.

In **Figure 5(c)**, with  $U = 6$  eV, the phase diagram of the competition between  $V_1$  and  $V_2$  is calculated. It is observed that when  $V_1$  and  $V_2$  are small, the SCDW phase occupies a large portion of the phase diagram. As the intersite Coulomb interactions increase, the system gradually transitions from the SCDW phase to the CDW phase. This result indicates that the intersite Coulomb interaction  $V$  is unfavorable for the formation and stabilization of magnetic order.

## 5. Conclusion

In summary, we employ the single-orbital extended Hubbard model for Kagome lattices to investigate the correlation between magnetic behavior and charge-density-wave (CDW). The results indicate that intersite Coulomb interaction  $V$  is essential for forming stable CDW and electronic nematic phases. A robust CDW phase emerges at  $V > 0.6$  eV, whereas onsite Coulomb interaction  $U$  strongly suppresses charge ordering. The competition between  $U$  and  $V$  dominates the stability of charge-ordered states. Strong onsite interaction ( $U \geq 6$  eV) induces stripe antiferromagnetic order on the CDW background and stabilizes the intertwined spin-charge density wave (SCDW). The intersite Coulomb interaction  $V$  is found to suppress magnetic ordering. This work offers a microscopic theoretical basis for the experimentally observed coexistence of CDW and SDW-CDW. It also highlights the vital role of nonlocal Coulomb interactions in modulating the ground-state properties of strongly correlated electron systems.

## Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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