Incommensurate Magnetic Ordering from One-Dimensional Correlated Topological Bulk States

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A phenomenological model accounts for the calculation of incommensurate ordering wave vectors (IC) in several Ce- and U-based f-electron itinerant compounds (CePtSn, CePdSn, CeNiSn, CeRhIn5, URu2Si2, CeNiAsO, CeCu(6−x)Au x, UNi2Al3, CeCuSn) as well as in BSSCO, Rb2ZnBr4, MnSi and prototypical IC system Chromium metal. This model is justified by a many-body topological one-dimensional (1-D) Dirac Hamiltonian after center of mass transformation on a chiral group symmetry in the basal plane plays a role in the establishment of the complex CDW in this compound. Still, the prototypical system for IC density waves is Cr metal where measurements at neutron and synchrotron sources reveal satellites that characterize the simultaneous occurrence of both a CDW and a SDW. In such 4f localized electrons systems, the non-local RKKY magnetic interaction propagates through the conduction band but the localized nature of the spins and nearest neighbor interactions give magnetic structures that are more CM in fashion.

When \( \tau \) is not a rational fraction, the order is said to be IC as it does not relate directly to the periodicities of the underlying crystalline lattice. In Rb2ZnBr4 there have been discussions about a “floating” IC order completely disconnected from the lattice periodicity. IC order stem from the onset of instabilities of the type: charge-density waves (CDW) and spin-density waves (SDW) if it is magnetized which arise from nesting of the Fermi surface when conduction electrons match and connect one side of the Fermi surface to the other. In density wave systems, theoretical work using free energy formulation focused on the IC to CM transition in term of strain waves and small lattice displacement. For example, neutron scattering studies on the insulating alloy 2H-TaSe2 reveal both IC and CM orderings observed simultaneously in the same crystalline phase at different wave vectors in the hexagonal basal plane. A particular space group representation of lattice displacements respecting the crystallographic group symmetry in the basal plane plays a role in the establishment of the complex CDW in this compound. Still, the prototypical system for IC density waves is Cr metal where measurements at neutron and synchrotron sources reveal satellites that characterize the simultaneous occurrence of both a CDW and a SDW.

However, the distinction between IC and CM wave vectors is less clear when experimental measurements show that IC wave vectors themselves tend to either “move” or are “fixed” in reciprocal space with temperature. Is
there a more direct role from the “commensurate” atomic positions of the underlying lattice to generate a “fixed” IC order?

In this paper, a phenomenological model accounts for the calculation of magnetic IC wave vectors in several crystallographic systems with metallic character. This ordering is different compared to standard models for IC order based on lattice distortions in the mean field approach\(^1\). Here the momenta defined by the scattering centers involved in the definition of the IC unit cell make the ordering "dynamic" and are not expected to move with temperature due to the topology of the crystalline lattice.

I. CORRELATED TOPOLOGICAL BULK STATES

The basis of topological effects in condensed matter is to associate a pseudo-spin \( \vec{d} \) to wave vector positions in reciprocal space where the Berry connection and curvature describe how this "magnetic pseudo-spin" is quantized and depends on geometric considerations of the reciprocal space \(^\text{14},\text{15}\). The pseudo-spins guide the alignment of the magnetic spins in a given band as can be seen by the magnetic interaction Hamiltonian of the form \(-d_i \sigma_i\) with \(\sigma_i\) the Pauli matrices. In a two-band model describing topological effects, the pseudo-spins have the form \((k \cos(n\theta), k \sin(n\theta), M - k^2/2)\) with \(M\) the energy gap appearing in the third dimension \(^\text{17}\). Furthermore, to take account of multi-band coupling in the simple model the pseudo-spins can be added in a weighted sum over different energy bands.

Equivalently, this formulation can be achieved using the Dirac equation as is very well presented by Shen\(^\text{19}\). The Dirac equation comes from the linearization of the relativistic energy-momentum 4-vectors to form a Hamiltonian. This equation is well known in particle physics and predicted the existence of positrons before its experimental observation. The success of this equation lays in its link between momentum and spin in the same framework. Recently, applications of a modified Dirac equation to condensed matter, which decouples topologically positive and negative energy solutions by adding a dynamic term to the rest mass energy, has a rich physics and may hint at the success of the many-body aspect of the Dirac equation.

As with the pseudo-spin representation, the modification to the Dirac Equation appears as a \(p^2\)-correction to the vacuum controlled by a gap parameter \(B\) as shown in Eq\(^\text{2}\). The usual notation for \(\alpha\) and \(\beta\) matrices is followed. The equation reduces to the standard Dirac equation when \(B = 0\) and \(v = c\), the speed of light.

\[
H = v \begin{pmatrix} p_x + (mv^2 - Bp_x^2) \end{pmatrix} \beta
\]

The parameter \(B\) change the sign of the \(\beta\) matrix term, or mass term and makes the +m and -m states different dynamically. The velocity \(v\) indicates the many body velocity associated with correlated behavior. For the one-dimensional (1-D) momentum, chosen along \(p_x\), Eq\(^\text{2}\) reduces to an independent set of equations summarized by Eq\(^\text{3}\)

\[
[vp_x σ_x + (mv^2 - Bp_x^2) σ_z] φ(x) = 0
\]

The wave function \(φ_\eta(x)\) is explicitly solved and shown in Eq\(^\text{3}\). The vector represents the spin state being here \(S_y\).

\[
φ_\eta(x) = \frac{C}{\sqrt{2}} \left( \begin{array}{c} \eta \gamma_0 \exp(-x/\xi+) \\ \eta \gamma_0 \exp(-x/\xi-) \end{array} \right)
\]

The end state solutions are labelled by the parameter \(\eta = \text{sgn}(B)\) and are controlled by two decay factor \(\xi_+ = |B| \hbar/v = |B| \hbar m/(\hbar Q')\) and \(\xi_- = \hbar/mv = \hbar/(\hbar Q')\). We change the variable interpretation from Shen\(^\text{19}\) by noting that \(m\) has the unit of momentum in the definitions of \(\xi\) and introduce a momentum variable \(h Q' = h(Q - q_{cm}) = mv\) to describe the solutions. The bulk state solutions are obtained by setting a closure of the gap with \(B \to 0\), or equivalently \(\xi \to 0\), which removes the \(\xi_+\) part of the wave function in Eq\(^\text{4}\). Writing explicitly the spin part, the general solution for the bulk state is reduced to Eq\(^\text{5}\)

\[
φ_\eta(x) = C_\eta e^{-x/(Q - q_{cm})}(\eta |+) + i |-\))
\]

As described in Shen\(^\text{19}\) the bulk state is further achieved by setting \(m \to 0\) or equivalently \(Q \to q_{cm}\) which sets the wave function independent of \(x\) and constant over the whole crystal. Before doing this last approximation, we will build the fermion Slater determinant wave function \(Ψ\) for several electrons involved in a many-body correlation. Doing so, the center of mass many body wave function leads to a product of the Eq.\(^\text{5}\) wave functions as expressed by Eq\(^\text{6}\)

\[
Ψ = Ce^{-Q_i(\Delta_i + x)}F(δ_j, Q_j)S(\eta, i)
\]

where \(Q_i = \sum_j (Q_j - q_{cm})\) with \(Q_j\) the different wave vectors of each correlated electron, \(q_{cm}\) the center of mass wave vector and \(\Delta_i = \sum_j δ_j\) if \(x_j = x + \delta_j\) where the spatial variables are all referenced to \(x\) (\(δ_0 = 0\)), which can be any electron involved in the superposition. The different spatial snapshots possible from one inertial frame to the other makes the momentum not a good quantum number (Heisenberg relation) and is a source of fluctuation. The function \(F\) is a sum of exponentials in \(Q_j's\) and \(δ_j's\) with different signs and is independent of \(x\). The spin part \(S\) is a sum of combinations of spin states with products of \(i^a j^b\) as pre-factors of the spin state \(|\alpha - b\rangle\). The topological bulk states for each electron involved in the correlated motion requires \(Q_i \to 0\) which removes the \(x\) dependence on the wave functions. Doing so, \(Q_i = 0\) leads to \(q_{cm} = (1/N) \sum_j Q_j\) (with \(N\) the number of electrons involved in the correlation). This average momentum corresponds to the IC wave vectors labeled in the
TABLE I. Crystal data for CeTSn (T=Pt,Pd,Ni) with the Pn2₁a space group

| Compound   | Atom | x       | y       | z       |
|------------|------|---------|---------|---------|
| CePtSn     | Ce   | 0.487907| 1/4     | 0.195807|
|            | Pt   | -0.290565| 0.24275| -0.409034|
|            | Sn   | -0.176328| 0.24627| -0.083228|
| CePdSn     | Ce   | 0.487894| 1/4     | 0.201234|
|            | Pd   | -0.299317| 0.24414| -0.41987|
|            | Sn   | -0.186585| 0.24674| -0.086806|
| CeNiSn     | Ce   | 0.481655| 1/4     | 0.197015|
|            | Ni   | -0.31081 | 0.25219| -0.41791|
|            | Sn   | -0.185726| 0.24334| -0.090766|

following as "topological dynamic ordering". The fluctuating properties of the wave functions $\Psi$ are discussed in section III.

In section II we show, from these 1-D solutions of the modified topological equation, that the $Q_j$'s can taken to be the local Bragg planes or crystallographic features in a crystal lattice. The average wave vector $q_{\text{cen}}$ corresponds to the IC magnetic ordering wave vector observed in compounds with different crystallographic space groups.

II. PHENOMENOLOGY FROM CRYSTALLOGRAPHY

A. Orthorhombic Symmetry

In the CePtSn, CePdSn and CeNiSn series, the crystal structure is that of the space group Pn2₁ labelled #33 in the crystallographic table. Published work has shown the space group Pn2₁a which is a permutation of the y- and z-axes. In this low-symmetry structure Pn2₁a has only one (4a) $(x,y,z)$ general symmetry position with atoms in the unit cell at $(x+1/2,y+1/2,z)$, $(x+1/2,y+1/2,z+1/2)$ and $(x+1/2,y+1/2,z+1/2)$. From the space group, the Ce atoms in this series of compounds occupy the $(x_{\text{Ce}},y_{\text{Ce}},z_{\text{Ce}})$ positions. The other crystallographic parameters appear in Table I. It is worth noting that the calculation of ordering wave vectors in these compounds needs precise crystallographic data for the phenomenological method described here to be effective.

CePtSn has two magnetic phases. At high temperatures, between $T_M$ and $T_N$, the magnetic order develops with a wave vector $(h,k,l)$ with $k=0.418b^*$. The second phase, at a low temperature below $T_M$, orders with a magnetic wave vector $k=0.466b^*$. The relevant positions of the Pt atoms along the $b^*$-direction are at $y_{\text{Pt}}=0.24275$ and at $y_{\text{Pt}}+1/2$. The reciprocal (1/distance) of these Bragg plane Pt positions leads to $4.11946$ and $1.34634$ wave vectors respectively. The average of the fractional part of these wave vectors does not lead to the observed ordering one. With nesting, even though the crystal structure has no inversion symmetry for the y-component but the cosine in Eq.1 has, these wave vectors are multiplied by two as the conduction electrons connect one side of the Fermi surface (at $-G$ to $G+\tau$), leading to $8.23893$ and $2.69270$ wave vectors. Both are wave vectors that can be translated to zero (because of the even integer part). Taking the average of the fractional parts of the two wave vectors, the predicted wave vector associated with the Pt atoms is 0.4658, very close to 0.466 (within 0.04%) seen experimentally as the IC wave vector for the low-temperature phase.

For the high-temperature phase, the Sn-atoms are at $y_{\text{Sn}}=0.24627$ and $y_{\text{Sn}}+1/2$. The associated wave vectors with the positions are 4.06058 and 1.34000. Nesting of the wave vectors leads to $8.12117$ and 2.68000. Translating the wave vectors in the same zone, 0 to 1 again, the average on the fractional part is 0.40058 for the magnetic ordering wave vector compared to 0.418 observed experimentally. The difference of 4% may come from an overlap of the averaging between the Pt and Sn sites 0.40658($1-x$)+0.4658$x=0.418$ which gives $x=27\%$ for the contribution from the Pt sites to the Sn sites averaging. It is possible to obtain $\tau=0.41978$ (a difference of 0.4% compared to 0.418) taking $y_{\text{Pt}}$, $y_{\text{Sn}}$, $y_{\text{Pt}}+1/2$, $y_{\text{Sn}}+1/2$, $y_{\text{Pt}}+1$, $y_{\text{Sn}}+1$ with associated nested wave vectors $8.23893$, $8.12117$, $2.6927$, $2.68$, $1.6093$ (2+0.3907), 1.60479 (2+0.39521). These results are attributed to the mixing of the Pt to the Sn Bragg planes at high temperature which vanishes at low temperature where the Pt Bragg planes alone drive the magnetic phase in CePtSn. It is worth noting that the $\tau$ of both magnetic phases require nesting of the wave vectors and an expression of the satellites near an "even" reciprocal lattice wave vector.

The case of CePdSn involves more atoms without nesting. Neutron scattering experiments have shown the magnetic wave vector is $k=0.473b^*$. Taking the Pd atoms, $y_{\text{Pd}}=0.24414$, $y_{\text{Pd}}+1/2$, $y_{\text{Pd}}+1$ and $y_{\text{Pd}}+3/2$ leads to the wave vectors 4.09601, 1.34383 (2+0.65617), 0.80377 and 0.57335. After translation of the wave vectors to the zero zone from 0 to 1, the average Pd satellite wave vector is 0.53232, or near the AF position as (1-0.46768) to follow the notation of published results. This result is lower but very close to the magnetic ordering wave vector 0.473 seen experimentally. Doing the same with the Sn sites, $y_{\text{Sn}}=0.24674$, $y_{\text{Sn}}+1/2$, $y_{\text{Sn}}+1$, $y_{\text{Sn}}+3/2$, the wave vectors are 4.05285, 1.33915 (2+0.66085), 0.802092 and 0.57250 respectively. The average of the Sn atoms is 0.52807 which can be rewritten as (1-0.47793), now higher than the observed magnetic ordering wave vector. Taking the average over the eight Pd and Sn atoms, or an equal contribution of each in the averaging, gives 1-0.472803 which is now very close (within 0.04%) to the experimental value 0.473 underlying the role of the Pt and Sn Bragg planes averaging in this series of compounds.

In the case of CeNiSn, it does not order magnetically but the method developed so far can be applied to find some justification for the gap zone centers at $(Q_n, 1/2+n, Q_c)$ with n an integer, found in neutron scattering.
The $y$-positions of the Ni Bragg planes over two unit cells at $y_{Ni}=0.25219$, $y_{Ni}+1/2$, $y_{Ni}+1$ and $y_{Ni}+3/2$ lead to the contributing wave vectors are $3.96526, 1.32945, 0.79860$ and $0.57071$. Nesting leads to $7.93053 (8 + 0.06947), 2.65890, 1.59720 (2 + 0.40280)$ and $1.14143 (2 + 0.85857)$. Taking the average over the fractional part of the four wave vectors leads to 0.497436 which is very close to the $y$-component of the wave vector at 1/2 (within 0.5%) of the insulating energy gaps observed experimentally. According to the phenomenological model ($Q_a, 1/2+n, Q_j$) are the zone centers due to scattering of the Ni Bragg planes over two unit cells in CeNiSn. Without nesting the atoms $y_{Ni}, y_{Ni}+1/2, y_{Ni}+1$ also lead to 0.501295 wave vector (an error of 0.3%).

Focusing on other orthorhombic compounds, CeRhIn$_5$ is a heavy fermion with a tetragonal P4/mmm #123 crystal structure with Ce atoms at the (1a) $(0, 0, 0)$ symmetry position, the Co at the (1b) $(0, 0, 1/2)$ symmetry position, and the In atoms at the (1c) $(1/2, 1/2, 0)$ and at the (4i) $(0, 1/2, z_{In}), (1/2, 0, z_{In}), (0, 1/2, -z_{In}), (1/2, 0, -z_{In})$ positions with $z_{In}=0.30592$ as published.

It orders magnetically below $T_N=3.8K$ with an IC wave vector $(1/2, 1/2, 0.297)$. Except for the (4i) positions, all the other atoms in the unit cell would contribute to reciprocal lattice wave vectors with no fractional part along the $c$-direction. With the $z_{In}$ components of the (4i) sites, there are two relevant positions: $z_{In}=0.30592$ and $1-z_{In}=0.69408$ in the folded reduced unit cell. The nested IC wave vector obtained are: 6.53766 and 2.88151. Translating these wave vectors to 0 leaves an average of 0.709595 $(1+0.290415)$ which compares favorably to the 0.297 ordering wave vector, an error of 2%. The translation to (0,0,1) as the zone center is the nearest reciprocal lattice wave vector to the satellite. In fact, the sum converges to 0.296889 (an error of 0.04%) after 7 Bragg planes if we consider the positions: $z_{In}, 1-z_{In}, 1+z_{In}, 2-z_{In}, 2+z_{In}, 3-z_{In}, 3+z_{In}$ which leads to the nested wave vectors: $6.53766, 2.88151, 2+0.46513, 2+0.819418, 0.867333, 0.742368, 0.604975$.

Another tetragonal compound that attracted a lot of attention is URu$_2$Si$_2$ due to the very small ordered magnetic moment size below 17K and large features in the specific heat at low temperature indicating other processes at play like multipole ordering. Inelastic fluctuations have been found at the AF (1,0,0) and an IC wave vector (1,4,0,0) = (0.4,0,0). The crystal structure is I4/mmm #139 with U-atoms at the (2a) $(0, 0, 0)$, the Ru-atoms at the (4i) $(0, 1/2, 1/4)$ and $(1/2, 0, 1/4)$ and the Si-atoms at the (4e) $(0, 0, z_{Si})$ and $(0, 0, -z_{Si})$ positions. All the atoms are translated by a body centered $(1/2, 1/2, 1/2)$. There are 2 Ru-atoms and 1 U-atom contributing to the body centered Bragg plane at the $x$-position=1/2. The difficulty here is that the expansion is at the $(1,0,0)$ wave vector which is a forbidden or AF wave vector of the magnetic structure. There are several ways to generate the CM 0.4 wave vector with the average of the 5- or 6-position sequence: 1/2, 1/2, 3/2, 3/2, 3/2, 5/2. One possible scenario involves of the 5 wave vector average 2, 2, 2/3 (2+1/3), 2/3 (2+1/3), 2/3 (2+1/3) without nesting gives an average, including the zeros, 2 + 2/5 (which is an IC satellite at 0.4). This suggests fluctuations of the 4 Ru-atoms in both unit cells with the addition of a single U-atom in the next nearest unit cell along the $x$-direction.

An interesting outcome arises from the analysis of the high-Tc superconductor Ba-Sr-Ca-Cu-O 2212. It exhibits an IC wave vector at $\tau=\pm 0.21a$ from the crystallographic reciprocal lattice position. BSCCO has an Amaa #66 space group crystal structure with atoms at, focusing on the $\tilde{a}$-direction: $x,-x,1/2+x,1/2-x,-x,1/2-x,1/2-x$ and the same atoms translated by $(0,1/2,1/2)$. Here all the atoms in BSSCO are at either $x=0, 0.25, 0.5, 0.75$ positions. The reciprocal of these positions lead to integer wave vectors but can serve as a basis for the IC wave vector. The metallic Cu atoms are at the general position $(0.5, 0.2498, 0.1967)$. From the space group these Cu-positions along the $\tilde{a}$-direction are at: 0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5, 0.5 (and the same sequence repeated after the (0.1/2,1/2) translation) leading to the wave vectors: 2, 2, 1, 1, 2, 2, (0), 0, 2, 2, 1, 1, 2, 2, (0), (0) respectively for the 16 atoms in the unit cell. The zeros in parenthesis stand for atoms contributing to reciprocal lattice wave vectors and can be translated to the 0. There are two types of average possible whether we include the zero wave vectors or not. The first average with the zeros is: $(8 \times 2 + 4 \times 1)/16 = 1.25 (1+0.25)$ and the second average without the zeros $(8 \times 2 + 4 \times 1)/12 = 1.6667$. Taking an AF SDW for the second wave vector gives $q=0.83333$ (or 1+0.6667 for the chiral satellite) after dividing by 2. The average of both satellites gives $(0.25+0.16667)/2=0.20833$ which is very close to 0.21 published (an error of 0.8%). The phenomenological model in BSSCO suggests an average dynamic IC order between competing SDW and CDW of slightly different origin in a moving reference frame. The IC order involves the unit cell with many atoms at commensurate positions in the unit cell which may highlight the special character of the physics of high-Tc’s in general.

The phenomenological model gives some insight into the IC order in the heavy fermion CeNiAsO. It has a P4/mmm #129 crystal structure with the Ce atoms at the Wyckoff (2c) positions $(1/4, 1/4, z_{Ce})$ with $z_{Ce}=0.1465$, the Ni atoms at the (2b) positions $(3/4, 1/4, 1/2)$, the As at the (2c) positions $(1/4, 1/4, z_{As})$ with $z_{As}=0.6434$ and the O atoms at the (2a) positions $(3/4, 1/4, 0)$ as published. CeNiAsO experience an IC phase transition attributed to a SDW below $T=7.6K$ with a wave vector $(0.444, 0, 0)$ The atomic positions involve a redundancy of 1/4 and 3/4 coordinates along the $\tilde{a}$-direction shared indistinctly by all the atoms. Taking the reciprocal of the say Ce-Bragg planes at 1/4, 3/4, 3/4 positions lead to the reciprocal wave vectors 4, 4/3 (2+2/3), and 4/3 (2+2/3). Translating all in the reciprocal zone from 0 to 1 and taking the average over the three satellites.
(0 + 2/3 + 2/3)/3 = 4/9 which is exactly the reciprocal wave vector found experimentally. It is worth mentioning that CeNiAsO has no superconductivity detected down to 30mK\textsuperscript{29} and that topological dynamic ordering may act as to prevent such occurrence.

Another system where electron correlations play an important role is CeCu\textsubscript{6}. In this compound, all the atoms exhibit metallic character complicating at first the analysis of IC “dynamic ordering” but it is worth noting that short-range Ce intersite correlations are observed\textsuperscript{30} qualitatively reminiscent of the phenomenological model presented here. It is a heavy fermion compound which displays no magnetic order but IC AF order is observed in the Au-doped version of the compound\textsuperscript{22} CeCu\textsubscript{6-\textit{p}}Au\textsubscript{\textit{p}}. With \textit{p}<0.5, the ordering wave vector remains stable at (0.625, 0, 0.275) while for \textit{p}>0.5 the IC wave vector is (0.59, 0, 0). In both the doped and undoped compound the crystal structure can be referred to the Pnma \textsuperscript{#62} space group\textsuperscript{23} even though there is a monoclinic phase at low T which can still be labeled according to the orthorhombic crystal structure. Focusing on the \textit{a}-direction, the Ce-atoms are distributed at the positions \textit{x}, -\textit{x}+1/2, -\textit{x}+(+1), \textit{x}+1/2 with varying \textit{x} = 0.2585 (1-\textit{p})+0.26078 \textit{p} with the concentration \textit{p} of the Au-atoms varying from 0 to 1. From the position of the fourth Ce-atom at \textit{x}+1/2 and \textit{x}+1/2+1, or after 2 unit cells, the wave vectors for \textit{p}=0.1 are 1.318 (2+0.682005) and 0.568593 for an average satellite of 0.625929. For \textit{p}=0.5 the wave vectors are 1.31641 (2+0.685387) and 0.568298 for an average wave vector 0.625943. Both average wave vectors are very close to the observed IC wave vector of 0.625 (an error of 0.05% to 0.2% over the concentration interval). For the \textit{c}-component of the IC wave vector found experimentally at 0.275 for \textit{p}>0.5 is also found by considering the fourth Ce-atom in the unit cell. The atomic positions along the \textit{c}-direction are at (following the listing order of the \textit{c} component): \textit{z}, \textit{z}+1/2, -\textit{z}+(+1), -\textit{z}+1/2 with \textit{z} = 0.4364 (1-\textit{p}) + 0.43593 \textit{p}. The fourth atom at -\textit{z}+1/2 gives a wave vector of 15.7233 (16+0.27673) at \textit{p}=0 which is close 0.275 (an error of 0.6%) but the calculated wave vector should have moved to \textit{τ}=0.334613 at \textit{p}=0.5 (an error of 22%). For the 0.59 IC wave vector observed experimentally along the \textit{a}-direction with \textit{p}>0.5, the correlations involve the whole unit cell. Taking \textit{p}=0.5, the wave vectors of the positions along the \textit{a}-direction (following the listing order already established for the Ce-atoms) are 3.85149 (4+1.48513), 4.16043, 1.35069 (2+0.649306), 1.31641 (2+0.683587) giving an average of 0.410458 (or 1-0.589542) an error of 0.08%. A similar result is obtained for \textit{p}=1.0 where the wave vectors 3.83465 (4+0.163535), 4.18025, 1.35278 (2+0.64722) and 1.31444 (2+0.68556) give an average of 0.419596 (or 1-0.580404) also very close to 0.59 with an error of 2%. In summary, the fourth atom in the unit cell at (x+1/2, y_{Cu}, \textit{z}+1/2) seems to drive the IC wave vector (with 2 unit cells along the \textit{a}-direction and 1 unit cell in the \textit{c}-direction) at low \textit{p} concentrations until correlations involving the whole unit cell are established with \textit{p}>0.5 along the \textit{a}-direction only. Topological dynamic ordering offers a relatively simple scenario of the short-range correlations in the doped CeCu\textsubscript{6} based on its crystallography.

To emphasize the role of metallic electrons in topological dynamic ordering, Rb\textsubscript{2}ZnBr\textsubscript{4} also offers an indication of crystallographic origin for an IC order\textsuperscript{31} Rb\textsubscript{2}ZnBr\textsubscript{4} has an ordered IC structure with \textit{q}=0.292 e\textsuperscript{a} at room temperature which locks-in at \textit{q}=-(1/3) e\textsuperscript{a} at low T, as published\textsuperscript{32}. It has a Penn\textsuperscript{#62} crystal structure with the room temperature metallic Zn positions at (0.923, 0.224, 0.774). The unit cell of Penn has eight atoms along the \textit{c}-axis: z, 1/2+z, z, 1/2-z, -z, 1/2-z, -z, 1/2+z which lead to the positions of the Bragg planes at 0.774, 0.726, 0.274, 0.226 (sorted in decreasing order in the reduced unit cell). Focusing on the first 2 positions of the list, the associated wave vectors without nesting are 1.29199 (1+0.29199) and 1.37741 (1+0.37741). The first 0.774 position gives the satellite observed for the room temperature phase with \textit{τ}=0.292. The interesting observation is by taking the average of these two satellites: (0.29199+0.37741)/2 = 0.3347 which is very close to 1/3 (an error of 0.4%), the wave vector of the low-temperature phase. Therefore, the phenomenological model in Rb\textsubscript{2}ZnBr\textsubscript{4} is that the electrons scattered by the metallic Zn atoms at z_{Zn}=0.774 drive the IC phase at room temperature while they become correlated with the electrons scattered by the atoms at z_{Zn}=0.726 at low T, leading to the nearly CM phase. A simple model for the phase transition can be built taking the average with weights w(T) dependent on temperature \textit{τ}=0.29199 w(T) + 0.37741 (1-w(T)). It is worth noting the low T \textit{c}-component of the Zn atomic positions at (0.924, 0.237, 0.781) lead to 0.28041 and 0.39082 satellites which give an average wave vector of 0.335615 also very close to 1/3.

B. Hexagonal Symmetry

The magnetic wave vectors in the heavy fermion UN\textsubscript{3}Al\textsubscript{3} have been observed by neutron scattering experiment\textsuperscript{33} as two satellites at (1/2±\textit{τ}, 0, 1/2) with \textit{τ}=0.110 which gives the IC satellites at 0.390 and 0.610 in the first zone without higher order satellites detected\textsuperscript{34}. The IC peaks did not move with temperature, giving a hint at their crystallographic origin\textsuperscript{35} \textsuperscript{36}. The crystal structure of UN\textsubscript{3}Al\textsubscript{3} is P6/mnm #191 and have U-atoms positions at (1a) \langle 0, 0, 0 \rangle, Al-atoms at the (3g) positions \langle 1/2, 0, 1/2 \rangle, \langle 0, 1/2, 1/2 \rangle, \langle 0, 1/2, 1/2 \rangle, \langle 0, 1/2, 1/2 \rangle and neighboring Ni atoms at the (2c) Wyckoff positions \langle 1/3, 2/3, 0 \rangle and \langle 2/3, 1/3, 0 \rangle in the hexagonal unit cell\textsuperscript{37}.

The \textit{a}-direction from the reference atom appears in Fig. 1. The red line indicates the distance associated with the largest 0.61 satellite which, by symmetry around the Al-atom along the \textit{b}-direction, lead to the Ch(n) CDW model in the figure. Ch(1) and Ch(2) in Fig. 1 intersect the \textit{b}-axis at Ch(1) (1/2, 3/2, 0) and Ch(2)
FIG. 1. Projection of atom positions onto the hexagonal basal plane of UNi$_2$Al$_3$. The dashed blue lines indicate the positions of the proposed CDW charged maxima (at Ch(n)) distributed along $\vec{a}$-direction. The dashed red line show the distance 1/0.61 from the satellite of the ordering wave vector along the $\vec{a}$-direction.

TABLE II. Calculation of the magnetic ordering wave vectors for Ch(n) maxima in UNi$_2$Al$_3$ based on a partial Ch(n) Bragg plane expansion. The values in bold are close to the observed experimental wave vectors in zero and in high magnetic field.

| Atoms                              | Average          | 1/2 ± $\tau$ |
|------------------------------------|------------------|--------------|
| Ch(1)+Ch(2)                        | $\frac{1}{2} + \frac{4}{5}$ | 0.15000     |
| Ch(1)+Ch(2)+Ch(3)                  | $\frac{1}{2} + \frac{4}{5} + \frac{3}{5}$ | 0.13333     |
| Ch(1)+Ch(2)+Ch(4)                  | $\frac{1}{2} + \frac{4}{5} + \frac{6}{11}$ | 0.11515     |
| Ch(1)+Ch(2)+Ch(3)+Ch(4)            | $\frac{1}{2} + \frac{4}{5} + \frac{3}{5} + \frac{6}{11}$ | 0.11136     |

At (1,1/3,0). Because of the hexagonal lattice, the projection of the Ch(1) onto the $\vec{a}$-direction gives a distance of $\langle 1 + \frac{2}{3} \cos(120^\circ), 0, 0 \rangle = \langle 2/3, 0, 0 \rangle$ and Ch(2) gives $\langle 1 + \frac{1}{3} \cos(120^\circ), 0, 0 \rangle = \langle 5/6, 0, 0 \rangle$. In reciprocal space, in units of $2\pi/a$ ($2/\sqrt{3}$), the q-vector is built by taking the reciprocal of the distance, or $1/distance$. For the Ch(1) the q-vector is $(3/2, 0, 0) = (1+1/2, 0, 0)$ and for the Ch(2) the q-vector is $(6/5, 0, 0) = (1+1/5, 0, 0)$. Putting the satellites in the 0 to 1 reciprocal zone, by taking the chiral satellites, the two fractional periodicities are 1-1/2 = 1/2 for Ch(1) and 1-1/5 = 4/5 for Ch(2) with reference to an even wave vector (here 0). The average of these wave vectors is 0.65, which is close to the ordering wave vector observed experimentally. It is possible to have a closer result by adding another unit cell along the $\vec{a}$-direction with Ch(3) and Ch(4) Bragg planes as shown in Fig.1. Doing so adds the positions at $\langle 2 + 2/3 \cos(120^\circ), 0, 0 \rangle = \langle 5/3, 0, 0 \rangle$ for the Ch(3) and $(2 + 1/3 \cos(120^\circ), 0, 0) = \langle 11/6, 0, 0 \rangle$ for the Ch(4). The q-vector for Ch(3) is $(3/5, 0, 0)$ and $(6/11, 0, 0)$ for Ch(4) all in the first reciprocal space zone (from zero to one). The average wave vector of the latter Ch(3) and Ch(4) gives 0.57273, lower than the 0.65 of the first two Bragg planes. Doing the average over the four Ch(n) Bragg planes gives a q=0.61135 which is very close to 0.610 observed experimentally (a difference of 0.3%). It is possible to refine this model by taking the weighted average 0.65x+0.57271(1-x)=0.610 which leads to x=48% for the mixing of the two sets of Bragg planes. Other ordering wave vectors obtained by taking different partial averages appear in Table II. These results do not require nesting. With nesting, Ch(2) alone generates wave vector 12/5=2+2/5 which, when translated to zero, gives a satellite at 0.4 which is very close (a difference of 3%) to the 0.39 IC satellite observed experimentally.

It is worth noting measurements in a high magnetic field up to 8 Tesla on this compound showed a transition between two “lock-in” wave vectors from 0.610 (1/2+0.110) to 0.613 (1/2+0.113) during a magnetic domain reorganization due to the change of strain in the magnetic field.$^{[22]}$ This result is very close to the loss of Ch(3) in the equal averaging of the four Ch(n) maxima as shown in Table II. This loss can be explained by the accidental correspondance between the Ch(3) wave vector of 3/5 (0.6) and the ordering wave vector of 0.61 and dampens the Ch(3) contribution to the average. It would be interesting to see if the other $\tau$ obtained in the table with this model appear at higher magnetic fields.

As a second example with hexagonal symmetry, Ce-CuSn has a $P6_3/mc$ #186 crystal structure with Ce-atoms at the (2a) $\langle 0, 0, 0 \rangle$ and (0,0,1/2) positions, Cu-atoms at the (2b) positions or Cu(1)=$\langle 1, 3, 2/3, z \rangle$ and Cu(2)=$\langle 2/3, 1/3, z + 1/2 \rangle$ with $z_{Cu}=0.27337$, and Sn-atoms are at the (2b) positions also but with $z_{Sn}=0.73435$ as published.$^{[39]}$ Since the Cu- and Sn-atoms have the same projections onto the hexagonal $\vec{a}$-direction as the Ni-atoms in UNi$_2$Al$_3$, the Cu- and Sn-nearest to the reference atom in Fig. 1 would only contribute to reciprocal lattice wave vectors. Magnetic ordering observed in this compound gives satellites at (1±$\tau$,0,0) with $\tau = 0.115$ as reported near each reciprocal lattice wave vector.$^{[39]}$ This value appears as the average of Ch(1), Ch(2) and Ch(4) in Table II, but the zone center is at 1/2 in reciprocal space and not near a structural reciprocal lattice wave vector. Following the Ch(n) model of UNi$_2$Al$_3$, nesting of the wave vectors involved in the sum leads to Ch(1) contributing to $\langle 3/2 \times 2, 0, 0 \rangle = \langle 3, 0, 0 \rangle$ with no fractional part (which will be ignored in the average). Ch(2) contributes to $\langle 6/5 \times 2, 0 \rangle = \langle 12/5, 0, 0 \rangle = \langle 2+2/5, 0, 0 \rangle$ which can be translated to $\langle 0+2/5, 0 \rangle$, Ch(3) to $\langle 3/5 \times 2, 0 \rangle = \langle 6/5, 0 \rangle = \langle 1+1/5, 0 \rangle = \langle 0+1/5, 0 \rangle$ and Ch(4) to $\langle 6/11 \times 2, 0 \rangle = \langle 12/11, 0 \rangle = \langle 1+1/11, 0 \rangle = \langle 0+1/11, 0 \rangle$. Note that the algorithm is changed to force a development near (0,0,0) by simple translation (not with the chiral satellites at (2,0,0)). The experimental result of 0.115 is the
average of $\text{Ch}(2)$, $\text{Ch}(3)$ and $\text{Ch}(4)$ divided by two, after a translation of the satellites back to $(1,0,0)$ as shown in Table IV. The last division by two is the result of an AF modulation of a CDW, i.e. a SDW which may come from the inclusion of 0 wave vectors in the sum from atoms contributing to reciprocal lattice positions. In this $\text{Ch}(n)$ phenomenological model, the ordering wave vectors in UNi$_2$Al$_3$ and CeCuSn can be made to have same type of SDW on the hexagonal lattice.

C. MnSi

MnSi has attracted a lot of attention recently because it can be considered a topological insulator and exhibits a Skyrmion lattice phase upon application of a magnetic field. Its crystal structure belongs to the tetrahedral $P\overline{2}13$ #198 space group with both Mn and Si ions sitting at the $(4a)$ symmetry position $(u,u,u)$, and the three coplanar sites perpendicular to the $(1,1,1)$ direction $\langle-u+1/2,-u,u+1/2\rangle, \langle-u+1/2,-u+1/2\rangle, \langle u+1/2,-u+1/2,-u\rangle$ with $u_{Mn}=0.138$ and $u_{Si}=0.845$. Below $T_N=29.5K$, the onset of a helical SDW is observed with a wavelength of 190Å along the $(1,1,1)$ direction which can be viewed, in reduced reciprocal lattice units, as $2\pi/190 = h/2\pi/a$ with $a=4.56\text{Å}$ and $h=0.024$. The crystal structure has no inversion symmetry, but the IC satellites at $G = 0$ are symmetric. The projection of the $(4a)$ lattice sites onto a unit vector along the $(1,1,1)$ leads to two periodicities: $1/\sqrt{3}u$ and $\sqrt{3}/(1-u)$, the latter coming from the three coplanar sites. For the Mn sites, the resulting wave vectors are 4.18370 and 2.00934 respectively. For the Si sites, the results are 0.683255 and 11.17452 (12±0.82548). By inspection, only the Mn coplanar sites, with 2.00934 has a small enough satellite wave vector to build the helical magnetic structure. If the experimental magnetic satellites are the third harmonic of the fractional part $3\times0.00934=0.28$, which is close to the 0.024 published, an error of 16%. The existence of the third harmonic indicates a squarer distribution for the helical structure in MnSi, from a Fourier series point of view. The first harmonic at the satellite position $\tau=0.00934$ near each reciprocal lattice wave vector could be observed experimentally with a higher resolution, like with resonant synchrotron X-ray probe for example. As an alternative analysis, with a weighted average of the satellites $0.00934 \times (1-x)$, $0.18370 = 0.024$ leads to $x=92\%$ mixing for the Mn sites. Nesting of the wave vectors does not lead to the observed value. Considering the other chiral pair for the Mn sites along the $(−1,−1,−1)$ direction with $u → 1-u$, $1/(\sqrt{3}(1-u))$ and $\sqrt{3}/u$ leads to the negative wave vectors -0.66978 and -12.5511 respectively. Taking the sum of the four satellite wave vectors for the Mn sites translated to 0, without averaging, leads to 0.1837 + 0.00934 - 0.66978 - 0.5511 = -1.02784, which gives a satellite near 0.028 also near to 0.024 seen experimentally. This latter result is obtained without a center of mass transformation but is a residual momentum from two chiral unit cells considering inversion in the crystal structure.

D. Chromium

Cr has long been known to exhibit IC ordering and has been intensely studied by neutron$^{14,15}$ and X-ray scattering experiments$^{14,15}$. In reciprocal space, a low temperature SDW is observed at $Q=(0.9515,0,0)$ with $\tau=0.0485$ near the AF $(1,0,0)$ zone center, a CDW at $2Q=(1.903,0,0)$ or $(2−2\tau,0,0)$ is observed as well as another CDW harmonic at 4$Q$, which can be relabeled as $(4−4\tau,0,0)$, also observed at 4$Q-2=(2±4\tau,0,0)$ positions. A 3$Q$ wave vector harmonic has also been observed$^{15}$. In the following analysis, simple crystallographic considerations can help gain insight about the experimental IC wave vectors observed. Cr has a BCC crystal structure #229 with atoms at $(0,0,0)$ and $(1/2,1/2,1/2)$ above $T=312K$ and experience structural phase transitions below $T=122K$ to a tetragonal phase $I4/mmm$ #139 also with atoms at the $(2a)$ symmetry positions $(0,0,0)$ and $(1/2,1/2,1/2)$ where the longitudinal incommensurate SDW develops. The tetragonal distortion does not change the reduced unit cell. Some recent theory describes Cr as a spin-split metal$^{23}$ where spin-up and spin-down bands move in opposite directions. The phenomenological model presented here also has broken inversion symmetry.

The Bragg plane expansion in Cr appears in Fig 2. Being spaced by 1/2 the Bragg planes at Cr(n) give a 2/n wave vector. Table IV shows the cumulative averaging from each Bragg plane addition. There are two wave vectors with experimental relevancy: the $1+\tau_0=1.04167$ gives a satellite at $1-\tau_0=0.95833$ which is 0.7% from 0.9515 of the observed Q-satellite experimental value, and the second remarkable value in the table is at 0.91333=1-2$\tau_0$ with $\tau_0=0.04333$, although not seen experimentally at the $(1,0,0)$ wave vector but at the $2-2\tau=1.9030$ wave vector, is nevertheless 0.5% from the calculated value at $2-2\tau_0=1.91333$ with $\tau_0=0.04333$ from
TABLE IV. Calculation of ordering wave vectors from the Cr(n) Bragg Plane expansion along the \( \bar{a} \)-direction in Cr metal (see Fig. 2). The values in bold are near the experimental wave vectors satellites near (1,0,0).

| Atoms                      | Average | Avg. Q |
|----------------------------|---------|--------|
| Cr(1)+Cr(2)                | \( \frac{2+1}{2} \) | 1.5    |
| Cr(1)+Cr(2)+Cr(3)          | \( \frac{2+1+2/3}{3} \) | 1.2222 |
| (1)+(2)+(3)+(4)            | \( \frac{2+1+2/3+1/2}{4} \) | 1.04166|
| (1)+(2)+(3)+(4)+(5)        | \( \frac{2+1+2/3+1/2+2/5}{5} \) | 0.91333|
| (1)+(2)+(3)+(4)+(5)+(6)    | \( \frac{2+1+2/3+1/2+2/5+1/3}{6} \) | 0.81666|

Table V

TABLE V. Relabeling of ordering wave vectors from the Cr(n) cumulative Bragg plane expansion along the \( \bar{a} \)-direction in Cr metal (see Fig. 2). The values in bold indicate averaging by group of three, six and nine Bragg planes that correspond to values of \( q_0 \) seen experimentally. Averaging above twelve Bragg planes slowly converges to zero as shown in Fig. 3.

| Atoms                      | Average | Harmonic | \( q_0 \) |
|----------------------------|---------|----------|----------|
| Cr(1)+Cr(2)                | \( \frac{2+1}{2} \) | 1+12\( q_0 \) | 0.0417   |
| Cr(1)+Cr(2)+Cr(3)          | \( \frac{2+1+2/3}{3} \) | 1+6\( q_0 \) | 0.0370   |
| (1)+(2)+(3)+(4)            | \( \frac{2+1+2/3+1/2}{4} \) | 1+\( q_0 \) | 0.0417   |
| (1)+...+(5)               | \( \frac{2+2/5}{6} \) | 1-2\( q_0 \) | 0.0433   |
| (1)+...+(6)               | \( \frac{2+1/3}{6} \) | 1-4\( q_0 \) | 0.0458   |
| (1)+...+(7)               | \( \frac{2+2/7}{6} \) | 1-6\( q_0 \) | 0.0432   |
| (1)+...+(8)               | \( \frac{2+1/4}{6} \) | 1-8\( q_0 \) | 0.0401   |
| (1)+...+(9)               | \( \frac{2+2/9}{6} \) | 1-10\( q_0 \) | 0.0371   |
| (1)+...+(10)              | \( \frac{2+1/5}{6} \) | 1-12\( q_0 \) | 0.03451  |
| (1)+...+(11)              | \( \frac{2+2/11}{6} \) | 1-14\( q_0 \) | 0.0322   |

It is interesting to expand this analysis further along the \( \bar{a} \)-axis as listed in Table V. The SDW satellites observed at \( 1\pm q_0 \) appear in the table as well as other even multiples of \( q_0 \) unobserved. The relative stability of \( q_0 \) in the table is remarkable and contains satellites near the experimental values for the CDW and SDW observed in Cr. The transition in Cr from \( \delta = 0.037 \) to \( \delta = 0.048 \) observed experimentally on decreasing temperature would come from a three Bragg plane averaging at high T (a doubling of the BCC/tetragonal unit cell when including the reference atom) to six at low T (a tripling and a half of the BCC/tetragonal unit cell). There is a periodicity by a group of three Bragg planes in the Table. It is the doubling of these SDW wave vectors in the table that would generate the CDW harmonics at 2\( \pm (2n)\tau \) seen in the X-ray experiment. From the table, there is a direct connection between the doubling of the 1\( \pm q_0 \) and the 2\( \pm 2q_0 \) satellites (labeled 2Q and 4-2Q in the X-ray paper). For the other satellites in the table, the doubling of 1\( \pm (2n)q_0 \) leads to the 2\( \pm (4n)q_0 \) satellites.

FIG. 2. Bragg Plane expansion, labeled Cr(n), for the calculation of the CDW and SDW in Cr. The third dimension of the crystal structure is projected onto the plane. All the planes are spaced by \( 1/2 \) lattice spacing from the reference atom at the left of the figure.

FIG. 3. Graph of \( q_0 \) from Table V in Chromium as function of the number of Bragg planes in the partial sum. Note the grouping by 3 of the first 6 sums near the experimental \( q_0 = \pm 0.04 \). The lowest values in the groupings are reminiscent of the experimental satellite wave vectors (containing 3 and 6 Bragg planes respectively) for high and low temperature.

III. SHORT AND LONG RANGE FLUCTUATIONS

The wave function \( \Psi \) in Eq. 6 contains many sources of fluctuations. There are magnetic fluctuations contained in the \( S(\eta, i) \) part of the wave function. The S-part, being a sum of eigenstates, is a superposition of \( S_y \) components and leads to magnetic fluctuations. Also, since the reference \( x \) can be taken on any electron involved in the sum, there is a fluctuation of the ever creation and destruction of the center of mass bulk states once it is achieved. The lifetime for these bulk states are short due to the Heisenberg relation since the electrons are moving away from the center of mass reducing their correlation lifetimes with increasing insulating character. The superposition of the many magnetically- and charge-fluctuating
Ψ wave functions in a crystal is the character of correlated electron systems, like heavy fermions, as seen in many U- and Ce-compounds. In CePdSn and Cr-metal, these correlations extend over many lattice spacings but much less than what is observed in superconductivity, for which the correlations extend over the scale of hundreds of nanometers (10^3 the lattice spacing). These two effects are competing on different length scales. In superconductivity, there is a softness in the dynamic response because the center of mass momentum of the Cooper pair with \( q_{cm} = (Q_0 + Q_1)/2 \) leads to the symmetric superconducting momenta \( k_a = (Q_0 - Q_1)/2 \) in the center of mass. With two wave vectors \( Q \), \( F(\delta_j, Q_j) = 2\sinh(k_a\delta_1/2) \) could extend over large length scales for large \( \delta_1 \) with the onset of bulk states. If the IC topological fluctuations are to be linked to superconductivity in the center of mass, the correlations need a relatively long lifetime, which in topological dynamic ordering depends strongly on the local crystallographic lattice environment. This would make this “tunable” superconducting state fundamentally different than BCS theory (which requires \( Q_0 = -Q_1 \) and a centrosymmetric structure with \( q_{cm} = 0 \) to couple with phonons of the crystallographic lattice). Topological dynamic ordering could apply to superconductivity in non-centrosymmetric structures if \( q_{cm} \) matches the momentum of a phonon.

**IV. CONCLUSION**

The phenomenological method for calculating the average IC unit cells applies favorably to itinerant electrons systems (itinerant f-electrons and metallic ions). The dynamic average wave vector \( q_{cm} \) restores inversion symmetry in a moving reference frame, the center of mass, for the correlated electrons. The correspondence to the IC magnetic ordering observed in materials and \( q_{cm} \) indicates an origin for fluctuations from topological effects. Such IC wave vectors are not expected to move with temperature except when there is a change in the number of electrons involved in the partial sums (see discussion of \( UNi_2Al_3 \) or Cr-metal). The algorithm to calculate the IC wave vector requires simple concepts like: a local expansion from crystallographic Bragg planes, nesting or not of the wave vectors, a division by two when there is AF order of a CDW is achieved and a reciprocal space reference wave vector chosen for the expansion of the satellites (usually an even multiple of a Bragg plane). The translation to zero wave vector represents standing waves without net velocity \( v \) in \( Q' = m v \).

In the few examples explored topological dynamic ordering gives an origin of the correlations in materials as shown in CePtSn, CePdSn, CeNiSn, CeRhIn5, CeNiAsO, URu2Si2, BSSCO, Rb2ZnBr4, CeCu(6−x)Au$_x$, Cr and in the hexagonal systems UNi$_2$Al$_3$ and CeCuSn. In MnSi, there is an explanation for the experimental wave vectors based on the fractional positions of atoms in the crystallographic unit cell without averaging. This study emphasizes the strong dependence on crystallography for the otherwise itinerant electrons and complements existing band-structure calculation methods to help improve the predictability of IC ordering wave vectors missed in some studies. It may help classify IC order in materials, especially when IC satellites do not move with changing temperature, and hence depends strongly on the commensurate crystalline environment.

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