Spin density wave order in interacting type-I and type-II Weyl semimetals

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Weyl semimetals (WSMs), featuring massless linearly dispersing chiral fermions in three dimensions, provide an excellent platform for studying the interplay of electronic interactions and topology, and exploring new correlated states of matter. Here, we examine the effect of a local repulsive interaction on an inversion-symmetry breaking Weyl semimetal model, using Cluster Dynamical Mean Field theory (CDMFT) and Variational Cluster Approximation (VCA) methods. Our analysis reveals a continuous transition from the gapless Weyl semimetal phase to a gapped spin density wave (SDW) ordered phase at a critical value of the interaction, which is determined by the band structure parameters. Further, we introduce a finite tilt in the linear dispersion and examine the corresponding behavior for a type-II Weyl semimetal model, where the critical interaction strength is found to be significantly diminished, indicating a greater susceptibility towards interactions. The behavior of different physical quantities, such as the double occupancy, the spectral function and the Berry curvature associated with the Weyl nodes are obtained in both the semimetallic and the magnetically ordered states. Finally, we provide an interaction-induced phase diagram for the Weyl semimetal model, as a function of the tilt parameter.

I. INTRODUCTION

The interplay of electronic correlations and band topology in strongly spin-orbit coupled systems [1,8] presents a topic of great interest in contemporary Condensed Matter Physics, with the potential to uncover new and exotic phases of matter. In this context, topological insulators [4-10] and Weyl semimetals [11,14] are examples of strongly spin-orbit coupled systems with low-energy degrees of freedom that are described by massless linearly dispersing electrons, and are suitable for studying the combination of many-body and band structure effects in topological materials. In particular, Weyl semimetals (WSMs) feature pairs of nondegenerate bands touching each other at isolated points in the band structure, with Weyl fermions as low-energy quasiparticles. Theoretically, this can be realized by breaking either inversion or time-reversal symmetry (TRS) or both. WSMs are characterized by open Fermi arcs [13,15,20] on their surfaces and a novel response to applied electric and magnetic fields [13,21,25]. A conventional or type-I Weyl semimetal has a conical spectrum and a point-like Fermi surface, but the energy dispersion at the node could also be tilted along a given direction. When the tilt exceeds a certain critical value, the Weyl node appears at an intersection of an electron and a hole pocket, giving rise to a type-II WSM [15,27,29]. The latter class of models are known to have properties qualitatively different from those of the former, some of which include a field-selective anomalous magnetotransport [30] and an intrinsic anomalous Hall effect [31]. On the experimental side, a number of material candidates for both type-I and type-II Weyl semimetals have been proposed, and confirmed in recent times [15,20,28,32,37].

Correlation effects are expected to be important for Weyl semimetal candidates, which often involve heavier elements with a strong spin-orbit interaction. Moreover, there have been experimental reports of collective many-body effects, such as superconductivity [33,38] or magnetism [39,41], in Weyl semimetals, necessitating the theoretical treatment of electronic instabilities. Other important questions involve the robustness of the topological properties of a Weyl semimetal in the presence of interactions [42,47], and the possibility of realizing interaction-induced topologically nontrivial phases [43-45]. The effects of electronic interactions in WSMs have been explored using various approaches [42,61] such as perturbative renormalization group (RG) [51,53,57,58,62], mean-field analyses [29,45,49,50,54,55,63], strong-coupling expansion methods [43] and, occasionally, numerical techniques [44,46,47,56]. Specific examples of possible broken-symmetry states have been considered, such as excitonic and charge-density wave (CDW) instabilities [43,45,50,51,53,57], as well as superconducting ground states [29,49,64,65]. There have been comparatively fewer studies of interaction effects in type-II WSMs, using similar approaches [54,57]. In order to complement the existing results, it is useful to employ a nonperturbative approach, that can describe the physical properties of the model by continuously varying the interaction strength, producing results that are highly illustrative in nature, and comprehensive as well. Besides, having a common framework to detect possible broken-symmetry phases and examine the changes in the topological properties of the system, makes it easier to characterize new and exotic types of order. Finally, one needs a simple way of introducing a linear tilt in the dispersion, and examining its effect on the properties of the interacting WSM model.

In this paper, we attempt to address these concerns, by studying the effect of a local, repulsive interaction on a simple inversion-symmetry breaking Weyl semimetal model, using two complementary methods, Cluster Dynamical Mean Field Theory (CDMFT) [56,59] and the Variational Cluster Approximation (VCA) [44,70,73]. Both of these belong to a set of closely related approaches known as Quantum Cluster Methods [24,75], which consider a finite cluster of sites embedded in an infinite lattice, and add to it additional fields or “bath” degrees of freedom, so as to best represent the effect of the surrounding infinite lattice. The values of these additional parameters are set using variational or self-consistency principles. In these approaches, broken symmetry states can appear even for the smallest clusters used, and unlike ordinary mean field theory, these are dynamical in nature, and retain the full effect of strong correlations. These methods allow us to obtain the full interacting Green’s function, spectral functions and topological properties as a function of the interaction strength, and include additional tuning parameters, such as a finite tilt in the dispersion, with relative ease.

Our main findings are as follows. At a critical value of the interaction strength, $U = U_c$, the Weyl semimetal undergoes a continuous transition to a topologically trivial spin density wave (SDW) ordered state. We find an ordering wavevector $Q = (0, 0, \pi)$, which connects Weyl nodes of opposite chiralities, with the magnetization pointing in the $z$ direction. In
the rest of the paper, we denote this particular SDW order as $M^{(0,0,\pi)}$. For the untiled Weyl dispersion, it is equivalent to a state with an ordering wavevector $Q = (\pi, 0, 0)$ (see Appendix A), with the magnetization pointing in the $x$ direction, which we henceforth denote as $M^{(\pi,0,0)}$. Besides, a different spin density wave order denoted as $M^{(\pi,\pi,\pi)}$, with an ordering wavevector $Q = (\pi, \pi, \pi)$, is also found to closely compete with $M^{(0,0,\pi)}$ in this analysis (see Appendix A for a pictorial depiction of the different types of magnetic order that can be realized in this system). These particular orders are presumably favored by the presence of nesting in the band structure, between Weyl nodes of opposite chiralities. Since our analysis is limited to the effect of repulsive local interactions at half-filling, we constrain our attention to various spin density wave instabilities. As expected, the magnetic order is accompanied by the gradual appearance of a spectral gap, and the destruction of the Berry curvature associated with the Weyl nodes, which we compute for the folded band structure, in the ordered state. As the interaction amplitude increases, the SDW order is found to become more robust, as indicated by a gradual increase in the magnitude of the order parameter. The critical interaction $U_c$, at which it appears, also depends on the details of the band structure and the model parameters considered. We introduce a finite tilt parameter $w_z$ (assumed to be along the $z$ direction for simplicity) and find that in the over-tilted type-II regime, the transition occurs at a significantly diminished value of the interaction, $U_c$. This is consistent with the expectation of an increased sensitivity towards interactions, when each Fermi point is replaced by an electron and a hole pocket (see Fig.1(B)). Once again, the SDW order $M^{(0,0,\pi)}$ (which is no longer equivalent to $M^{(0,0,0)}$ for $w_z \neq 0$) is found to be favored for the type-II WSM model. In general, the magnitude of the tilt parameter strongly affects the critical amplitude for the transition, and its orientation may decide the specific nature of the magnetic order. We have independently verified our results for the order of the phase transition and the competing density-wave instabilities, using both the CDMFT and the VCA approaches.

The paper is organized as follows. In Sec. II we introduce the model Hamiltonian, and provide a brief overview of the CDMFT and VCA methods that are used in our analysis. In Sec. III we present the results of our CDMFT computations for the double occupancy and the dominant SDW order parameter, as a function of the interaction. We also pictorially illustrate the behavior of the spectral function and the Berry curvature associated with the Weyl nodes. We then present the results of our VCA calculations, which confirm the nature of the spin density wave instability occurring in this system, as well as order of the transition. We also present the corresponding results as a function of the increasing tilt parameter $w_z$, which pushes the critical interaction strength $U_c$ to smaller values. Based on these results, we present the interaction-induced phase diagram of the WSM model considered by us, as a function of $w_z$. Finally, in Sec. IV we summarize our results, discuss some relevant observations, and present the conclusions of our study.

II. MODEL AND METHODS

A. Model Hamiltonian

Consider the general form of the Hamiltonian in the vicinity of a Weyl point, along with a possible tilt in the dispersion, given by

$$H_0(k) = w_z k_z + v_x k_x \sigma_x + v_y k_y \sigma_y + v_z k_z \sigma_z,$$

where $\sigma_{x,y,z}$ are the Pauli matrices. The corresponding eigenvalues are

$$E_{\pm}(k) = w_z k_z \pm \sqrt{v_x^2 k_x^2 + v_y^2 k_y^2 + v_z^2 k_z^2}.$$

The first term is a linear tilting term, which is crucial for the emergence of type-II Weyl fermions. Once $|w_z| > |v_z|$, the Weyl cone is over-tilted and the Fermi surface changes from a point to an electron and a hole pocket, touching each other at the type-II Weyl node. Throughout our analysis, we consider $v_x = v_y = v_z = 1$ and tune the tilt parameter $w_z$, to explore different regimes. When $|w_z| < |v_z| = 1$, we
have a conventional type-I Weyl semimetal, while \(|w_j| > 1\) corresponds to the over-tilted type-II regime. In principle, one could also have a non-linear dispersion in one or more directions in Eq. (1) above, and include a quadratic tilt term (referred to as a Type-III WSM \cite{Weyl-points}). This model has its own peculiar properties and will be studied in a future work.

For the purpose of our analysis, we study models defined on the cubic lattice. Using Eq. (1) above, we consider the following noninteracting lattice model for a Weyl semimetal with a linear dispersion,

\[
H_0 = \sum_{k} c_k^\dagger (w_x \sin k_x + v_x \sigma_x \sin k_x \\
+ v_y \sigma_y \sin k_y + v_z \sigma_z \sin k_z) c_k, \tag{2}
\]

where the lattice spacing has been set to unity, and the fermion operators are spin doublets, i.e. \(c_k \equiv (c_{kT}, c_{kI})\). The Weyl nodes for the above model occur at the points \((0, 0, 0)\), \((\pi, 0, 0)\), \((0, \pi, 0)\), \((\pi, \pi, 0)\) and \((\pi, \pi, \pi)\) and permutations thereof. One of the consequences of the presence of Weyl nodes at these high-symmetry points is the absence of Fermi arcs in the orthogonal \(\hat{x}\), \(\hat{y}\) or \(\hat{z}\)-directions. This is due to the fact that the projected Weyl points on the surfaces in all of these directions are formed by Weyl points of opposite chiralities (see Fig. 5). However, we do see Fermi arcs in the \((110)\) direction for this model. We also introduce a tilt parameter, \(\hat{v}_i\) into account by a set of uncorrelated, additional orbitals which break inversion symmetry. For a finite value of \(w_z\), it also violates time-reversal symmetry, although this has no effect on the positions of the Weyl nodes.

In the real-space representation, the noninteracting Hamiltonian takes the following form

\[
H_0 = -\frac{i}{2} \sum_{r, \alpha, \beta} \left( w_r c_{r\alpha}^\dagger c_{r+\hat{\alpha}+\hat{\beta}} + v_x c_{r\alpha}^\dagger \sigma_x^{\alpha\beta} c_{r+\hat{\alpha}+\hat{\beta}} \\
+ v_y c_{r\alpha}^\dagger \sigma_y^{\alpha\beta} c_{r+\hat{\alpha}+\hat{\beta}} + v_z c_{r\alpha}^\dagger \sigma_z^{\alpha\beta} c_{r+\hat{\alpha}+\hat{\beta}} \right) - \mu \sum_{r, \sigma} n_{r, \sigma}, \tag{3}
\]

Here, \(\hat{x}, \hat{y}\) and \(\hat{z}\) are the lattice unit vectors along the \(x, y\) and \(z\) directions, the operator \(c_{r\alpha}\) annihilates a particle with spin \(\alpha\) on site \(r\), while \(\sigma^\mu (\mu = x, y, z)\) denotes the three Pauli matrices corresponding to the spin degree of freedom, and the number density per spin projection of the spin-1/2 electrons is \(n_{r, \sigma} = c_{r\alpha}^\dagger \sigma_{r, \sigma}\). In the following analysis, we investigate the effect of local Hubbard interactions on the model defined above. The resulting Hamiltonian is as follows,

\[
H = H_0 + U \sum_{r} n_{r, \uparrow} n_{r, \downarrow}, \tag{4}
\]

where \(H_0\) is defined in Eq. (3) above. \(U\) is the Hubbard interaction parameter which is taken to be positive, or repulsive. For the purpose of our analysis, the chemical potential is fixed at \(\mu = U/2\) throughout, which corresponds to half-filling.

As mentioned earlier, we examine the possibility of spin density wave (SDW) orders as prototypical many-body instabilities of the WSM model at half-filling with repulsive interactions. A general SDW operator with wavevector \(Q\) is defined as follows-

\[
\Psi_{SDW} = \lambda \sum_{r} A_r \cos[Q.r + \phi], \tag{5}
\]

where \(A_r = S_r^x, S_r^y\) and \(\lambda\) is a variational parameter. In the following analysis, we probe the presence of SDW orders with wavevectors \(Q = (\pi, 0, 0), (0, 0, \pi), (\pi, \pi, 0)\) and \((\pi, \pi, \pi)\), and observe stable solutions for multiple values of \(Q\) in the strongly interacting regime, depending on the parameters chosen.

\[\text{Figure 3. Evolution of the double occupancy and the spin density wave (SDW) order parameter } \langle \langle M^{(0,0,\pi)} \rangle \rangle \text{ with an ordering wavevector } Q = (0,0,\pi), \text{ as a function of the interaction parameter } U \text{ for two sets of model parameters (A) } v_x = v_y = v_z = 1, w_x = 0 \text{ (type-I, above) and (B) } v_x = v_y = v_z = 1, w_x = 1.5 \text{ (type-II, below).}

For the untilted dispersion, this is equivalent to the order \(M^{(x,0,0)}\), with \(Q = (\pi, 0, 0)\). In both cases, we observe a continuous transition to an SDW ordered state, for a critical value of the interaction strength, \(U_c\). For \(w_x = 0\), we find \(U_c \approx 3\), whereas for \(w_x = 1.5 > v_x\), the system reacts much more strongly to the presence of interactions, with \(U_c \approx 0.1\). This is expected due to the appearance of a finite Fermi surface for an over-tilted dispersion. As explained in the text, we find a jump in the order parameter \(M^{(x,0,0)}\) as a function of increasing \(U\) in our CDQFT calculations for a value of \(U > U_c\), which leads to an apparent hysteresis behavior. However, as we decrease \(U\), the system seems to undergo a continuous transition at \(U = U_c\).

\[\text{B. Methods: CDQFT and VCA}

Here, we provide a brief overview of the Quantum Cluster Methods used in our analysis. For a more detailed discussion on the principles and the mathematical background of these methods, please see Ref. \cite{Weyl-points}.

Cluster Dynamical Mean Field Theory (CDQFT) is an extension of the Dynamical Mean Field Theory (DMFT) method, where the single-site impurity is replaced with a cluster of sites with open boundary conditions, which takes into account short-range spatial correlations exactly. In this approach, the effect of the cluster’s environment is taken into account by a set of uncorrelated, additional orbitals hybridized with the cluster, known as the “bath”. The infl-
nite lattice is thus tiled into small clusters, each of which is coupled to a bath of uncorrelated, auxiliary orbitals. These bath orbitals have their own (possibly spin-dependent) energy levels \( E_{\sigma} \) and are hybridized with the cluster sites \( r \) with amplitudes \( \Theta_{ir} \). The bath parameters \( (E_{\sigma}, \Theta_{ir}) \) are determined by a self-consistency condition (see Ref. [74] for details).

In our analysis, we use a 12-site \((4 \times 8)\) cluster-bath system, which is illustrated in Fig. 2. An effective model is solved on the cluster, and the self-energy associated with that cluster is then applied to the whole lattice. The lattice Green’s function is computed from the cluster’s self-energy \( \Sigma(\omega) \)

\[
G^{-1}(\tilde{k}, \omega) = G_0^{-1}(\tilde{k}, \omega) - \Sigma(\omega)
\]

where \( \tilde{k} \) denotes a reduced wavevector (defined in the Brillouin zone of the super-lattice), and \( G_0 \) is the noninteracting Green’s function. Once a solution is found for a given set of model parameters, average values of one-body operators defined on the lattice can then be obtained from the above Green’s function \( G \). An exact diagonalization solver is used (at zero temperature), and the complexity of the computation is determined by the total number of cluster and bath orbitals. For the type-I WSM model with \( |w| < 1 \), we consider a particle-hole symmetric ansatz for the bath parameters, and every cluster site is hybridized with every bath site in the system by a hopping parameter. For the type-II WSM model with \( |w| > 1 \), on the other hand, we no longer impose particle-hole symmetry on the bath parameters, and for simplicity, each cluster site is now only hybridized with the two bath sites that are adjacent to it.

The Variational Cluster Approximation (VCA) method involves solving a model exactly on a small cluster of lattice sites, adding fields that represent the effect of the cluster’s environment. The essence of this method lies in Potthoff’s self-energy functional approach [77], which involves a functional \( \Omega(\Sigma) \), of the self-energy \( \Sigma \), parameterized by the one-body terms collectively labeled by \( h \). The original Hamiltonian \( H \), defined on the infinite lattice, is considered along with a reference Hamiltonian \( H' \), which is often a restriction of \( H \) to the cluster. A finite number of Weiss fields may be added to the latter, in order to probe different broken symmetries. Any one-body term can be added to \( H' \), since the basic requirement is that \( H' \) and \( H \) must share the same interaction term. The electron self-energy \( \Sigma(\omega) \) associated with \( H' \) is then used as a variational self-energy, in order to construct the Potthoff self-energy functional (see Ref. [74] for a detailed mathematical explanation of the VCA approach):

\[
\Omega(\Sigma(h)) = \Omega(\Sigma(h)) + \text{Tr} \ln \left( - (G_0^{-1} - \Sigma(h))^{-1} \right) - \text{Tr} \ln \left( - G'(h) \right),
\]

where \( G' \) is the physical Green’s function of the cluster, \( G_0 \) is the noninteracting Green’s function of the original lattice model, and \( h \) denotes collectively the coefficients of all the adjustable one-body terms added to \( H' \), acting as variational parameters. The symbol \( \text{Tr} \) stands for a sum over all degrees of freedom and frequencies. \( \Omega' \) is the ground-state energy of the cluster which, along with the associated Green’s function \( G' \), is computed numerically, in our case via the exact diagonalization method at zero temperature. The best possible self-energy \( \Sigma(\omega) \) corresponds to the stationary point of the functional. The latter is then combined with \( G_0 \) to form an approximate Green’s function \( G \) for the original Hamiltonian \( H \), from which any one-body term, such as the order parameters associated with various SDW orders, can be computed. We define our reference Hamiltonian on an eight-site cubic cluster.

III. RESULTS AND DISCUSSION

In this section, we discuss the behavior of different physical quantities associated with the WSM model defined in Eq. (2), as a function of the interaction strength \( U \), obtained from our analyses. Using CDMFT, we examine the double occupancy, the relevant SDW order parameters, the spectral function and the Berry curvature associated with the Weyl nodes, for both the type-I and type-II WSM models. In the VCA approach, we first obtain the behavior of the Potthoff functional \( \Omega \) as a function of the relevant Weiss fields, corresponding to different types of order. The stationary point of the functional is then used to approximately evaluate the Green’s function for the lattice model, and calculate different physical properties as a function of the interaction amplitude. We also compare the critical interaction strength for different values of the tilt parameter \( w \).

A. CDMFT: Numerical results

1. Type-I:

   Here, we discuss our CDMFT results for a type-I Weyl semimetal model, with \( v_x = v_y = v_z = 1 \) and \( w = 0 \). These results remain qualitatively unchanged for all \( |w| < |v| \).

   a. Double occupancy and order parameter: For the above values of the band structure parameters, our CDMFT solutions indicate that the Weyl semimetal undergoes a continuous transition to the spin-density wave (SDW) ordered state \( M_0^{(0,0,0)} \), at a critical interaction amplitude \( U = U_{\text{c1}} \approx 3 \). We find clear signatures of a phase transition in the double occupancy, as well as the magnitude of the SDW order parameter \( |M_0^{(0,0,0)}| \) calculated as a function of \( U \) (see Fig. 3). However, there is an apparent discrepancy between the behavior of these quantities for increasing and decreasing values of \( U \). In the former case, we observe a jump in the double occupancy as well as the order parameter \( |M_0^{(0,0,0)}| \), for \( U \approx 5 > U_{\text{c1}} \). This is evident from Fig. 3(A). However, as we decrease the magnitude of \( U \), no such jump is observed, and the transition appears to be continuous. Therefore, an apparent hysteresis behavior is observed in the transition region of \( U_{\text{c1}} < U < U_{\text{c2}} \) where \( U_{\text{c1}} \approx 3 \) and \( U_{\text{c2}} \approx 5 \), which also shows up in the double occupancy. The reason for observing a finite jump in the order parameter is unclear, but it could potentially be due to a false minimum generated in the self-consistency procedure employed in CDMFT. In the next section, we find that our VCA results clearly point towards a second-order phase transition in this system.

   b. Spectral function: We also calculate the spectral function \( A(\omega, k_x, k_y, k_z) = -\frac{1}{\pi} \text{Im} G(\omega, k_x, k_y, k_z) \) for the WSM model, and illustrate our results for two different values of the interaction parameter \( U \), representative of the semimetallic and \( M_0^{(0,0,0)} \) phases respectively (see the upper panel in Fig. 4). At \( U = 1 < U_{\text{c1}} \), the spectrum is found to be gapless, as expected, and the dispersion resembles that of a noninteracting type-I WSM. At \( U = 5 > U_{\text{c1}} \), a large spec-
A central gap is observed, along with a nontrivial value for the SDW order parameter \( \langle M^{(0,0,\pi)} \rangle \). This is consistent with the expectation of a phase transition at \( U = U_c \approx 3 \).

c. Topological properties: In order to verify the topological properties of the WSM model in the presence of interactions, we calculate the Berry phases associated with the Weyl nodes, using an approach introduced in Ref. [47] which we briefly describe below.

In a noninteracting WSM, the Weyl points can be identified as hedgehog singularities of the Berry curvature, \( \nabla \times a(k) \), where \( a \) is the Berry connection defined in terms of the occupied Bloch states. In the presence of interactions, a many-body Berry connection \( A(k) \) and associated Berry curvature \( \nabla \times A \) are analogously defined in Ref. [47], using the zero-frequency Green’s function. A topological Hamiltonian is defined as,

\[
H_i(k) = -G(0,k)^{-1} = H(k) + \Sigma(0,k)
\]

where \( H \) is the Bloch Hamiltonian for the noninteracting case, while \( \Sigma(\omega,k) \) is the self-energy matrix. \( H_i \) plays the role of an effective Bloch Hamiltonian for the interacting system, and its eigenstates are used to define the many-body Berry connection, as \( A(k) = -i \sum (nk|\nabla|nk) \), where \( H_i(k)|nk\rangle = \epsilon_i(k)|nk\rangle \), \( \{\epsilon_i(k)\} \) being the band structure of \( H_i \). Here the sum is restricted to eigenstates with \( \epsilon_i(k) \leq 0 \). It has been argued that the monopoles of \( \nabla \times A \) correspond to the Weyl points of the interacting system.

Using the above approach, we have calculated the Berry curvature for different band structure parameters, and a range of values of \( U \). Fig. [5] shows the field lines of \( \nabla \times A \) in the \( k_\parallel = 0 \) plane, for \( U = 2 < U_c \), which illustrates the topological properties of the WSM model in the presence of interactions. In the ordered state, we consider a folded Brillouin zone for calculating the Berry curvature, which is found to vanish. Backfolding due to an ordering vector \( Q \) maps Weyl nodes to regions of the Brillouin Zone with nodes of opposite chirality, where they meet and gap out. We have also verified that the Fermi arcs in this system vanish in the gapped state.

2. Type-II (over-tilted):

Next, we consider the WSM model in the over-tilted type-II regime, i.e. when the tilt parameter \( |w_z| > |v_y| \). As an illustrative example, we discuss our results for the band structure parameters \( v_x = v_y = v_z = 1 \) and \( w_x = 0 \), considering \( U = 2 < U_c \), where the system is still in the semimetallic state. As expected, we obtain the same result for the type-II WSM model in the gapless regime. In this plane, the Weyl nodes are present at the points \((0,0,0), (\pm \pi,0,0), (0,\pm \pi,0)\) and \((\pm \pi, \pm \pi,0)\). The directions of the arrows and the colors (red or blue) indicate the chiralities associated with the different nodes.

At a critical interaction strength \( U_c \), we observe a transition to an SDW order \( M^{(0,0,\pi)} \), with an ordering wavevector \( Q = (\pi,0,0) \) (or, equivalently \( M^{(0,0,\pi)} \) with \( Q = (0,0,\pi) \)) which connects Weyl nodes of opposite chiralities. In the ordered state, backfolding due to the ordering wavevector \( Q \) maps these Weyl nodes to one another, leading to a gapped spectrum, and the Berry curvature vanishes.

Figure 4. The spectral function, obtained from our CDMFT calculations, for the gapless Weyl semimetal phase, as well as the magnetically ordered phase. The panels above and below correspond to the type-I and type-II regime of parameters, respectively. In the upper panel, we present the spectral functions for the band structure parameters \( v_x = v_y = v_z = 1 \) and \( w_x = 0 \), considering \( U = 1 < U_c \), where the system is still gapless, and \( U = 5 > U_c \), where a finite gap has appeared in the spectrum. The lower panel shows the corresponding results for \( w_x = 1.5 \), with the interaction amplitudes \( U = 0.05 < U_c \) and \( U = 3 > U_c \). From Fig. [3][B], we observe that the order parameter \( \langle M^{0.0.\pi} \rangle \) varies very slowly as a function of \( U \) in the over-tilted regime, which may lead to a more gradual appearance of the spectral gap.

Figure 5. The field lines of the Berry curvature \( \nabla \times A \) in the \( k_\parallel = 0 \) plane, for the type-I WSM model with parameters \( v_x = v_y = v_z = 1 \) and \( w_x = 0 \), considering \( U = 2 < U_c \), where the system is still in the semimetallic state. As expected, we obtain the same result for the type-II WSM model in the gapless regime. In this plane, the Weyl nodes are present at the points \((0,0,0), (\pm \pi,0,0), (0,\pm \pi,0)\) and \((\pm \pi, \pm \pi,0)\). The directions of the arrows and the colors (red or blue) indicate the chiralities associated with the different nodes. At a critical interaction strength \( U_c \), we observe a transition to an SDW order \( M^{0.0.\pi} \), with an ordering wavevector \( Q = (\pi,0,0) \) (or, equivalently \( M^{0.0.\pi} \) with \( Q = (0,0,\pi) \)) which connects Weyl nodes of opposite chiralities. In the ordered state, backfolding due to the ordering wavevector \( Q \) maps these Weyl nodes to one another, leading to a gapped spectrum, and the Berry curvature vanishes.

\[ H_i(k) = -G(0,k)^{-1} = H(k) + \Sigma(0,k) \]

where \( H \) is the Bloch Hamiltonian for the noninteracting case, while \( \Sigma(\omega,k) \) is the self-energy matrix. \( H_i \) plays the role of an effective Bloch Hamiltonian for the interacting system, and its eigenstates are used to define the many-body Berry connection, as \( A(k) = -i \sum (nk|\nabla|nk) \), where \( H_i(k)|nk\rangle = \epsilon_i(k)|nk\rangle \), \( \{\epsilon_i(k)\} \) being the band structure of \( H_i \). Here the sum is restricted to eigenstates with \( \epsilon_i(k) \leq 0 \). It has been argued that the monopoles of \( \nabla \times A \) correspond to the Weyl points of the interacting system.

Using the above approach, we have calculated the Berry curvature for different band structure parameters, and a range of values of \( U \). Fig. [5] shows the field lines of \( \nabla \times A \) in the \( k_\parallel = 0 \) plane, for \( U = 2 < U_c \), which illustrates the topological properties of the WSM model in the presence of interactions. In the ordered state, we consider a folded Brillouin zone for calculating the Berry curvature, which is found to vanish. Backfolding due to an ordering vector \( Q \) maps Weyl nodes to regions of the Brillouin Zone with nodes of opposite chirality, where they meet and gap out. We have also verified that the Fermi arcs in this system vanish in the gapped state.
of a type-I WSM. As we decrease the magnitude of $U$, no such jump is observed and the transition appears to be continuous (see Fig. 3(B)).

b. Spectral function: We also show the spectral function obtained in this case for two representative values of $U$, i.e., $U = 0.05 < U_c$ and $U = 3 > U_c$, in the lower panel in Fig. 4. In this case, we find a relatively gradual opening of the spectral gap, as compared to the upper panel with $w_z = 0$, which may be due to a much slower variation in the magnitude of the order parameter $\langle M_z^{(0,0,\pi)} \rangle$ in this case.

To conclude this part of our analysis, our CDMFT solutions for the WSM model in Eq. (2), with interactions, indicate a second-order phase transition to a spin density wave ordered state at a critical interaction strength $U = U_c$. This is accompanied by the appearance of a gap in the spectral function and the vanishing of the Berry curvature associated with the Weyl nodes. For both the type-I and type-II WSM models considered above, we observe an apparent jump in the magnitude of the order parameter for increasing values of $U$, which is absent for decreasing $U$. This could be due to a false minimum in the CDMFT procedure, which is prone to first-order transitions. The SDW order is found to become more robust for larger values of $U$, as indicated by a slow increase in the magnitude of the order parameter for $U > U_c$. In the next section, we confirm the order of the transition using the VCA approach.

B. VCA: Numerical results

We have also used the Variational Cluster Approximation (VCA) method to investigate the effect of local repulsive interactions on the WSM model. As stated earlier, we limit our considerations to spin density wave instabilities, and probe the relevant SDW orders by solving the following Hamiltonian on an 8-site cubic cluster,

$$H' = H'_0 + hM_z^{(0,0,\pi)},$$

where $H'_0$ and $M_z^{(0,0,\pi)}$ are the restriction to the cluster of the kinetic energy operator, and the SDW operator $M_z^{(0,0,\pi)}$ defined in Eq. 5, respectively. The coefficient $h$ is the corresponding Weiss field, which is the only variational parameter used in optimizing the Potthoff functional $\Omega$. We study the evolution of the Potthoff functional $\Omega$, as a function of $h$, for different values of $U$. Initially, for a weakly interacting system, $\Omega$ has a single minimum at $h = 0$, indicating the absence of the corresponding SDW order. At a critical value $U = U_c$, it develops a new minimum at a finite value of $h$ (with a maximum at $h = 0$), indicating a continuous transition to the corresponding magnetically ordered state. Likewise, we find competing minima in the functional for the SDW orders $M_z^{(\pi,0,0)}$ and $M_z^{(\pi,\pi,\pi)}$ and select the solution with the lowest value of $\Omega$ at the stationary point. We then calculate various physical properties of the model, and in particular, the order parameter $\langle M_z^{(0,0,\pi)} \rangle$ as a function of $U$, which goes to zero at the critical value $U = U_c$, as illustrated in Fig. 4(B). The magnitude of $\langle M_z^{(0,0,\pi)} \rangle$ increases slowly as a function of $U$, and is found to be sensitive to the band structure parameters.

2. Type-II (over-tilted):

Here, we discuss our VCA results for the WSM model parameters $v_x = v_y = v_z = 1$ and $w_z = 1.5$. We find that the Potthoff functional $\Omega$ once again develops a minimum at a nonzero value, with a maximum at $h = 0$ for a critical interaction strength $U_c \sim 0.7$ (see Fig. 5(C)), which is significantly lower than the one obtained for the type-I regime. The solution corresponding to the stationary point of $\Omega$ is used to calculate the order parameter $\langle M_z^{(0,0,\pi)} \rangle$ as a function of $U$ (see Fig. 5(D)). Overall, the behavior of the system in this regime is found to be qualitatively similar to that of the type-I WSM model, though evidently more sensitive to interaction effects. This is consistent with the CDMFT results obtained for this model.

In Fig. 7 we use our VCA results for different sets of band structure parameters to plot the magnitude of the order parameter $\langle M_z^{(0,0,\pi)} \rangle$ as a function of $U$, for different values of $w_z$. As the tilt $w_z$ is increased, the critical interaction strength $U_c$ decreases. In particular, we find a significant change in the value of $U_c$ when $|w_z| > 1 = |v_z|$. Fig. 8 shows the interaction-induced phase diagram for the WSM model defined in Eq. (2), as a function of the parameter $w_z$, for $v_x = v_y = v_z = 1$. The value of the tilt parameter $w_z$ at which the system undergoes a transition from the type-I to the type-II regime (dictated by a singularity in derivative of the critical interaction $U_c$) is also found to be slightly renormalized in the presence of interactions, as indicated by the dashed red line in Fig. 8. In general, for a nontrivial tilt term, the position in the phase diagram where the order appears is highly sensitive to the magnitude of the tilt, and the nature of the magnetic order may depend on its direction.

To conclude this part, we find from our VCA analysis that the WSM model defined by us in Sec. II shows a continuous transition to an SDW ordered state at a critical value of the interaction strength $U_c$, and this order becomes more robust for increasing values of $U$. The position in the phase diagram where the order appears depends on the band structure parameters, and is found to be particularly sensitive to the value of the tilt parameter $w_z$. While $M_z^{(0,0,\pi)}$ is found to be the dominant SDW order in most the cases we consider, in general one could also have competing orders such as $M_z^{(\pi,0,0)}$ or $M_z^{(\pi,\pi,\pi)}$, depending on the model parameters and the orientation of the tilt.

IV. CONCLUSIONS

In summary, we have studied the effect of a local repulsive interaction $U$ on an inversion-symmetry breaking Weyl semimetal (WSM) model using the Cluster Dynamical Mean
Field Theory (CDMFT) and Variational Cluster Approximation (VCA) methods. We examine the evolution of the system as a function of the interaction strength $U$, taking into account the effect of a nonzero tilt parameter $w_z$. We find that the system undergoes a second-order transition at a critical value of the interaction $U = U_c$, to a spin density wave (SDW) ordered state, with an ordering wavevector $Q = (0, 0, \pi)$ and magnetization in the $z$-direction. For the untilted dispersion, this is equivalent to the corresponding state with a wavevector $Q = (\pi, 0, 0)$ and magnetization in the $x$-direction. These wavevectors connect Weyl...
nodes of opposite chiralities, and such instabilities are favored by the nesting between these points in the band structure. This result makes sense from a physical point of view, since the Weyl nodes are pinned to high-symmetry points in our model, preventing the movement of nodes of opposite chiralities towards each other. The phase transition is accompanied by the gradual appearance of a gap in the spectrum. The Berry flux associated with the Weyl nodes is also found to disappear in the ordered state due to the backfolding of the Weyl nodes with opposite chiralities onto each other.

In the type-II or over-tilted regime, the corresponding phase transition occurs at a significantly lower value of $U_c$, indicating that the WSM phase is more susceptible to interactions in this case. The nature of the transition as well as the magnetic order is confirmed by the results of our VCA calculations. We then obtain the ground-state phase diagram for the WSM model, as a function of the tilt parameter $w_c$, and find that the critical value of the tilt at which the system undergoes a transition from the type-I to the type-II WSM phase is renormalized in the presence of interactions. Spin-density-wave instabilities have also appeared in previous studies on type-I and type-II WSM models, using different methods, and a prominent example, similar in spirit to our work, is Ref. 44, where the Quantum Cluster Methods used in this analysis have the advantage of being nonperturbative and are especially useful in the strongly interacting limit, they only take into account short-range correlations, and may therefore overemphasize the order.

Our treatment may easily be generalized to more complicated Weyl semimetals, such as for multi-Weyl systems with quadratic tilt terms, and such problems will be addressed in future studies.

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Figure 9. The arrangement of the 4-site clusters employed for our CDMFT calculations, with superlattice vectors that can accommodate the SDW orders considered by us, i.e. (a) $M_z^{(0,0,π)}$ with wave vector $Q = (0,0,π)$ and (b) $M_z^{(π,π,π)}$ with wave vector $Q = (π,π,π)$. Here, we consider a cluster of side $α$, where $α$ is the lattice constant and the superlattice vectors are $(1,1,0)$, $(0,2,0)$ and $(0,0,2)$, with distances measured in units of $α$.

Figure 10. The 8-site cubic cluster employed by us for our VCA computations with an illustration of the competing solutions for SDW orders, i.e. (a) $M_z^{(0,0,π)}$ with wavevector $Q = (0,0,π)$ and (b) $M_z^{(π,π,π)}$ with wavevector $Q = (π,π,π)$. Here, we consider a cluster of side $α$, where $α$ is the lattice constant, and the superlattice vectors are $(2,0,0)$, $(0,2,0)$ and $(0,0,2)$, with distances measured in units of $α$.

APPENDIX A: EFFECTIVE HAMILTONIAN AT LARGE $U$

We use the strong-coupling expansion method to obtain the effective spin Hamiltonian for our model in the large-$U$ limit. For $w_z = 0$, the effective Hamiltonian is given by

$$H_{\text{eff}} = J_z \sum_{\langle ij \rangle_z} (S_i^z S_j^z - S_i^+ S_j^-) + J_x \sum_{\langle ij \rangle_x} (-S_i^+ S_j^+ + S_i^- S_j^- - S_i^x S_j^y) + J_y \sum_{\langle ij \rangle_y} (-S_i^y S_j^y - S_i^+ S_j^- + S_i^x S_j^x),$$

where $J_x = J_y = \frac{4v^2}{u}$, $J_z = \frac{4v^2}{u}$ and $J_y = \frac{4v^2}{u}$ in terms of our WSM model parameters. For $J_z \gg J_x$, a ferromagnetic order along $z$ is favored with spins in the $xy$ plane, with an antiferromagnetic order along $(π,0,0)$, as a correction, if $S$ is along $x$. The same behavior would be observed in the other two directions if we have $J_z \gg J_x$, for instance, so the ratios $J_x^z$ or $J_x^y$ do not have a qualitative effect on the behavior of the above Hamiltonian. This is consistent with the equivalence that we observe, for $w_z = 0$, between the SDW order $M_z^{(0,0,π)}$ (with wavevector $(0,0,π)$ and magnetization in the $z$ direction) and $M_z^{(π,π,π)}$ (with wavevector $(π,π,π)$ and magnetization in the $x$-direction). However, we find no such equivalence to be present in either the noninteracting or the large-$U$ limit, when $w_z \neq 0$. 