

Antiferromagnetism, spin liquid, and plaquette singlet phases in the Shastry-Sutherland model: A variational cluster approximation approach

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We study the half-filled single-band Hubbard model on the Shastry-Sutherland lattice with nearest-neighbor hopping t , incorporating (i) a frustrating diagonal hopping t' to probe the emergence of spin-liquid behavior, and (ii) an additional Heisenberg exchange J that explicitly stabilizes plaquette-singlet correlations. Using the variational cluster approximation (VCA) with exact diagonalization at zero temperature on an eight-site cluster, we map the phase diagrams in the $(U/t, t'/t)$ and $(U/t, J/t)$ parameter planes. In the $(U/t, t'/t)$ plane, our analysis uncovers a competition between Néel antiferromagnetic (AFM) order with staggered magnetization and a nonmagnetic regime lacking conventional order, consistent with a nonmagnetic insulating phase that may be related to the spin-liquid-like regimes reported in previous studies. In contrast, the $(U/t, J/t)$ phase diagram exhibits a competition between the Néel antiferromagnet and a solid valence-bonding valence bond plaquette (PS), where spins form localized singlet plaquettes. Most notably, we observe that the transition from the PS phase to the Néel AFM phase is a first-order phase transition, with a discontinuous jump of the order parameters at the phase boundary, in quantitative agreement with high-pressure heat-capacity measurements on $\text{SrCu}_2(\text{BO}_3)_2$ [J. Guo *et al.*, *Commun. Phys.* **8**, 75 (2025)]. Thus, our VCA analysis underscores the subtle interplay of geometric frustration, quantum fluctuations, and dimensionality, and elucidates the crucial role of short-range correlations in stabilizing and competing ground states of frustrated quantum magnets.

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I. INTRODUCTION

Frustrated quantum magnets provide fertile ground for the emergence of novel phases of matter, where strong quantum fluctuations suppress conventional symmetry breaking and stabilize unconventional collective states [1]. Unlike classical Néel antiferromagnets, frustrated systems often host ground states with no long-range magnetic order, including quantum spin liquids (QSLs) [2,3] and valence-bond solids (VBSs) [4,5]. These states exemplify exotic forms of quantum order, ranging from long-range entanglement to spontaneously broken lattice symmetries. More recently, frustrated magnets have also been identified as promising candidates for realizing deconfined quantum critical points (DQCPs)—continuous transitions between phases with unrelated broken symmetries, beyond the Landau paradigm [6–12]. Establishing the microscopic fingerprints of such criticality remains one of the central open challenges in modern condensed matter physics.

A paradigmatic setting for investigating these ideas is the Shastry-Sutherland lattice (SSL), a two-dimensional geometry formed by orthogonal diagonal dimers embedded in

a square lattice [1]. This arrangement creates strong competition between nearest-neighbor and diagonal exchange couplings, leading to pronounced geometric frustration. The SSL was originally introduced as an exactly solvable model with a singlet-dimer ground state in the strong-diagonal limit [13], and has since become a cornerstone of low-dimensional quantum magnetism [4]. Subsequent studies established a rich phase diagram containing dimer, plaquette-singlet, and antiferromagnetic phases, together with possible intermediate nonmagnetic regimes depending on the coupling ratios and microscopic model considered [14,15]. Its material realization in $\text{SrCu}_2(\text{BO}_3)_2$, a layered copper borate where Cu^{2+} spin- $\frac{1}{2}$ ions occupy the SSL vertices, has established a rare experimental platform in which to probe these theoretical predictions [5,16–18]. Remarkably, $\text{SrCu}_2(\text{BO}_3)_2$ exhibits magnetization plateaus, proximate QSL behavior, and field-induced transitions, making it an indispensable case study in frustrated magnetism.

Recent numerical and analytical efforts have provided increasingly detailed insights into the competing orders of the SSL. Variational Monte Carlo studies employing Gutzwiller-projected wave functions have identified a gapless $\mathbb{Z}_2$ Dirac spin liquid, characterized by algebraically decaying correlations and emergent Dirac-like excitations [19]. Large-scale tensor-network simulations using infinite projected entangled-pair states have mapped out the phase diagram, which reveals a narrow QSL region separating plaquette and antiferromagnetic phases [20]. Meanwhile, pseudofermion functional renormalization group calculations have provided access to dynamical properties, uncovering signatures of Dirac cones

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in the spin structure factor—further supporting the case for fractionalized excitations [21]. Taken together, these results suggest that the SSL hosts a remarkably delicate balance between dimer, VBS, QSL, and Néel orders, with transitions that may exemplify DQCP physics.

Despite these advances, several fundamental questions remain unresolved. The precise stability of the QSL phase, its competition with antiferromagnetism, and the nature of the criticality at their boundaries are still under debate. Moreover, most prior studies have neglected the role of electron-electron interactions and, in particular, the explicit treatment of the on-site Coulomb repulsion within the Hubbard framework. Bridging this gap is crucial, as a faithful description of correlated electrons requires methods capable of handling interaction effects beyond effective spin models. Equally important is the reconciliation of numerical predictions with experimental observables, where a complete characterization of the phase diagram in the $(U/t, t'/t)$ and $(U/t, J/t)$ parameter planes remains elusive. Developing approaches that can treat the Coulomb interaction on equal footing with frustration therefore constitutes a pressing challenge for theory.

In this work, we employ the variational cluster approximation (VCA), combined with exact diagonalization on an eight-site cluster at zero temperature, to investigate these open questions. Our analysis focuses on the interplay between magnetization processes, spin-liquid behavior, singlet-plaquette phases, and the emergence of competing ordered states in the Shastry-Sutherland lattice. By systematically mapping out the phase diagrams in the $(U/t, t'/t)$ and $(U/t, J/t)$ parameter planes, we reveal distinct regimes of competing orders. In the $(U/t, t'/t)$ plane, our results uncover a competition between Néel antiferromagnetic order—characterized by finite staggered magnetization—and a nonmagnetic regime devoid of conventional long-range order. The latter is consistent with an algebraic spin-liquid (ASL) phase, distinguished by a gapped excitation spectrum and vanishing staggered magnetization. In contrast, the $(U/t, J/t)$ phase diagram exhibits a competition between the Néel antiferromagnet and a plaquette-singlet (PS) valence-bond solid, where spins preferentially form localized singlet plaquettes. Most notably, we find that the transition between the PS and Néel phases is of first-order character, with a discontinuous jump in the order parameters at the phase boundary. This prediction is in quantitative agreement with recent high-pressure heat-capacity measurements on $\text{SrCu}_2(\text{BO}_3)_2$ [22].

The paper is organized as follows: in Sec. II, we define the model and review the VCA method. We present and discuss our results in Sec. III and conclusion in Sec. IV.

II. MODEL AND METHOD

We consider the half-filled single-band Hubbard model on the Shastry-Sutherland lattice a two-dimensional geometry formed by orthogonal dimers embedded within a square lattice. The Hamiltonian can be written in the following form:

$$H_{\text{ASL}} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) - t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma}, \quad (1)$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) an electron of spin σ on site i , and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ counts the number of electrons of spin σ at that site. The nearest-neighbor hopping amplitude on the square lattice is denoted by t , while the frustration-inducing diagonal hopping is t' . The on-site Coulomb repulsion is U , and μ is the chemical potential, chosen as $\mu = U/2$ at half-filling. In Eq. (1), nearest-neighbor pairs are denoted by $\langle \dots \rangle$ while the second-neighbor (diagonal) pairs are indicated by $\langle\langle \dots \rangle\rangle$ and H.c. is the Hermitian conjugate.

To explicitly capture plaquette correlations, we also study the extended Hubbard-Heisenberg Hamiltonian,

$$H_{\text{PS}} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + J \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma}, \quad (2)$$

where $(\mathbf{S}_i)$ is the spin operator at site (i) , and (J) denotes the interdimer Heisenberg exchange interaction that favors plaquette-singlet formation. The other parameters of the model are taken to be the same as those specified in Eq. (1).

The primary purpose of Eq. (2) is not to represent the exact strong-coupling limit of Eq. (1), but rather to introduce an additional Heisenberg interaction that promotes plaquette-singlet correlations. In the actual strong-coupling expansion of the Hubbard model, exchange interactions proportional to $(4t^2/U)$ and $(4t'^2/U)$ are generated on the corresponding bonds. Therefore, Eq. (2) should be viewed as an extended Hubbard-Heisenberg model in which the exchange coupling (J) is treated as an independent control parameter. This construction allows us to directly investigate the competition between antiferromagnetic and plaquette-singlet correlations.

To explore possible symmetry-breaking phases—such as antiferromagnetic order, plaquette-singlet phases, and insulating phases—in the models of Eqs. (1) and (2), we employ the VCA with an exact diagonalization solver at zero temperature [23]. This method has been successfully applied to a wide range of strongly correlated electron systems to study the emergence of broken-symmetry phases, most notably unconventional superconductivity [24,25]. In particular, Sénéchal *et al.* [24] demonstrated how VCA can capture d -wave superconducting order in the two-dimensional Hubbard model, while Aichhorn *et al.* [25] extended the approach to investigate competing orders and phase diagrams in related systems.

VCA studies of the half-filled frustrated Hubbard model on the square lattice have revealed competing Néel and collinear antiferromagnetic phases, a paramagnetic region, and a d -wave superconducting phase stabilized by frustration, with possible coexistence between antiferromagnetism and superconductivity [26]. In stacked Hubbard models, VCA has shown that the interplay between frustration and interlayer coupling induces transitions between Néel and collinear antiferromagnetic phases and a paramagnetic Mott insulating state, with both first- and second-order transitions depending on dimensionality [27]. For the two-dimensional symmetric periodic Anderson model at half-filling, VCA reveals a quantum phase transition between a Kondo insulating state and an antiferromagnetically ordered phase as the interaction

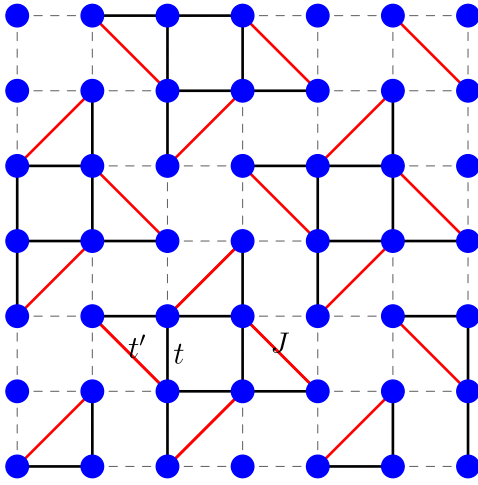


FIG. 1. Schematic of the eight-site cluster of the Shastry-Sutherland lattice used in the VCA calculations. Blue circles denote Cu sites, and black solid lines represent the nearest-neighbor hopping t . In the $(U/t, t'/t)$ phase diagram, the red diagonal bonds indicate the frustrating hopping t' , while in the $(U/t, J/t)$ phase diagram they represent the Heisenberg exchange J that favors plaquette-singlet formation. Dashed black lines denote intercluster links.

strength is increased [28]. Moreover, VCA studies of Dirac Hubbard models on honeycomb and π -flux lattices indicate that the metal-insulator transition is strongly affected by cluster geometry and that antiferromagnetic order preempts the nonmagnetic Mott insulating phase, excluding a spin-liquid phase in these systems [29].

The VCA approach provides a nonperturbative treatment of short-range electronic correlations by exactly solving finite-size clusters while treating intercluster effects at the variational level. However, VCA also has intrinsic limitations. In particular, results may depend on the choice of cluster geometry and size, and the restricted variational space of the self-energy can introduce biases in the determination of phase boundaries and long-range order. Furthermore, finite-cluster approximations may underestimate long-wavelength fluctuations. These limitations should be kept in mind when interpreting the present results. Despite these limitations, the VCA has been shown to reliably capture qualitative phase competition in a wide class of correlated electron systems. Comprehensive reviews of the theoretical foundations and applications of VCA are provided by Potthoff [30,31], where the method is presented within the self-energy functional framework and its ability to describe symmetry breaking and phase transitions in correlated systems is emphasized.

Like other quantum cluster approaches, such as cellular dynamical mean-field theory (CDMFT) [32,33] and the dynamical cluster approximation [34], the VCA begins by partitioning the infinite lattice into a tiling of identical finite clusters. In this work, we adopt the eight-site cluster geometry shown in Fig. 1, which is and must be commensurate with the Shastry-Sutherland lattice and captures the essential short-range correlations arising from both nearest-neighbor and diagonal interactions. The choice of an eight-site cluster strikes a balance between computational tractability and the

ability to resolve the competition between Néel antiferromagnetism, spin-liquid behavior, and plaquette-singlet order.

The eight-site cluster employed in this work preserves the point-group and translational symmetries relevant to the Shastry-Sutherland lattice. Therefore, the cluster geometry does not explicitly favor any particular broken-symmetry state. Nevertheless, as in all cluster approaches, finite-size effects may influence the quantitative location of phase boundaries. A systematic finite-size scaling analysis would require larger symmetry-preserving clusters. However, the next available cluster contains 16 sites and is computationally inaccessible within the present exact-diagonalization-based VCA implementation. Consequently, while the existence of competing phases can be addressed reliably, the precise location and nature of the phase boundaries should be interpreted with the usual caution associated with finite-cluster calculations.

Within the VCA framework, one considers two systems. The first is the original lattice problem, described by the Hamiltonian H_{ASL} or H_{PS} (denoted simply as H for brevity), defined on the infinite Shastry-Sutherland lattice. The second is the *reference system*, governed by a Hamiltonian H' , which is restricted to the finite cluster but shares the same interaction terms as H .

In practice, the reference Hamiltonian H' is obtained by restricting H to the finite cluster, i.e., by removing all intercluster hopping terms. Additional one-body terms, such as Weiss fields, may then be introduced to probe potential broken symmetries. More generally, any one-body operator can be added to H' as a variational parameter. The cluster size must be chosen such that the single-particle Green's function can still be computed exactly, typically by exact diagonalization, while remaining large enough to faithfully capture the relevant short-range correlations. An important point in model (2) is that the Heisenberg interaction is confined to the cluster, like t' in model (1).

The optimal one-body terms of H' are determined through a variational principle. Specifically, the electron self-energy Σ generated by the reference system is employed as a variational ansatz to construct the Potthoff self-energy functional [35]:

$$\Omega[\Sigma(\xi)] = \Omega'[\Sigma(\xi)] + \text{Tr} \ln \left\{ -[\mathbf{G}_0^{-1} - \Sigma(\xi)]^{-1} \right\} - \text{Tr} \ln[-\mathbf{G}'(\xi)], \quad (3)$$

where $\mathbf{G}_0$ is the noninteracting Green's function of the original lattice, and $\mathbf{G}'$ is the interacting Green's function of the cluster. The parameter set ξ denotes the variational one-body fields introduced in H' . The symbol Tr represents a functional trace, i.e., a sum over frequencies, momenta, and band indices. The cluster grand potential Ω' corresponds to its ground-state energy, since the chemical potential μ is included explicitly in H' . Both $\mathbf{G}'(\omega)$ and Ω' are evaluated numerically using Lanczos exact diagonalization at zero temperature.

The Potthoff functional $\Omega[\Sigma(\xi)]$ in Eq. (3) can be evaluated exactly, but only within the restricted manifold of self-energies $\Sigma(\xi)$ generated by the reference Hamiltonian H' . The physical solution is obtained by locating the stationary point of $\Omega[\Sigma(\xi)]$ with respect to the variational parameters ξ , i.e.,

$$\frac{\partial \Omega(\xi)}{\partial \xi} = 0. \quad (4)$$

In practice, this condition is solved using standard optimization techniques (e.g., Newton-Raphson). The resulting stationary self-energy Σ is then combined with the noninteracting lattice Green's function $\mathbf{G}_0$ to construct an approximate interacting Green's function $\mathbf{G}$ for the original Hamiltonian H . From $\mathbf{G}$ one may evaluate expectation values of any one-body operator, including order parameters associated with magnetism. Finally, the value of $\Omega(\xi)$ at the stationary point provides a variational estimate of the lattice grand potential, ensuring thermodynamic consistency within the VCA framework.

Equation (4) may in general admit multiple stationary solutions. For example, one may obtain a *normal-state* solution in which all Weiss fields vanish, as well as a symmetry-broken solution characterized by a finite Weiss field. Following the variational principle of self-energy functional theory [36], the physically realized phase is identified with the stationary solution that yields the lowest value of the Potthoff functional (3). In this way, competing phases can be systematically compared by introducing different Weiss fields and evaluating their corresponding grand potentials Ω . Moreover, the nature of the phase transition can be inferred from the behavior of Ω and the corresponding order parameters: a continuous evolution signals a second-order transition, whereas a discontinuous jump indicates a first-order transition.

This framework enables an unbiased investigation of AFM long-range order, PS correlations, and possible spin-liquid regimes, while faithfully treating quantum fluctuations at the cluster level. In contrast to mean-field approaches, which approximate interactions by static averages, VCA incorporates the full dynamics of short-range correlations within the reference cluster. This makes it particularly well suited for frustrated systems such as the Shastry-Sutherland lattice, where competing interactions and quantum fluctuations play a decisive role in selecting the ground state. In the following, we apply this framework to map out the phase diagrams of the Shastry-Sutherland model in the $(U/t, t'/t)$ and $(U/t, J/t)$ model parameter planes.

Numerical computations for this paper were performed using the PYQCM package [37].

III. RESULTS AND DISCUSSIONS

In this section we present and analyze our results. We first demonstrate how the VCA framework can be employed to identify the transition line separating metallic and insulating phases. We then turn to the suppression of AFM order and the emergence of an ASL regime. Finally, we investigate the competition between AFM order and the PS phase, focusing on the nature of the corresponding phase transition.

A. Metal-insulator transition

While CDMFT is well known for its ability to capture the Mott transition through the behavior of bath parameters [38], VCA provides an alternative route to describe the evolution from a correlated metal to an insulating regime. In this approach, the cluster chemical potential μ' is treated as a variational parameter, allowing the metal-insulator transition (MIT) to be identified from the electronic density. For each

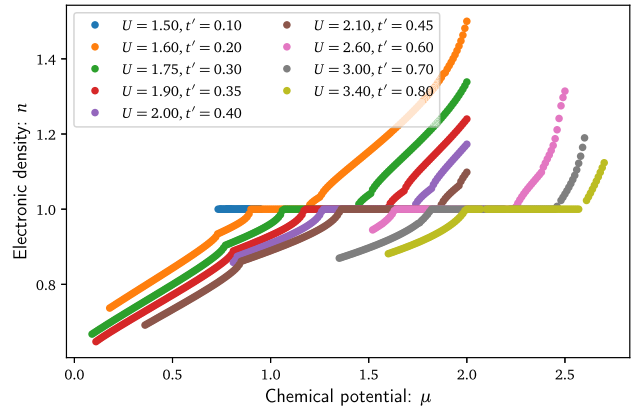


FIG. 2. Electronic density n vs Coulomb interaction U/t for different frustrating hoppings t'/t at fixed chemical potential $\mu = U/2$ in model (1). The approach to half-filling is shown as a function of increasing interaction strength.

value of t' , we compute the density n as a function of the chemical potential μ . In the insulating regime, $n(\mu)$ exhibits a robust plateau at $n = 1$, which persists as long as the system remains insulating. The breakdown of this plateau signals the onset of metallic behavior, as illustrated in Fig. 2.

The critical interaction strength for the MIT increases with frustration, since a larger t' enhances electronic delocalization and counteracts localization due to the Coulomb repulsion. This highlights the cooperative role of frustration and electron correlations in stabilizing unconventional insulating phases. At fixed t'/t , the spectral gap opens continuously as U/t increases, yielding a continuous Mott transition. The corresponding MIT line, shown in Fig. 4, delineates the boundary separating the metallic state from the insulator phase. This continuous character stands in sharp contrast to the first-order PS-AFM transition observed in the $(U/t, J/t)$ phase diagram, underscoring the rich interplay between frustration, interactions, and quantum fluctuations in the Shastry-Sutherland lattice.

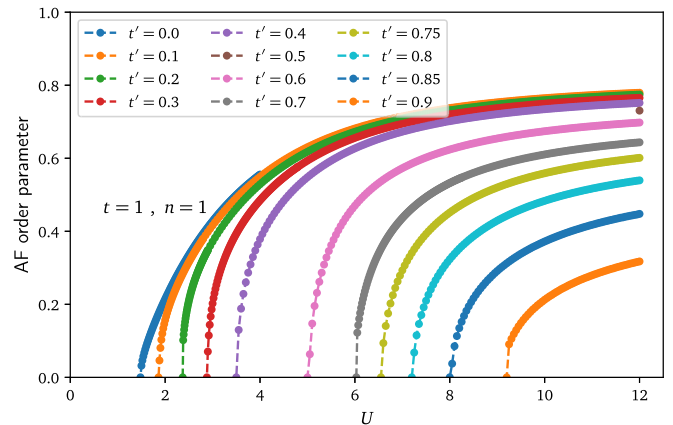


FIG. 3. Staggered AFM order parameter as a function of U/t for different values of t'/t in model (1). Increasing frustration suppresses AFM order and shifts the critical interaction where magnetism vanishes.

B. Antiferromagnetism and spin liquid

We next turn to the competition between antiferromagnetism and spin-liquid behavior in the $(U/t, t'/t)$ parameter plane. The staggered AFM order parameter can be defined as

$$m_{\text{AFM}} = \frac{1}{N} \sum_i (-1)^i \langle n_{i\uparrow} - n_{i\downarrow} \rangle, \quad (5)$$

where N is the total number of lattice sites, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the local density operator, and $(-1)^i$ distinguishes the two sublattices of the Shastry-Sutherland lattice. Equivalently, one may write

$$m_{\text{AFM}} = \frac{2}{N} \sum_i (-1)^i \langle S_i^z \rangle, \quad (6)$$

with $S_i^z = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$. Within the VCA framework, m_{AFM} is obtained by introducing a staggered Weiss field h_{AFM} as a variational parameter in the reference Hamiltonian,

$$H'_{\text{AFM}} = h_{\text{AFM}} \sum_i (-1)^i (n_{i\uparrow} - n_{i\downarrow}), \quad (7)$$

and then computing the expectation value of H'_{AFM} with the optimized Green's function at the stationary point of the Potthoff functional.

Figure 3 displays the evolution of the staggered AFM order parameter as a function of interaction strength U/t for several values of the frustrating diagonal hopping t'/t . For weak frustration, AFM order develops robustly and increases monotonically with U/t , as expected for a Mott insulating state dominated by local moments. However, as t'/t is increased, frustration strongly suppresses magnetic order, and beyond a critical threshold the staggered magnetization vanishes altogether. This identifies a critical line in the $(U/t, t'/t)$ plane beyond which no long-range AFM order can be stabilized.

The resulting phase diagram, shown in Fig. 4, highlights the emergence of an intermediate nonmagnetic regime separating the AFM and metallic phases. Within VCA, this phase is characterized by the absence of long-range order, a vanishing staggered magnetization, and the presence of a finite single-particle excitation gap. These features indicate the presence of a nonmagnetic insulating phase. Within the present VCA framework, the absence of long-range magnetic order and the existence of a finite gap are consistent with a spin-liquid-like regime. However, the precise nature of this phase cannot be determined conclusively from the present calculations, since VCA on a finite cluster does not provide direct access to the long-distance correlations, topological properties, or critical exponents required for an unambiguous identification of an algebraic spin liquid. The observed phase may therefore be viewed as a nonmagnetic insulating state compatible with previous proposals of spin-liquid behavior on the Shastry-Sutherland lattice. Importantly, the AFM-ASL transition obtained within the VCA is continuous: the order parameter decreases smoothly to zero as the transition line

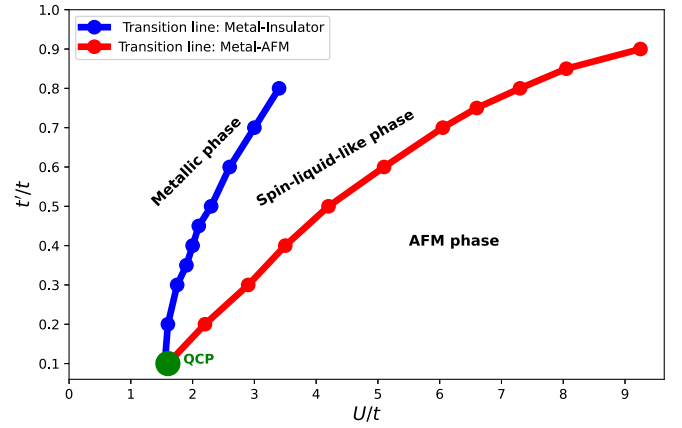


FIG. 4. Phase diagram in the $(U/t, t'/t)$ plane for model (1). The diagram shows the AFM, algebraic spin liquid (ASL), and metallic phases, together with the corresponding metal-insulator and AFM transition lines. A quantum critical point (QCP) separates the AFM and spin-liquid-like phase regimes.

is crossed. This continuous character is compatible with the theoretical scenario of a deconfined quantum critical point (DQCP), in which fractionalized excitations and emergent gauge fields mediate the transition between Néel order and a quantum paramagnet. The identification of such a continuous AFM-ASL transition in the Shastry-Sutherland model underscores the role of geometric frustration in driving unconventional quantum criticality and provides a natural link to recent tensor-network and Monte Carlo studies that have reported similar behavior in related frustrated lattices.

Moreover, the existence of a nonmagnetic insulating regime is directly relevant to the physics of $\text{SrCu}_2(\text{BO}_3)_2$, the canonical realization of the Shastry-Sutherland lattice. Inelastic neutron scattering and thermodynamic measurements in this material have revealed suppression of long-range order under pressure and signatures consistent with proximate spin-liquid behavior. Our results therefore suggest that the ASL phase identified within VCA may provide a theoretical explanation for these experimental anomalies, highlighting the Shastry-Sutherland compound as a promising platform for realizing deconfined quantum criticality in the laboratory.

C. Plaquette singlet and antiferromagnetism

We now turn to the $(U/t, J/t)$ plane, where the explicit Heisenberg exchange on diagonal bonds is introduced as an additional source of frustration. Figure 5 shows the staggered AFM order parameter as a function of J/t . At small J/t , AFM order remains stable and increases smoothly with interaction strength. However, as J/t grows, the AFM order parameter is abruptly suppressed and displays a discontinuous drop at a critical coupling. This behavior identifies a first-order transition into the PS valence-bond solid, a phase in which spins preferentially form localized singlets on elementary plaquettes rather than establishing long-range magnetic order.

We note that the first-order character is inferred from the discontinuous behavior of the variational solution and the corresponding order parameters. Since the present study is restricted to a single cluster geometry, a systematic finite-size

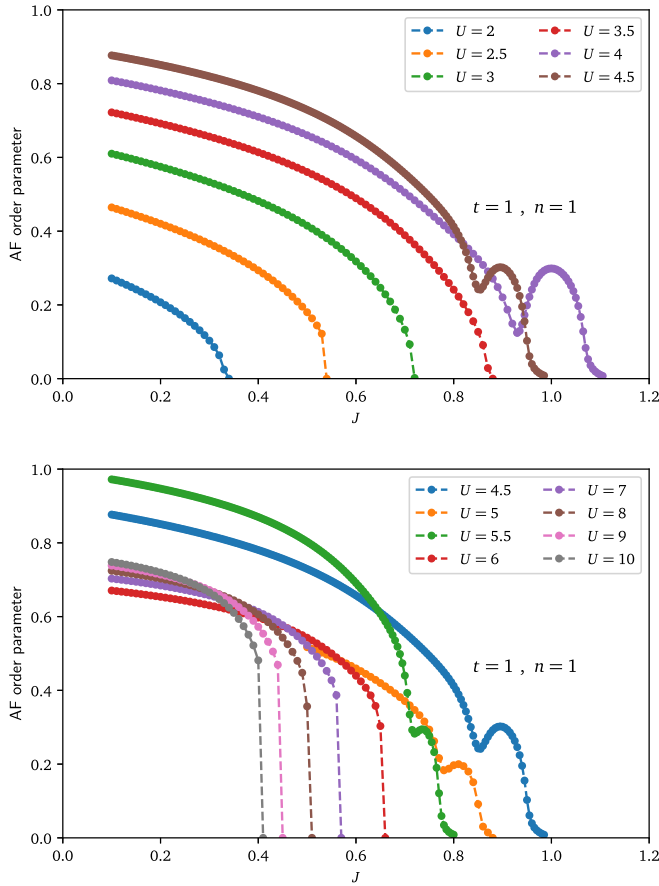


FIG. 5. Antiferromagnetic order parameter as a function of Heisenberg exchange J for several values of U/t in model (2). The curves show the suppression of AFM order at large J/t , indicating competition with plaquette-singlet correlations.

scaling analysis cannot be performed. Therefore, although the observed discontinuity is consistent with a first-order transition, finite-size effects may influence its precise location and strength.

From Fig. 5, we observe oscillations in the magnetic order parameter in the range $4t \leq U \leq 5.5t$. As shown in Fig. 3, these oscillations appear to be driven by the Heisenberg coupling J , indicating its role in inducing quantum fluctuations. In a similar spirit, the theory of quantum oscillations reported in Ref. [39] predicts de Haas–van Alphen oscillations of the magnetization in the intermediate to weak Kondo coupling regime. In our model, this oscillatory behavior arises as a direct consequence of the coupling J .

The global phase diagram in Fig. 6 illustrates the interplay between metallic, AFM, and PS phases. While the AFM-metal boundary remains continuous, the AFM-PS transition is strongly first order, as evidenced by the discontinuity of the order parameter. The stabilization of the PS phase at large J/t underscores the importance of interdimer exchange processes, which favor singlet formation and weaken long-range AFM correlations. This result is consistent with previous tensor-network studies and exact-diagonalization work, which also reported PS phases in proximity to AFM order in the Shastry-Sutherland model. The existence of a plaquette-singlet phase between the dimer and Néel phases was proposed by

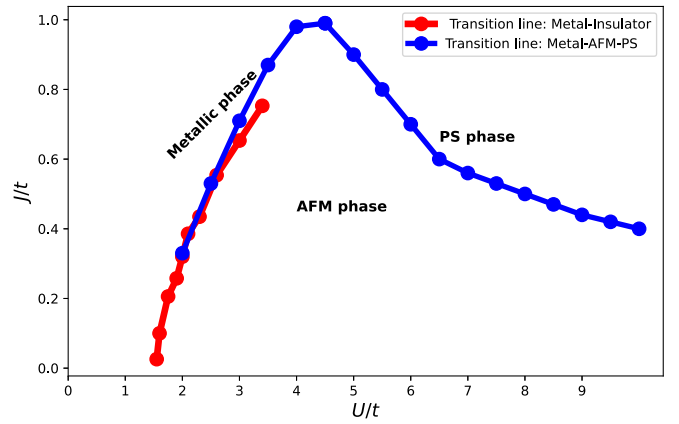


FIG. 6. Phase diagram in the $(U/t, J/t)$ plane in model (2). The system exhibits AFM, PS, and metallic phases, separated by well-defined transition lines. The PS-AFM boundary is first order, while the AFM-metal boundary is continuous.

Koga and Kawakami using series expansion and numerical approaches [15].

A notable feature of the present phase diagrams is the absence of an explicit dimer phase, which is known to constitute the exact ground state of the Shastry-Sutherland model in the strong-frustration regime. This absence should not be interpreted as evidence that the dimer phase is absent from the model itself. Rather, it reflects the limitations of the present variational space and cluster geometry. The VCA calculations were designed to probe antiferromagnetic and plaquette-singlet ordering through the corresponding Weiss fields, whereas no dedicated dimer order parameter was introduced. Consequently, the present analysis is restricted to the competition among the phases accessible within this variational framework. The exact dimer phase and its competition with plaquette and antiferromagnetic phases have been extensively investigated in previous studies and remain an important part of the broader Shastry-Sutherland phase diagram.

From an experimental perspective, the first-order character of the AFM-PS transition provides a natural explanation for the abrupt anomalies observed in thermodynamic measurements on $\text{SrCu}_2(\text{BO}_3)_2$ under applied pressure [22]. In particular, the discontinuous jump in the specific heat and the sharp change in the magnetic response are in quantitative agreement with our VCA results, which reveal a first-order transition between the AFM and PS states. This close correspondence emphasizes the predictive power of cluster approaches in capturing the subtle balance of competing interactions in geometrically frustrated materials.

Taken together with our analysis of the AFM–spin-liquid-like phase and metal-insulator transitions, these results highlight the rich diversity of critical phenomena in the Shastry-Sutherland lattice: while the AFM–spin-liquid-like phase and MIT boundaries are continuous, the AFM-PS transition is sharply first order, underscoring the coexistence of conventional and unconventional quantum criticality within the same frustrated model.

D. Comparison with previous studies

Our results are broadly consistent with previous studies of the Shastry-Sutherland lattice. The exact dimer phase established by Shastry and Sutherland and later analyzed by Miyahara and Ueda lies outside the set of phases explicitly considered in the present VCA study. Previous investigations have also reported plaquette-singlet phases and intermediate nonmagnetic regimes separating antiferromagnetic and dimerized states. More recently, tensor-network, variational Monte Carlo, and pseudofermion functional renormalization-group calculations have emphasized the competition among antiferromagnetic, plaquette, and spin-liquid-like phases. Within the limitations imposed by the finite cluster size, our VCA calculations reproduce this overall competition and provide a complementary perspective based on correlated-electron Hubbard and Hubbard-Heisenberg models. In particular, the competition between antiferromagnetic and plaquette-singlet order and the identification of a nonmagnetic insulating regime are in qualitative agreement with these previous studies, while extending the analysis to a variational cluster framework capable of treating electronic correlations explicitly.

IV. CONCLUSION

In this work, we have investigated the Shastry-Sutherland model within the framework of the variational cluster approximation, focusing on the interplay between magnetization processes, spin-liquid behavior, and plaquette-singlet correlations. By treating the cluster chemical potential and symmetry-breaking Weiss fields as variational parameters, we have mapped out the phase diagrams in the $(U/t, t'/t)$ and $(U/t, J/t)$ planes.

Our results reveal three distinct classes of quantum phase transitions. First, the metal-insulator transition is continuous and driven by the opening of a Mott gap, with the critical interaction strength increasing under geometric frustration. Second, in the $(U/t, t'/t)$ plane, we identified a continuous transition between Néel antiferromagnetism and a nonmagnetic insulating phase consistent with previously

proposed spin-liquid-like regimes, providing evidence for a possible deconfined quantum critical point. Third, in the $(U/t, J/t)$ plane, we observed a strongly first-order transition from antiferromagnetism to a plaquette-singlet valence-bond solid, in quantitative agreement with high-pressure thermodynamic experiments on $\text{SrCu}_2(\text{BO}_3)_2$.

Taken together, these findings demonstrate that the Shastry-Sutherland lattice hosts both continuous and discontinuous transitions, illustrating the coexistence of unconventional quantum criticality and first-order physics within a single frustrated geometry. Beyond their conceptual significance, our results establish a direct theoretical link to experimental observations in $\text{SrCu}_2(\text{BO}_3)_2$ and underscore the utility of quantum cluster methods in capturing the essential physics of strongly correlated and frustrated magnets.

Future work could extend the present study in several directions. Finite-temperature VCA or cluster extensions could provide access to thermodynamic properties and the evolution of magnetization plateaus. Dynamical extensions, including the calculation of spin structure factors, would enable a more detailed comparison with inelastic neutron scattering experiments. Finally, incorporating long-range Coulomb interactions or external fields may shed further light on the stability of spin-liquid regimes and the potential realization of exotic excitations such as fractionalized spinons and emergent gauge fields in the Shastry-Sutherland lattice.

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DATA AVAILABILITY

The data that support the findings of this article and the PYTHON code for generating the figures are publicly available [40].

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- [1] F. Ferrari and R. Valentí, Antiferromagnetism on the Shastry-Sutherland lattice, *Phys. Rev. B* **110**, 205140 (2024).
 - [2] L. Balents, Spin liquids in frustrated magnets, *Nature (London)* **464**, 199 (2010).
 - [3] R. Ma and C. Wang, Average symmetry-protected topological phases, *Phys. Rev. X* **13**, 031016 (2023).
 - [4] H.-D. Liu, Y.-H. Chen, H.-F. Lin, H.-S. Tao, and W.-M. Liu, Antiferromagnetic metal and Mott transition on Shastry-Sutherland lattice, *Sci. Rep.* **4**, 4829 (2014).
 - [5] M. E. Zayed, C. Rüegg, J. Larrea J., A. M. Läuchli, C. Panagopoulos, S. S. Saxena, M. Ellerby, D. F. McMorrow, T. Strässle, S. Klotz, *et al.*, 4-spin plaquette singlet state in the Shastry-Sutherland compound $\text{SrCu}_2(\text{BO}_3)_2$, *Nat. Phys.* **13**, 962 (2017).
 - [6] T. Senthil, A. Vishwanath, L. Balents, S. Sachdev, and M. P. Fisher, Deconfined quantum critical points, *Science* **303**, 1490 (2004).
 - [7] S. Sachdev, Quantum magnetism and criticality, *Nat. Phys.* **4**, 173 (2008).
 - [8] A. W. Sandvik, Evidence for deconfined quantum criticality in a two-dimensional Heisenberg model with four-spin interactions, *Phys. Rev. Lett.* **98**, 227202 (2007).
 - [9] N. Xi, H. Chen, Z. Y. Xie, and R. Yu, Plaquette valence bond solid to antiferromagnet transition and deconfined quantum critical point of the Shastry-Sutherland model, *Phys. Rev. B* **107**, L220408 (2023).
 - [10] J. Y. Lee, Y.-Z. You, S. Sachdev, and A. Vishwanath, Signatures of a deconfined phase transition on the Shastry-Sutherland lattice: Applications to quantum critical $\text{SrCu}_2(\text{BO}_3)_2$, *Phys. Rev. X* **9**, 041037 (2019).
 - [11] H. Kageyama, K. Yoshimura, R. Stern, N. V. Mushnikov, K. Onizuka, M. Kato, K. Kosuge, C. P. Slichter, T. Goto, and Y. Ueda, Exact dimer ground state and quantized magnetization plateaus in the two-dimensional spin system $\text{SrCu}_2(\text{BO}_3)_2$, *Phys. Rev. Lett.* **82**, 3168 (1999).
 - [12] R. W. Smith and D. A. Keszler, Synthesis, structure, and properties of the orthoborate $\text{SrCu}_2(\text{BO}_3)_2$, *J. Solid State Chem.* **93**, 430 (1991).

- [13] B. S. Shastry and B. Sutherland, Exact ground state of a quantum mechanical antiferromagnet, *Physica B+C* **108**, 1069 (1981).
- [14] S. Miyahara and K. Ueda, Theory of the orthogonal dimer Heisenberg spin model for $\text{SrCu}_2(\text{BO}_3)_2$, *J. Phys.: Condens. Matter* **15**, R327 (2003).
- [15] A. Koga and N. Kawakami, Quantum phase transitions in the Shastry-Sutherland model for $\text{SrCu}_2(\text{BO}_3)_2$, *Phys. Rev. Lett.* **84**, 4461 (2000).
- [16] Y. Cui, L. Liu, H. Lin, K.-H. Wu, W. Hong, X. Liu, C. Li, Z. Hu, N. Xi, S. Li, *et al.*, Proximate deconfined quantum critical point in $\text{SrCu}_2(\text{BO}_3)_2$, *Science* **380**, 1179 (2023).
- [17] J. Guo, G. Sun, B. Zhao, L. Wang, W. Hong, V. A. Sidorov, N. Ma, Q. Wu, S. Li, Z. Y. Meng, A. W. Sandvik, and L. Sun, Quantum phases of $\text{SrCu}_2(\text{BO}_3)_2$ from high-pressure thermodynamics, *Phys. Rev. Lett.* **124**, 206602 (2020).
- [18] J. L. Jiménez, S. P. G. Crone, E. Fogh, M. E. Zayed, R. Lortz, E. Pomjakushina, K. Conder, A. M. Läuchli, L. Weber, S. Wessel, *et al.*, A quantum magnetic analogue to the critical point of water, *Nature (London)* **592**, 370 (2021).
- [19] A. Maity, F. Ferrari, J. Y. Lee, J. Potten, T. Müller, R. Thomale, R. Samajdar, and Y. Iqbal, Evidence for a $\mathbb{Z}_2$ Dirac spin liquid in the generalized Shastry-Sutherland model, [arXiv:2501.00096](https://arxiv.org/abs/2501.00096).
- [20] P. Corboz, Y. Zhang, B. Ponsioen, and F. Mila, Quantum spin liquid phase in the Shastry-Sutherland model revealed by high-precision infinite projected entangled-pair states, *Phys. Rev. Lett.* **136**, 186701 (2026).
- [21] S. Wessel, I. Niesen, J. Stapmanns, B. Normand, F. Mila, P. Corboz, and A. Honecker, Thermodynamic properties of the Shastry-Sutherland model from quantum Monte Carlo simulations, *Phys. Rev. B* **98**, 174432 (2018).
- [22] J. Guo *et al.*, Deconfined quantum critical point lost in pressurized $\text{SrCu}_2(\text{BO}_3)_2$, *Commun. Phys.* **8**, 75 (2025).
- [23] C. Dahnken, M. Aichhorn, W. Hanke, E. Arrigoni, and M. Potthoff, Variational cluster approach to spontaneous symmetry breaking: The itinerant antiferromagnet in two dimensions, *Phys. Rev. B* **70**, 245110 (2004).
- [24] D. Sénéchal, P.-L. Lavertu, M.-A. Marois, and A.-M. S. Tremblay, Competition between antiferromagnetism and superconductivity in high- T_c cuprates, *Phys. Rev. Lett.* **94**, 156404 (2005).
- [25] M. Aichhorn, E. Arrigoni, M. Potthoff, and W. Hanke, Variational cluster approach to the Hubbard model: Phase-separation tendency and finite-size effects, *Phys. Rev. B* **74**, 235117 (2006).
- [26] A. H. Nevidomskyy, C. Scheiber, D. Sénéchal, and A.-M. S. Tremblay, Magnetism and d -wave superconductivity on the half-filled square lattice with frustration, *Phys. Rev. B* **77**, 064427 (2008).
- [27] T. Yoshikawa and M. Ogata, Role of frustration and dimensionality in the Hubbard model on the stacked square lattice: Variational cluster approach, *Phys. Rev. B* **79**, 144429 (2009).
- [28] S. Horiuchi, S. Kudo, T. Shirakawa, and Y. Ohta, Antiferromagnetism versus Kondo screening in the two-dimensional periodic Anderson model at half filling: Variational cluster approach, *Phys. Rev. B* **78**, 155128 (2008).
- [29] M. Ebato, T. Kaneko, and Y. Ohta, Metal-insulator transition of Dirac fermions: Variational cluster study, *J. Phys. Soc. Jpn.* **84**, 044714 (2015).
- [30] M. Potthoff, Self-energy-functional theory, in *Theoretical methods for Strongly Correlated Systems*, edited by A. Avella and F. Mancini, Springer Series in Solid-State Sciences Vol. 171, (Springer, New York, 2012), Chap. 9.
- [31] M. Potthoff, Variational cluster approximation, in *DMFT at 25: Infinite dimensions, Lecture Notes of the Autumn School on Correlated Electrons 2014*, edited by E. Pavarini, E. Koch, D. Vollhardt, and A. Lichtenstein (Forschungszentrum Jülich, 2014).
- [32] H. Park, K. Haule, and G. Kotliar, Cluster dynamical mean field theory of the Mott transition, *Phys. Rev. Lett.* **101**, 186403 (2008).
- [33] D. Sénéchal, Cluster dynamical mean field theory, in *Strongly Correlated Systems: Theoretical Methods* (Springer-Verlag, Berlin, 2012), pp. 341–371.
- [34] M. H. Hettler, M. Mukherjee, M. Jarrell, and H. R. Krishnamurthy, Dynamical cluster approximation: Nonlocal dynamics of correlated electron systems, *Phys. Rev. B* **61**, 12739 (2000).
- [35] M. Potthoff, Self-energy-functional approach to systems of correlated electrons, *Eur. Phys. J. B* **32**, 429 (2003).
- [36] M. Potthoff, Systematics of approximations constructed from dynamical variational principles, in *Effective Models for Low-Dimensional Strongly Correlated Systems*, AIP Conf. Proc. No. 816 (AIP, Melville, NY, 2006), pp. 41–54.
- [37] T. N. Dionne, A. Foley, M. Rousseau, and D. Sénéchal, PYQCM: An open-source Python library for quantum cluster methods, *SciPost Phys. Codebases* **23** (2023).
- [38] J. P. L. Faye, D. Sénéchal, and S. R. Hassan, Topological phases of the Kitaev-Hubbard model at half filling, *Phys. Rev. B* **89**, 115130 (2014).
- [39] P. Ram and B. Kumar, Theory of quantum oscillations of magnetization in Kondo insulators, *Phys. Rev. B* **96**, 075115 (2017).
- [40] J. P. L. Faye, O. Ndiaye, and D. Senechal, Antiferromagnetism, spin liquid, and plaquette singlet phases in the Shastry-Sutherland model: A variational cluster approximation approach, OSF, 2026, <https://osf.io/ty2cz/>.