Integer and fractional quantum hall effects in lattice magnets

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Chapter 10

Introduction to triplet states: spin-density waves

10.1 General considerations

The purpose of the present section is to provide more insight into triplet particle-hole condensates, i.e. density wave states which break spin rotation symmetry. Up until this point spin triplet states have been mentioned only occasionally and briefly, such as QSH effects obtained from QAH effects (see for instance section 9.3.1), or uniaxial spin density waves obtained from charge order (see section 9.4.1). All of these examples have in common that they constitute the simplest class of spin triplet states, more or less trivially obtained from spinless states. Indeed, in essence they can be thought of as two copies of spinless states, one for each spin species, but with opposite sign for the two species. To put this more succinctly, they are obtained from the singlet states by replacing all $\delta_{\sigma\sigma'}$ with $\sigma^3_{\sigma\sigma'}$.

In quite a number of cases, such as the QSH effects, these triplet states are degenerate with the singlet states on a mean field level, precisely because the former comprise two copies of the latter. A notable exception are the uniaxial spin density waves of section 9.4.1, where the relative sign difference of the two copies is reflected in a different energy spectrum for the two species. Spinful condensates proportional to σ^3 break spin rotation symmetry partially, and for this reason are certainly proper triplet states. However, the unbroken generator of spin rotations σ^3 signals that they far from exhaust the possible triplet condensates. Therefore, we take a closer look at spin triplet states in this section. We stress that we have no intention of being complete, but merely wish to present some of the general aspects of spinful condensates which go beyond the partial breaking of spin rotation reflected in the exchange $\delta_{\sigma\sigma'} \leftrightarrow \sigma^3_{\sigma\sigma'}$. We will do so with the help of selected lattices and example condensates. We will restrict ourselves to lattices with hexagonal symmetry and focus exclusively on ordering at the M-points. This will serve the purpose of demonstrating the most salient features characteristic of nontrivial triplet states. Specifically, the focus will be on two main concepts connected to the full breaking of spin rotation symmetry. The first is the possibility to dress lattice symmetries which are broken in the condensed state with a unitary global spin rotation, restoring them as symmetries. The second is the existance of time-reversal invariant spin-bond density waves, which will be introduced as a novel class of candidate interaction-induced topological insulators as well as topological semimetals. Both of these concepts will be shown to illustrate how the symmetry structure of spin density waves can be lifted from the spinless (spin rotation invariant) density waves.

In section 9.2.2 the foundations for a spinful mean field theory were presented, providing a possible context for the emergence of spinful density waves from electronic correlations in the same way as for spinless (or spin rotation invariant) case. Indeed, the triplet condensates may be taken as candidate ground states for mean field treatments, or considered variational states in the context of other approaches. In this section we repeatedly seek to establish a connection between a systematic development of spin rotation symmetry broken density waves and results from recent literature, which has reported a number of such density waves as dominant electronic instabilities or mean field ground states.

When it comes to lattice symmetries in two dimensions, the symmetry groups D_n and C_{nv} are distinct in the presence of spin degrees of freedom. In section 9.1.1 we have mentioned this distinction briefly and referred to the Appendix for details. As the differences do not significantly alter the observations and conclusions to come, we do the same here and content ourselves with focusing on the main features of lattice symmetries in the presence of spin, which are shared between the groups D_n and C_{nv}. Lattice symmetries act in spin space as a unitary $SU(2)$ matrix associated to the $SO(3)$ element acting on spatial coordinates. In addition, time-reversal symmetry now takes the form $\mathcal{T} = e^{i\pi\sigma^2/2}\mathcal{K}$, which has important the property $\mathcal{T}^2 = -1$. Triplet condensates therefore necessarily break time-reversal invariance, as all the three Pauli matrices σ^i are odd under time-reversal. Notice however that in case of the uniaxial density waves, i.e. $\sim \sigma^3$, applying a global spin rotation after time-reversal (a rotation of π around for instance the x axis) brings the state back to itself. Hence, the time-reversed mean field Hamiltonian is unitarily equivalent to itself, effectively restoring time-reversal symmetry.

This brings us to the broader principle of spin rotation equivalence, which we take some time to introduce here before zooming in on specific lattices and particular states. For any spinful condensate a global spin rotation cannot change the spectrum or the free energy as the interacting Hamiltonian is $SU(2)$ invariant. For the mean field Hamiltonian this means that a global spin rotation yields a unitarily equivalent Hamiltonian which necessarily has the same spectrum. When considering lattice symmetries such as rotation, reflection and translation, global spin rotation equivalence comes into play in an important and consequential way. There are spinful density waves which have the property that the application of a lattice operation can be compensated by a global spin rotation. To put it in a different way, application of a lattice operation may result in a physical state which is related to the initial state by a global spin rotation. Let us make this statement more specific and tangible. We are going to study condensates of hexagonal lattices with M-point ordering only, and we therefore recall that the real space M-point modulation functions have been defined as $\vec{\zeta}\cdot\vec{\xi}(\vec{x})$ and fully specify a given type of M-point order. A general spinful ordering needs three of these functions, one for each spin direction. Instead of a vector $\vec{\zeta}$ it therefore makes sense to use a matrix $\mathcal{M} = \mathcal{M}_{i\mu}$ to encode the degrees of freedom for spinful M-point order, where $i = 1, 2, 3$ corresponding to σ^i, i.e.

$$\sigma^i \mathcal{M}_{i\mu} \xi_\mu(\vec{x}), \tag{10.1}$$

which can alternatively and more concisely written as $\vec{\sigma}\cdot\vec{\mathcal{M}}(\vec{x}) = \vec{\sigma}\cdot\vec{\mathcal{M}}_\mu \xi_\mu(\vec{x})$. Lattice symmetries can be represented by their action on $\vec{\xi}$. For instance, we have seen that $X\vec{\xi}(C_3\vec{x}) = \vec{\xi}(\vec{x})$ and $G_1\vec{\xi}(\vec{x}+\vec{x}_1) = \vec{\xi}(\vec{x})$. In particular translational symmetry was always broken for M-point modulations. To see how global spin rotations can come to the rescue, let us take such a translation, i.e. $T(\vec{x}_1)$, as an example. The effect of the translation on the spin order is

$$\vec{\sigma}\cdot\vec{\mathcal{M}}(\vec{x}+\vec{x}_1) = \sigma^i \mathcal{M}_{i\mu}[G_1]_{\mu\nu}\xi_\nu(\vec{x}). \tag{10.2}$$

We would like this to be equal to a global spin rotation $\mathcal{R}$ (depending on G_1) of the form

$$\vec{\sigma}\cdot\mathcal{R}\vec{\mathcal{M}}(\vec{x}). \tag{10.3}$$

Therefore, the translation $T(\vec{x}_1)$ can be compensated by a global spin rotation if and only if the following relation is satisfied

$$\sigma^i \mathcal{M}_{i\mu}[G_1]_{\mu\nu}\xi_\nu(\vec{x}) = \sigma^i \mathcal{R}_{ij}\mathcal{M}_{j\mu}\xi_\mu(\vec{x}). \tag{10.4}$$

This relation expresses the condition that the action on $\vec{\xi}$ can be carried over to $\vec{\mathcal{M}}$ and therefore to $\vec{\sigma}$. In other words, the translation can be compensated by a global rotation if G_1 acting on $\mathcal{M}$ from the right is identical to some $O(3)$ matrix $\widetilde{G}_1$ acting on $\mathcal{M}$ from the left, i.e. on its spin indices. Suppose for instance we have $\mathcal{M}_{11} = \mathcal{M}_{22} = \mathcal{M}_{33} = 1$ and all other elements zero. Then $\mathcal{M}$ is simply the identity and G_1 commutes with it so that $\mathcal{R} = G_1$. The translation can be compensated by a rotation of π around the z-axis, as this is the interpretation of G_1 as an element of $O(3)$. This follows from the fact that a general $O(3)$ matrix $\mathcal{R}$ acting on $\mathcal{M}$ gives $\vec{\sigma} \cdot \mathcal{R}\vec{\mathcal{M}}(\vec{x})$, and we can associate an $SU(2)$ matrix U with $\mathcal{R}$ such that

$$\vec{\sigma} \cdot \vec{\mathcal{M}} = U^{\dagger}\vec{\sigma} \cdot (\mathcal{R}\vec{\mathcal{M}})U. \tag{10.5}$$

In contrast, had we chosen instead $\mathcal{M}_{31} = \mathcal{M}_{32} = \mathcal{M}_{33} = 1$ and all other elements zero, the condition of equation (10.4) cannot be fulfilled and translational symmetry is manifestly broken. The physical significance of these two seemingly arbitrary choices for $\mathcal{M}$ will be clarified below when discussing the triangular lattice.

The concept of global spin rotation equivalence and its connection to lattice symmetries has appeared before in the context of classical spin models [208]. There it was employed to derive classical spin states which are invariant under all lattice operations, modulo a global spin rotation. Since translations are a subset of the lattice operations, these "classical spin liquids" must necessarily have a uniform spin length at every site. In the present case, where we study electronic density wave states, we find these fully symmetric spin density waves as a subset of a larger class of spinful density waves, which also includes spin-bond density waves and translational symmetry broken spin density waves, the uniaxial spin density waves being an example of the latter.

A key difference between the classical spin liquids of [208], i.e. classical spin states invariant under all lattice operations up to an $O(3)$ rotation, and electronic spinful density waves is the treatment of improper global rotations needed to promote lattice operations to symmetries. Elements of $O(3)$ are divided into two groups, the proper and improper rotations, which are distinguished by their determinant, i.e. $\mathrm{Det}\,[\mathcal{R}] = \pm 1$. Improper elements can always be written as the product of a proper rotation $\mathcal{R}' \in SO(3)$ and the inversion operations, $\mathcal{R} = -\mathcal{R}'$. The relevance if this distinction follows from the need to associate an $SU(2)$ matrix U with $\mathcal{R}$, which is only possible for proper $\mathcal{R}$. In particular this means that if $\mathcal{R}$ is improper, the state is odd under the operations corresponding to $\mathcal{R}$, i.e.

$$\vec{\sigma} \cdot (\mathcal{R}\vec{\mathcal{M}}) \to -\vec{\sigma} \cdot (\mathcal{R}'\vec{\mathcal{M}}) = -U\vec{\sigma} \cdot \vec{\mathcal{M}}U^{\dagger}, \tag{10.6}$$

where the matrix U is the $SU(2)$ equivalent of $\mathcal{R}'$. In case of hexagonal lattice M-point we already observed in Section 9.4.1 that an $O(3)$ representation of the group of lattice symmetries is generated by their action on $\vec{\xi}(\vec{x})$. The generators of this representation are G_i, X, X^T and Y. Equation (10.4) states that it is these generators which determine $\mathcal{R}$. Only the element Y is improper, implying that all reflections are associated with an improper rotation. Below we will illustrate in specific cases how this affects the electronic symmetries of given density waves.

10.2 Triangular lattice triplet states

Spin density waves in hexagonal lattice systems modulated by the M-piont vectors are currently attracting much attention, with the triangular lattice being one of the most prominent represenatives of lattices with hexagonal symmetry. One of the first examples of such a novel spin density wave state, proposed in the context of preformed classical local moments coupled to electrons, has been a noncoplanar chiral spin state [30]. It was shown in [30] that this state can also be thought of as a proper density wave spontaneously formed by onsite Hubbard-like interactions, in the same spirit which is at the heart of the present framework. The chiral spin density wave gaps out the electronic spectrum and leads to a Quantum Anomalous Hall ground state. In later works, the problem of spin density wave physics was revisited in a broader setting, pertaining to more general lattices with hexagonal lattices with hexagonal symmetry [160], but taking the honeycomb lattice as an example. Already briefly mentioned in section 9.4.1, the main result of this work and subsequent studies [162, 163] was the prediction of a thermal phase transition to a uniaxial translational symmetry broken spin density wave. In all of the hexagonal lattices we consider in this work, both types of spin density wave states, the uniaxial and the chiral density waves, fit into the scheme of lifting particle-hole triplet condensates with specific symmetry from the corresponding spinless site ordered states. More specifically, they can be understood by consering a single root state, the A_1 symmetric site ordered state for each of the lattices. This is most easily demonstrated for the case of the triangular lattice.

10.2.1 Spin density wave states

The A_1 symmetric site ordered state was given in equation (9.234). There are two rather straightforward ways to take this as a root state and make it spinful. One is obvious: just create two copies for both spin species and give them a relative minus sign. This yields

$$\langle \hat{\psi}^\dagger_\sigma(\vec{k}+\vec{Q}_\mu)\hat{\psi}_{\sigma'}(\vec{k})\rangle = \frac{1}{\sqrt{3}}\Delta_{\text{uniax}}\ \sigma^3_{\sigma\sigma'}, \tag{10.7}$$

and it exactly corresponds to the uniaxial spin density wave. It represents a manifestly translational symmetry broken state, preserving however C_{6v} (or alternatively D_6) symmetry, up to global rotation. In real space we can denote it as

$$\sigma^3 \mathcal{M}_{3\mu} \xi_\mu(\vec{x}), \quad \mathcal{M}_{31} = \mathcal{M}_{32} = \mathcal{M}_{33} = 1. \tag{10.8}$$

Following equation (10.4) we have already discussed this possibility as a case where translations cannot be saved by global spin rotations. This is different for the second way of incorporatig the spin degree of freedom, which is

$$\langle \hat{\psi}^\dagger_\sigma(\vec{k} + \vec{Q}_\mu) \hat{\psi}_{\sigma'}(\vec{k}) \rangle = \frac{1}{\sqrt{3}} \Delta_{\text{chiral}} \, \sigma^\mu_{\sigma\sigma'}. \tag{10.9}$$

Each of the order parameter components $\vec{Q}_\mu$ is associated with a different spin Pauli matrix, and in real space this can be represented as

$$\sigma^i \mathcal{M}_{i\mu} \xi_\mu(\vec{x}), \quad \mathcal{M} = I, \tag{10.10}$$

where I is the unit matrix. Now translations can be compensated by global spin rotations and the point group operations must be combined with global spin rotations as well to leave the spin density wave invariant. In particular, the effect of reflections on $\vec{\xi}$ always contains the element Y, which we have mentioned to be an improper element of $O(3)$. Indeed, $-Y$ is a rotation of π around the z-axis, followed by a rotation of $-\pi/2$ around the y-axis. Hence, the chiral spin density wave state is odd under all reflections, indeed a necessary condition to host a QAH effect which is a property well-established for this particular spin density wave [30] and its generalizations to other hexagonal lattices [40, 209, 210].

10.2.2 Spin-flux ordered states

As a second class of spinful condensates on the triangular lattice, we now focus on a particularly interesting combination of spin and flux ordered states. Spin density waves break time-reversal symmetry and so does flux order. Above we have seen that the chiral spin density waveof equation (10.9) causes a spectral gap and leads to a QAH effect. The same is true for the flux ordered state contained in the decomposition (9.232) and explicitly defined in equation (9.239). This motivates the question whether symmetric combinations of spin and flux order exist, which are possibly energetically favorable and host nontrivial physical effects. Since both constituents of such spinful flux ordered states, i.e. the spin part and the flux part, are time-reversal odd, the combination of the two should be time-reversal symmetric. Even more strikingly, not only are such states be time-reversal invariant, lattice symmetries such as reflections and translations which are broken by the constituent orders may be resurrected, as global spin rotations can be employed to bring the mean field Hamiltonian back to itself. We will now demonstrate this using two examples on the triangular lattice, which however easily generalize to other well-known hexagonal lattices, i.e. the honeycomb and kagome lattices.

In case the triangular lattice we have derived a flux ordered state transforming as A_1 and given in equation (9.239). Translational symmetry is manifestly broken in this state. To see how appropriate spinful versions of this state can be constructed which recover (part of) the broken lattice symmetries, it is most convenient to adopt the real space perspective [see also equation (9.238)]. This requires three matrices $\mathcal{M}_i$, one for each bond direction, in the same way as three $\vec{\zeta}_j$ are required for any bond order including flux order. Following equation (9.238) it was shown that flux order is specified by $\vec{\zeta}_1 = \vec{\zeta}$, $\vec{\zeta}_2 = X\vec{\zeta}$ and $\vec{\zeta}_3 = X^T\vec{\zeta}$ with $\vec{\zeta} = [1, -1, 0]^T$. Spin-bond ordered states are then generically specified by

$$\sigma^i [\mathcal{M}_j]_{i\mu} \xi_\mu(\vec{x}), \tag{10.11}$$

and here we construct them explicitly by embedding the $\vec{\zeta}_j$ in the matrices $\mathcal{M}_j$. One such embedding yields a highly symmetric electronic state and it is obtained by putting the $\vec{\zeta}_j$ on the diagonal of the corresponding $\mathcal{M}_j$, with all off-diagonal elements zero. As both the $\mathcal{M}_j$ matrices and the G_j matrices representating the translations only have diagonal elements, they commute, having the consequence that translations can be compensated by global proper spin rotations. Mathematically this embedding can be concisely written as

$$[\mathcal{M}_j]_{i\mu} = \zeta_j^\mu \delta_{i\mu}. \tag{10.12}$$

The flux ordered state of equations (9.238) and (9.239) is odd under all reflections. In the presence of spin structure global spin rotations can recover these symmetries. Taking the reflection σ_v as an example, we have that

$$\vec{\sigma} \cdot \mathcal{M}_j \cdot \vec{\xi}(\vec{x}) \to \vec{\sigma} \cdot \mathcal{M}_j \cdot Y \vec{\xi}(\vec{x}), \tag{10.13}$$

where it is important to note that the reflection exchanges $j = 1$ and $j = 2$ and maps $j = 3$ to itself. We then find that $\mathcal{M}_3 Y = -Y\mathcal{M}_3$ and $\mathcal{M}_1 Y = -Y\mathcal{M}_2$, which proves that the proper rotation $-Y$ compensates for the reflection, reinstitating it as a symmetry. Hence, the only symmetry broken by this particular density wave state is spin-rotation symmetry.

A second natural embedding of the $\vec{\zeta}_j$ is to associate each of the $\vec{\zeta}_j$ with a different direction in spin space, i.e. to choose a different spin projection for each bond direction $\vec{x}_j$. This can be concisely captured by the expression

$$[\mathcal{M}_j]_{i\mu} = \zeta_j^\mu \delta_{ij}, \tag{10.14}$$

where δ_{ij} associates the spin label i with the bond label j. This however has the consequence that the matrices $\mathcal{M}_j$ are not diagonal, which precludes the recovery of translational invariance. Even though translational invariance is now manifestly broken, we can recover the reflections as $\mathcal{M}_3 Y = -Y\mathcal{M}_3$ and $\mathcal{M}_1 Y = -Y\mathcal{M}_2$ still holds. We conclude that this embedding yields a spin-rotation symmetry and translational symmetry broken state, which preserves the C_{6v} (or D_6) operations.

The real space perspective is perhaps the most convenient in highlighting the symmetry properties. Transforming to momentum space gives the condensate functions given by

$$\langle \hat{\psi}^\dagger_\sigma(\vec{k}+\vec{Q}_\mu)\hat{\psi}_{\sigma'}(\vec{k})\rangle = i\Delta_{\text{Dirac}}\zeta^\mu_j \cos k_j \; \sigma^\mu_{\sigma\sigma'}, \tag{10.15}$$

(no summation over μ on the right hand side) in case of the first embedding, and

$$\langle \hat{\psi}^\dagger_\sigma(\vec{k}+\vec{Q}_\mu)\hat{\psi}_{\sigma'}(\vec{k})\rangle = i\Delta_{\text{QSH}}\sum_j \zeta^\mu_j \cos k_j \; \sigma^j_{\sigma\sigma'}, \tag{10.16}$$

in case of the second embedding. The spectral properties of the mean field Hamiltonian corresponding to these spin-flux (or spin-bond) ordered states turn out to be rather intriguing. We now discuss them in more detail, which will explain the labeling Δ_{Dirac} and Δ_{QSH}. We start with the highly symmetric state given in equation 10.15.

The mean field spectrum of the highly symmetric state given in equation (10.15) is presented in Fig. 10.4. We observe that the spectrum consists of four bands, which is a consequence of a combined time-reversal symmetry and inversion symmetry, mandating a two-fold degeneracy for each energy level at every $\vec{k}$. The high symmetry of this state leads to additional spectral degeneracies, the most notable being the four-fold degeneracy at all the M' points. The nested Fermi surface at filling $n = 3/4$ is gapped out except for these isolated remaining degeneracies at the M' points, which we soon show follows from the fact that all lattice symmetries are essentially preserved. In that sense, the remaining degeneracies are very similar to the isolated degeneracies of the staggered flux order on the square lattice [see equation (9.100) and Section 9.3.2]. In the latter case, degeneracies at isolated points in the reduced Brillouin zone define Dirac nodes, i.e. in the vicinity of these points the dispersion is linear. The same is true in the present case. At each of the three M' points of the low-energy excitations are described a pair of Dirac nodes transforming into each other under the time-reversal operation, which is the reason we have denoted the state as Δ_{Dirac}. The square lattice staggered flux state breaks some lattice symmetries, in addition to time-reversal symmetry, but preserves spin rotation symmetry. The present spin-flux ordered state does not break any lattice symmetries and preserves time-reversal, but it breaks spin rotation symmetry. Furthermore, the low-energy theory of the staggered flux state consists of two Dirac nodes instead of

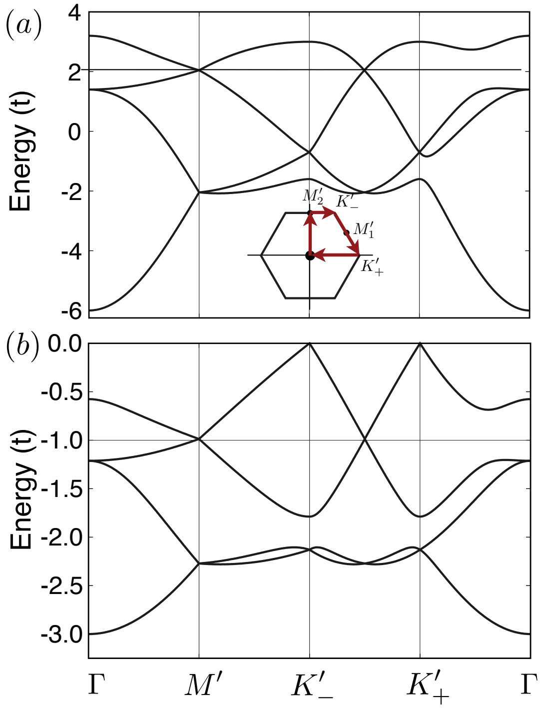

Figure 10.1: (a) Energy bands of the triangular lattice in the presence of the triplet density wave state given in equation (10.15). At the $\vec{M}'$ points in the reduced Brillouin zone the red circles point to the Dirac nodes. (b) Mean field spectrum of the equivalent state on the honeycomb lattice.

six (two for each of the three M' points). In that respect, the spin-flux ordered state is reminiscent of the three dimensional spin-orbit coupled diamond lattice model [3], which at half filling gives rise to a low-energy $3D$ Dirac theory at three inquivalent points in the $3D$ Brillouin zone. We come back to this reminiscence below.

We first show explicitly that the Dirac nodes at the $\vec{M}'$ points are protected by the symmetries which leave them invariant. Crucially, this includes the translations combined with global spin rotations and we use the relation between lattice operations and spin rotations establsihed in Appendix C.3. For the sake of definiteness we choose $\vec{M}'_2$ to demonstrate the degeneracy. The basis state at the $\vec{M}'_2$ point takes the form

$$\hat{\Phi}_{\vec{M}'} = \begin{bmatrix} \hat{\psi}_\sigma(\vec{M}'_2) \\ \hat{\psi}_\sigma(\vec{M}'_2 + \vec{Q}_1) \\ \hat{\psi}_\sigma(\vec{M}'_2 + \vec{Q}_2) \\ \hat{\psi}_\sigma(\vec{M}'_3 + \vec{Q}_3) \end{bmatrix}, \tag{10.17}$$

where σ labels the spin degree of freedom. In order to analyse the effect of lattice symmetries we choose a set of Pauli matrices σ^i to act on the spin degree of freedom, a set of matrices τ^i to act within the blocks $(\vec{M}'_2, \vec{M}'_2+\vec{Q}_1)$ and $(\vec{M}'_2+\vec{Q}_2, \vec{M}'_2+\vec{Q}_3)$, and a set matrices ν^i to act on the block degree of freedom. It turn out to be convenient to start with the inversion C_2, which has the effect

$$C_2 \quad \rightarrow \quad \begin{bmatrix} \hat{\psi}_\sigma(-\vec{M}'_2) \\ \hat{\psi}_\sigma(-\vec{M}'_2 + \vec{Q}_1) \\ \hat{\psi}_\sigma(-\vec{M}'_2 + \vec{Q}_2) \\ \hat{\psi}_\sigma(-\vec{M}'_3 + \vec{Q}_3) \end{bmatrix} = \nu^1 \hat{\Phi}_{\vec{M}'}. \tag{10.18}$$

From this we conclude that the Hamiltonian at $\vec{M}'_2$ can only have terms $\sigma^i\tau^j$ or $\sigma^i\tau^j\nu^1$, where it is understood that $i, j = 0, 1, 2, 3$. The translation $T(\vec{x}_2)$ is associated with G_2 and can be compensated by a rotation around the x-axis by π, which gives

$$T(\vec{x}_2) \quad \rightarrow \quad -i\sigma^1\nu^3\hat{\Phi}_{\vec{M}'}. \tag{10.19}$$

This leaves us with allowed terms τ^j, $\sigma^1\tau^j$, $\sigma^2\tau^j\nu^1$ and $\sigma^3\tau^j\nu^1$. The translation $T(\vec{x}_3)$ is associated with G_3 and a rotation by π around the y-axis will make it a symmetry. The action on the basis state is

$$T(\vec{x}_3) \quad \rightarrow \quad -i\sigma^2\tau^3\hat{\Phi}_{\vec{M}'}, \tag{10.20}$$

which leaves us with the following allowed terms

$$\tau^3,\ \sigma^1\tau^1,\ \sigma^1\tau^2,\ \sigma^2\nu^1,\ \sigma^2\tau^3\nu^1,\\ \sigma^3\tau^1\nu^1,\ \sigma^3\tau^2\nu^1. \tag{10.21}$$

What is left to consider is the two reflections which leave $\vec{M}'_2$ invariant. We consider $C_2\sigma_v$, which leads to

$$C_2\sigma_v \quad \rightarrow \quad -ie^{i\pi\sigma^2/4}\sigma^3 \begin{bmatrix} 1 & & & \\ & & & 1 \\ & & 1 & \\ & 1 & & \end{bmatrix} \hat{\Phi}_{\vec{M}'}. \tag{10.22}$$

The spin rotation $-ie^{i\pi\sigma^2/4}\sigma^3$ is the global spin rotation necessary to compensate Y. This transformation leads to the immediate exclusion of the terms $\sigma^2\tau^3\nu^1$ and $\sigma^2\nu^1$. The term τ^3 is clearly left invariant. The other four terms must be combined in order to represent invariant terms, and the final terms which are allowed by symmetry are

$$\tau^3,\ \tau^1(\sigma^1 - \sigma^3\nu^1),\ \tau^2(\sigma^1 - \sigma^3\nu^1). \tag{10.23}$$

Subjecting them to a basis transformation $e^{-i\pi\sigma^1\nu^1/4}e^{i\pi\sigma^3/8}$ brings them into a very simple form, and we obtain $\sigma^1\tau^1$, $\sigma^1\tau^2$ and τ^3. These three matrices anti-commute between each other and this leads to the conclusion that the most general symmetry allowed Hamiltonian at the $\vec{M}'$-points, $\mathcal{H} = m_1\sigma^1\tau^1 + m_2\sigma^1\tau^2 + m_3\tau^3$, has two eigenvalues $\pm\sqrt{m_1^2 + m_2^2 + m_3^2}$, with each eigenvalue being fourfould degenerate.

This proves that the fourfold degeneracy at the $\vec{M}'$ points is in fact symmetry protected. As we have already shown in quite a number of cases before, such as the square lattice π-flux state in Section 9.3.2, one can take the low-energy Dirac description of this spin-flux state as a starting point for studying the effect of additional symmetry breaking. We recall that in case of the square lattice π-flux state all lattice symmetries were left unbroken, because a gauge transformation could be employed to bring the Hamiltonian back to itself. In the present case a global spin rotation acts as the unitary operation bringing the Hamiltonian back to itself, and in the same way as was presented in Section 9.3.2 we can list the effect of lattice symmetry breaking in terms of the Dirac language. A key aspect of the lattice symmetric spin-flux state is the need to be careful to account for the spin rotation symmetry breaking and the nontrivial spin structure of the Dirac spinors. We leave such a detailed account of the low-energy Dirac theory following from the spin-fux state for future study.

Let us now come to the second spin-flux state given in equation (10.16) and in equation (10.14). We had already observed that translational symmetry is broken

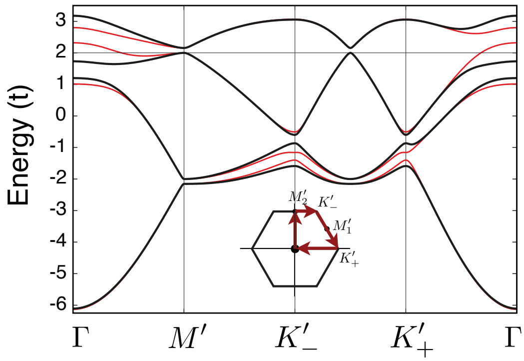

Figure 10.2: Energy bands of the triangular lattice in the presence of the triplet density wave state given in equation (10.16). The black (red) spectrum corresponds to the density wave strength $\Delta_{\text{QSH}} = -0.4$ ($\Delta_{\text{QSH}} = 0.4$). An energy gap emerges in case of $\Delta_{\text{QSH}} < 0$ at the $\vec{M}'$ points in the reduced Brillouin zone and an evaluation of the inversion eigenvalues (C_2 eigenvalues) at these $\vec{M}'$ shows that the insulating ground state is a QSH state. Note that all bands are doubly degenerate due to the presence of both time-reversal and inversion symmetry. Inset shows the path through the reduced BZ.

in this state and we therefore do not a priori expect any degeneracies at the M'-points other than the ones required by the presence of both time-reversal and inversion symmetry. The mean field energy bands are presented in Fig. 10.2, where we show two different spectra corresponding to positive and negative sign of the density wave strength. The spectra show that indeed no additional degeneracies exist and in case of $\Delta_{\text{QSH}} < 0$ a full energy gap is emerges, which is however second order in the density wave strength. For the resulting insulating state we can calculate the $\mathbb{Z}_2$ topological invariant written in equation (9.42) and we find that this state is a non-trivial QSH state.

This shows that embedding flux order in a spinful setting can lead to two distinct time-reversal invariant topological states of matter: a $2D$ symmetry protected Weyl semimetal and an insulating QSH state. Both of these spinful density waves preserve all point group symmetries, but they differ with respect to translations. The $2D$ Weyl semimetal preserves all translations, which is the origin of its symmetry protection.

10.3 Honeycomb lattice

In order to inspire confidence in the general applicability of the results on M-point ordered triplet density waves in systems with hexagonal symmetry, which we have presented with the help of the triangular lattice above, we briefly show how these results carry over to the honeycomb lattice. Specifically, we will discuss the honeycomb lattice realizations of the uniaxial and chiral spin density waves, as they have generated considerable interest recently [40, 160, 162, 163]. In addition, we show explicitly that the fully symmetric spin-flux ordered state exists on the honeycomb lattice as well and has the same key properties as on the triangular lattice.

In the same way as for the triangular lattice, the starting point for the spin density waves are the expressions for the site ordered states derived in Section 9.4.1. Site ordered states transforming as irreducible representations of the lattice symmetry group were specified by two vectors, i.e. $\vec{\zeta}_A$ and $\vec{\zeta}_B$ [see equations (9.169) and (9.170)], and the job here is to embed them in two matrices $\mathcal{M}_A$ and $\mathcal{M}_B$ representing the spin order. With this sublattice degree of freedom taken into account, the general spin ordered state is written as

$$\sigma^i[\mathcal{M}_j]_{i\mu}\xi_\mu, \tag{10.24}$$

and using that general form we can write the uniaxial spin density waves obtained from the site order expressions as

$$[\mathcal{M}_A]_{3\mu} = \zeta_A^\mu, \quad [\mathcal{M}_B]_{3\mu} = \pm\zeta_B^\mu. \tag{10.25}$$

We had found two site ordered states transforming as $1D$ representations of C_{6v}, an A_1 state and a B_2, which are distinguished by the relative sign between the sublattices. In case of uniaxial spin density wave order, this is captured by the overall sign of $\mathcal{M}_B$, as equation (10.25) shows. The specific uniaxial spin density wave reported in [160, 162, 163] is corresponds to the choice $[\mathcal{M}_B]_{3\mu} = +\zeta_B^\mu$ and breaks translational symmetry but preserves the rotations and reflections. The mean field spectral properties, in particular the emergence of a QBC point at Γ [163], have been mentioned already in Section 9.4.1, as they follow straightforwardly from considering the two spin species separately.

The second choice for embedding the $\vec{\zeta}_j$ in the matrices $\mathcal{M}_j$ is to put the vectors on the diagonal of the corresponding matrices. This can be simply written as

$$[\mathcal{M}_A]_{i\mu} = \zeta_A^\mu \delta_{i\mu}, \quad [\mathcal{M}_B]_{i\mu} = \pm\zeta_B^\mu \delta_{i\mu}. \tag{10.26}$$

As we have already observed in case of the triangular lattice spin density waves, the fact that the matrices $\mathcal{M}_j$ only have diagonal entries has the consequence that the effects of lattice translations can be compensated by global spin rotations. Both spin states (distinguished by $\pm$) are therefore translationally invariant. The state constructed from the A_1 site ordered state, i.e. the $+$ choice, still preserves all rotations, but breaks all reflections as they can only be compensated by improper elements of $O(3)$ and therefore this spin density wave has lower symmetry then its site ordered parent state (A_2 instead of A_1). The other spin density wave, coming from the B_2 site ordered state, becomes a B_1-symmetric state. The broken reflections become good symmetries again, as the improper $O(3)$ rotation necessary to bring the state back to itself provides an additional minus sign. In turn, the minus sign coming from the improper rotation is respondible for the breaking of the σ_d reflections.

The spin density wave transforming as A_2 first appeared in the literature as the honeycomb lattice generalization of the chiral triangular lattice spin density wave [40]. Indeed, it has the same symmetry properties and since it breaks all reflections in addition to time-reversal, it can host a Quantum Anomalous Hall effect. In [40] it was demonstrated that the formation of this noncoplanar spin density wave gaps out the Fermi surface at the van Hove singularities and the the insulating ground state is indeed a Chern insulator. Furthermore, it was shown in [163] that the emergence of the noncoplanar electronically insulating spin density wave at very low temperatures can be understood starting from the uniaxial spin density wave. The low-energy theory of the electronic degrees of freedom takes the form of a QBC point, as was noted in Section 9.4.1, and when the uniaxial spin density wave starts to develop noncoplanar components at low temperatures [160] this introduces a time-reversal breaking mass in the low-energy description. A gapped QBC point necessarily leads to a QAH ground state. Hence, we see how the spin density waves we simply obtained from site ordered states transforming as $1D$ representations of the point group, are related to each other and are found to be the lowest energy states in both a mean-field treatment [40] and a Ginsburg-Landau free energy approach [160].

It is interesting to note another property of the noncoplanar spin density waves specified by equation 10.26 and which transform as A_2 and B_1 under rotations and reflections. As was mentioned, these spin density waves are translationally invariant up to global spin rotations. In fact, if one considers them as classical spin states, they are invariant under all lattice symmetries, as the proper or improrer nature of the $O(3)$ rotation needed to compensate a given lattice operation is immaterial. As such, these two spin states are examples of what has been named *regular magnetic orders* [208], i.e. classical spin states which preserve all lattice symmetries up to a global spin rotation. In [208] all regular magnetic orders were derived for the triangular, honeycomb and kagome lattices and it is a simple matter to check that all spin states with a quadrupled unit cell, meaning ordering at the M-points, coincide with the spin density waves we construct from site-order by embedding them in a translationally invariant way. The formalism developed and presented in Section 9.4.1 to find the ordered M-point states thus systematically yields the specific subset of regular magnetic orders modulated by M-point vectors.

We conclude this brief overview of honeycomb lattice spin triplet density waves by commenting on the honeycomb lattice version of the spin-flux state which we introduced above for the triangular lattice. We simlpy start from the M-point ordered flux state which transforms as A_2, which was obtained from triplet F_2 in Section 9.4.1. The spinful version of this state, which preserves all lattice symmetries and time-reversal symmetry, is straightforwardly obtained by associating each $\vec{Q}_\mu$ with a different σ^μ, giving

$$\langle \hat{\psi}^\dagger_{i\sigma}(\vec{k}+\vec{Q}_\mu)\hat{\psi}_{j\sigma'}(\vec{k})\rangle = [\hat{\Delta}_\mu(\vec{k})]_{ij}\sigma^\mu_{\sigma\sigma'}, \tag{10.27}$$

(no sum implied on the RHS). The explicit expression of the $\hat{\Delta}_\mu(\vec{k})$ have been given in 9.4.1 following equation 9.186 and can just be taken from there. The mean field energy bands of the honeycomb spin-flux ordered state are presented in Fig. 10.4(b), which immediately shows the resemblance between the honeycomb and triangular lattice spectra. In fact, the main point we wish to stress here is that the key features of the electronic symmetries and spectra are shared between these hexagonal symmetry spin-flux orders. While spin-rotation symmetry is broken, lattice symmetries are all preserved up to global spin rotation and time-reversal symmetry is recovered by combining flux and spin type order. At the same time, the low-energy theory is in both cases (in all cases in fact) governed by a Dirac equation at each of the M'-points.

10.4 Common features of condensates with M-point order

To conclude this section on M-point spin triplet density waves with hexagonal symmetry, we the take the opportunity to summarize and review some of the key features of such density waves.

The exposition of spinful density waves presented above has made it clear how spin density waves with specific symmetry, i.e. transforming according to irreducible representations of the lattice symmetry group, can be obtained from corresponding spinless density waves. In case of the pure spin density waves (no bond or flux order), we have demonstrated both for the triangular and the honeycomb lattices that site ordered states can be taken as "parent" states, by embedding them in a spinful setting. Site ordered states with M-point ordering vectors on the triangular lattice transform according to the representation $F_1 = A_1 \oplus E_2$ (see Section 9.4.3), while honeycomb lattice site order was shown to be decomposed as $F_1 \oplus = A_1 \oplus B_2 \oplus E_1 \oplus E_2$ (see Section 9.4.1). Only focusing on the $1D$ representations (it would work in the same way for $2D$ representations), i.e. the two A_1 states and the B_2 state, we have outlined two ways of constructing spin density waves of dinstinct symmetry. The first may be referred to as the uniaxial scheme, in which the spin density waves inherit the symmetry from the site ordered states, i.e. they are also A_1 and B_2 states but break spin-rotation invariance partially. The second would be chiral scheme, in which the symmetry of the spin density waves changes from A_1 to A_2 and B_2 to B_1 $(= B_2 \otimes A_2)$ as compared to the parent site order. In the chiral scheme the resulting spin density wave states are non-coplanar. These schemes can be directly applied to the kagome lattice, for which we derived the $1D$ site order representations A_1, B_1 and B_2. From these we can construct a set of uniaxial spin density waves of the same symmetry (A_1, B_1 and B_2), or a set of chiral spin density waves with representations obtained from multiplication by A_2 (A_2, B_2 and B_1).

Let us take a closer look at the unaxial A_1 and chiral A_2 spin density waves on each of these three lattices. The spin density waves are graphically represented in Fig. 10.3. On the left side of (a)-(c) we show the uniaxial A_1 states, from which we see that while on the triangular and honeycomb lattices the spin lengths are not equal, the spin moments of the kagome lattice state are of equal length. The spin length of all the states on the right side of Fig. 10.3(a)-(c) is necessarily equal due to translational invariance. We observe a deep connection between the three unaxial A_1 and chiral A_2 spin density waves, as we find that they not only have the same symmetry, but also the same electronic properties. The uniaxial spin density waves (see also Section 9.4.1) all share the same low-energy description at Γ of the reduced (folded) Brillouin zone. Specifically, for appropriate fillings these are semimetallic states with a QBC point for

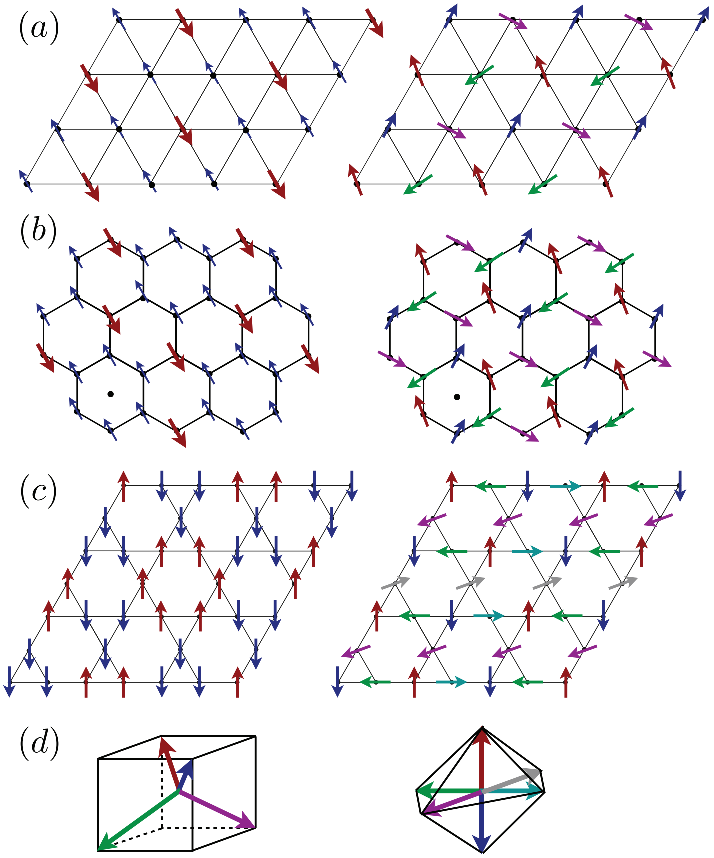

Figure 10.3: Spin density waves of hexagonal lattices with A_1 and A_2 symmetry obtained from embedding site order in a spinful setting (a) A_1 (left) and A_2 (right) density waves of the triangular lattice, and the same for (b) the honeycomb lattice and (c) the kahome lattice. (d) shows the non-coplanar spins of the A_2 states of the triangular and honeycomb lattices (left), and the kagome lattice (right).

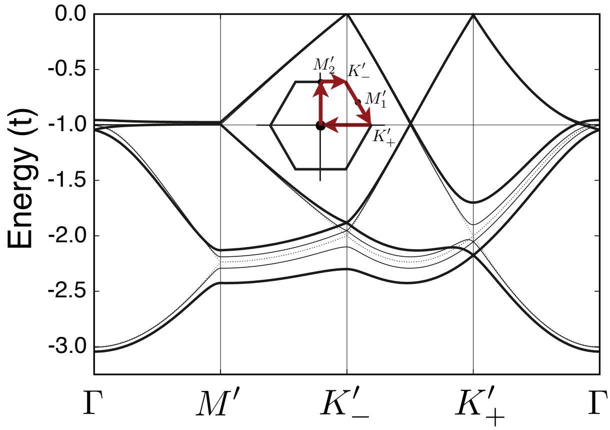

Figure 10.4: Honeycomb lattice energy bands for the B_1 chiral spin density wave. Thin dashed lines correspond to the free honeycomb band structure, solid thin lines to a weakly developed B_1 spin density wave and thick solid lines to a density wave with considerable strength. Between the lowest two bands a (doubly degenerate) Dirac node appears at K'_+.

one of the spin species, also referred to as half metallic states [160], while excitations involving the other spin species are gapped. Instead, the chiral spin density waves are all gapped for appropriate fillings and the insulating ground state is a QAH state. As was pointed out in [163], the A_1 and A_2 spin density waves are closely related in the sense that a smooth interpolation from the A_1 state to the gapped A_2 exists, which has the low-energy interpretation of gapping out the QBC point by a manifest breaking of time-reversal symmetry. The symmetry perspective developed in this work reveals and formalizes both the deep connection between the A_1 and A_2 density waves and the lattice independence of their (low-energy) electronic properties.

Interestingly, not only the A_1 and A_2 spin density waves have properties which transcend the lattice specific setting, but also the two chiral B_1 spin density waves on the honeycomb and kagome lattices. Incidentally, such a state does not exist for the triangular lattice. At the van Hove fillings these states lead to a change in shape of the Fermi surface that is schematically captured by the lower left part of Fig. 9.7. This is in agreement with symmetry, as time-reversal symmetry is broken by the spin density wave and B_1 symmetry implies that the reflection planes bisecting the vertices of the BZ are still good reflection planes, while the other set of reflections is broken. The most important feature of the mean field spectrum corresponding to these states, both on the hobeycomb and the kagome lattice, is the appearance of Dirac nodes at K'_+ (or K'_-, depending on the sign of the order parameter) in the form isolated touchings between the *lowest two* bands. That they should appear only at one of the two valleys which are each others time-reversal partners is again in agreement with the breaking of this symmetry.

A different class of spinful density waves is derived from spin rotation invariant bond ordered states, or, more specifically flux ordered states. The structure of this derivation is essentially the same as for the pure spin density waves. Starting from the A_2 flux ordered states, which exist for all three hexagonal lattices considered in this work and come from the F_2 representation, we have discussed three schemes of constructing spin rotation symmetry breaking density waves. The first is straightforward and involves the global exhange of $\delta_{\sigma\sigma'}$ and $\sigma^3_{\sigma\sigma'}$ (the "two copies with opposite sign" scenario), creating an insulating time-reversal invariant density wave with the same mean field spectrum for up and down electrons, but opposite Chern numbers $C_\uparrow - C_\downarrow \neq 0$. The second scheme amounts to assigning a different spin Pauli matrix σ^i to each of the three hopping directions of a hexagonal lattice, i.e. $\vec{x}_i$. This spin-flux ordered state fully breaks spin rotation symmetry, and translational symmetry, while preserving all point group operations. The mean field spectrum is gapped and corresponds to a QSH state. In the third scheme one assigns a different Pauli matrix σ^i to each of the three M-point ordering momenta $\vec{Q}_\mu$. For the triangular lattice we showed in detail how such an embedding preserved all lattice symmetries, including the translations that are broken in the M-point flux ordered state. As a consequence of this high degree of symmetry there are protected degeneracies at the M' points of the reduced Brillouin zone, in addition the Kramers degeneracy mandated by time-reversal symmetry. The spectrum disperses linearly in all directions around these M' points making this particular spin-flux ordered state a Dirac semimetal. Time-reversal symmetry requires two degenerate Dirac nodes per M' point. To summarize these three schemes, all of them yield time-reversal invariant yet spin rotation symmetry broken density waves. In case of the first two, they transform as A_1 but break translational symmetry. The third scheme of constructing spinful bond density waves results in a fully lattice symmetric state. Again, these statements apply to all three lattices and should be considered a property of the hexagonal symmetry class more than of particular lattices.

The highly symmetric nature of the Dirac semimetal is a result of the embedding of the A_2 flux ordered state in a spinful setting. It allows for translations to be dressed with global spin rotation to be become good symmetries again, inspite of the underlying M-point order. Furthermore, the reflections broken in the flux state become good symmetries again, because they come dressed with improper rotations restoring the them as symmetries. The protection of the Dirac semital at the M' critically relies on the presence of translational symmetry, as we have seen in Section 9.4.1. This not

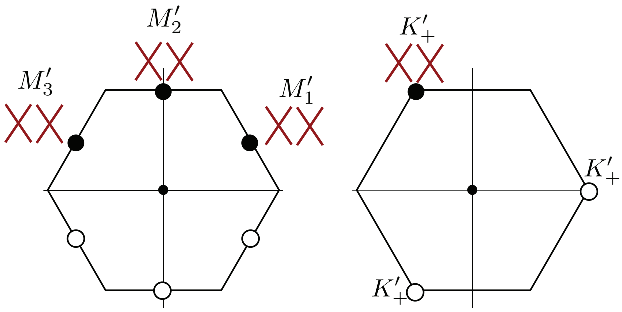

Figure 10.5: (left) Schematic representation of the double Dirac nodes at the three *inequivalent* M'-points of the reduced hexagonal Brillouin zone in the presence of the spin-flux density wave. (right) Schematic representation of the double Dirac nodes at the three *equivalent* K'_+-points in the presence of B_1 symmetric spin density wave order on for instance the honeycomb or kagome lattice.

only illustrates the principle of global spin rotation equivalenceitself, i.e. applying lattice operations yields a unitarily equivalent Hamiltonian, but it also exemplifies its importance for protecting topological semimetals.

The fully lattice symmetric spin-flux density wave states and the B_1 spin density wave states are two examples of classes of states for which translational symmetry is preserved. In both cases translational invariance plays a role in the protection of the semimetallic Dirac points and their twofold degeneracy. Both semimetallic states constitute new symmetry-protected topological semimetals. One breaks time-reversal symmetry the other preserves it. The two Dirac theories are schematically summarized in Fig. 10.5. In case of the time-reversal symmetric spin-flux state the low-energy Dirac theory consists of six Dirac nodes, two for each inequivalent M' point. Instead, the B_1 symmetric time-reversal breaking states have a double node at the K'_+ (or K'_-) point.

The concept of global spin rotation equivalence in relation to lattice symmetries was introduced for classical spin models in [208], which coined the notion of classical spin liquids. They are defined as classical spin states which do not break any lattice symmetries, up to a global $O(3)$ spin rotation. In [208] a projective symmetry group analysis was employed to systematically derive spin states which satisfy this condition for selected lattices. For hexagonal lattices, a subset of these classical spin liquids is build from M-point ordering vectors. This subset of classical spin liquids is automatically generated as a by-product of the symmetry organization of density waves detailed in this work. To see this, let us go back again to spin density waves obtained from site order. In the second scheme of embedding, i.e. the chiral scheme, we put the vectors specifying site order $\vec{\zeta}_i$ (i labeling the sublattice) on the diagonal of the corresponding matrix $\mathcal{M}_i$, which restores translational invariance. If instead of constructing a an electronic spin density wave, i.e. $\vec{\sigma} \cdot \vec{\mathcal{M}}_i$, for the which the $\mathbb{Z}_2$ content of $O(3) = \mathbb{Z}_2 \times SO(3)$ matters, we construct a classical spin state $\vec{\mathcal{S}}_j(\vec{x})$ of the form

$$\vec{\mathcal{S}}_j(\vec{x}) = \vec{\mathcal{M}}_j(\vec{x}) = [\vec{\mathcal{M}}_j]_\mu \xi_\mu(\vec{x}), \tag{10.28}$$

we have obtained a classical spin liquid. To put it differently, if we interpret the chiral spin density waves as classical spin states, they satisfy the criteria for a classical spin liquid. Take for instance the kagome lattice. The kagome lattice allows for three M-point ordered classical spin liquids [208], which are immediately obtained from the three site ordered states A_1, B_1 and B_2 by putting the vectors $\vec{\zeta}_i$ (see Section) on the diagonal of $\mathcal{M}_i$. We therefore close by mentioning that classical spin liquids may be obtained in straightforward manner by taking the $1D$ site order representations and embedding appropriately in spin space. Of course this requires specifying M-point order ahead of time.