Implications of the B20 crystal structure for the magnetoelectronic structure of MnSi

T. Jeong and W. E. Pickett

Department of Physics, University of California, Davis, California 95616, USA

(Received 18 March 2004)

Due to increased interest in the unusual magnetic and transport behavior of MnSi and its possible relation to its crystal structure (B20) which has unusual coordination and lacks inversion symmetry, we provide a detailed analysis of the electronic and magnetic structure of MnSi. The nonsymmorphic P2\(_1\)3 spacegroup leads to unusual fourfold degenerate states at the zone corner R point, as well as “sticking” of pairs of bands throughout the entire Brillouin zone surface. The resulting Fermi surface acquires unusual features as a result of the band sticking. For the ferromagnetic system (neglecting the long wavelength spin spiral) with the observed moment of 0.4\(\mu_B/\text{Mn}\), one of the fourfold levels at R in the minority bands falls at the Fermi energy \((E_F)\), and a threefold majority level at \(k=0\) also falls at \(E_F\). The band sticking and presence of bands with vanishing velocity at \(E_F\) imply an unusually large phase space for long wavelength, low energy interband transitions that will be important for understanding the unusual resistivity and far infrared optical behavior.

DOI: XXXX

PACS number(s): 71.28.+d, 75.10.Lp, 71.18.+y, 71.20.Lp

I. INTRODUCTION

Although the binary compound MnSi has been of interest for some time, unusual behavior of this material has led to accumulating evidence that it is a novel type of weak ferromagnet. MnSi shares the B20 structure with low symmetry occupied sites with the monosilicides of Cr, Fe, and Co that is particularly interesting because of its lack of a center of inversion. Isosctructural FeSi has attracted substantial interest as a correlated electron insulator (sometimes referred to as “Kondo insulator”) and although the gap of 0.13 eV is reproduced very well by usual density functional based (unpolarized) band theory as shown by Mattheiss and Hamann (MH),\(^1\) a local moment is evident at elevated temperature and correlation effects are obvious. The existence of the gap in band theory seems to be a rather delicate one depending strongly on the internal structural parameters and Fe-Si hybridization, yet the gap persists in (paramagnetic) MnSi where it lies above the Fermi level. Since transition metal silicides (CrSi and CoSi, besides the two mentioned) with varying electron concentrations take this structure, the gap cannot be instrumental in stabilizing this structure.

While FeSi remains paramagnetic in spite of displaying local moment behavior, MnSi becomes magnetically ordered below 29 K. At higher temperatures its susceptibility is Curie-Weiss-like, with a Mn moment of 2.2\(\mu_B\).\(^2\) It was established by Ishikawa et al.\(^3\) that the order is that of a long-wavelength heliomagnet \(^4\) [wavelength \(2\pi/q=190\text{ Å, } q=1/20(\pi/a)\)] with an ordered moment of 0.4\(\mu_B/\text{Mn}\). The spiral structure has been attributed to the lack of inversion symmetry in its B20 crystal structure, which brings the Dzyaloshinski-Moriya interaction into play.\(^5\) The Curie temperature drops with pressure until magnetic order disappears\(^6,7\) at the quantum critical point (QCP) of \(P_c=1.46\text{ GPa}\), a modest pressure that corresponds to a rather small volume change from ambient pressure. A magnetic field of 1 kOe leads to a conical ordered phase, while 6 kOe is sufficient to transform the system to ferromagnetic (FM) order.\(^5\) The resistivity \(\rho(T)\) under pressure and field has attracted considerable attention. Thessieu et al.\(^8\) reported magnetoresistance that showed strong structure in the 0.5–1.2 T range for pressures of 0.7–1.7 GPa.\(^9\) Near the critical pressure \(P_c\), they observed \(\rho\propto T^{1.7}\) behavior in zero field that reverted to \(T^2\) at 3.3 T. Initially the resistivity \(\rho\) which is Fermi-liquid-like \((T^2)\) in the FM phase, was reported to be linear-in-\(T\) for \(P>P_c\),\(^7\) but recent data show it to be \(\rho\propto T^{3/2}\) up to 30 kbar (twice \(P_c\)).\(^9\) This scaling suggests something different from both normal Fermi liquid behavior \((\rho\propto T^2)\) and the T-linear non-Fermi-liquid dependence seen in several metals near the quantum critical point, and nonuniversal. Recent zero-field \(^29\)Si NMR data\(^10\) have been interpreted in terms of an onset of inhomogeneous magnetism at 1.2 GPa which extends at least to 1.75 GPa, completely encompassing the QCP. Earlier Thessieu et al.\(^8\) had reported,\(^11\) also from \(^29\)Si NMR studies, that some kind of local magnetic order remained above \(P_c\). For strong inhomogeneity, such as in a two-phase system, non-Fermi-liquid behavior in \(\rho(T)\) would not be so surprising.

There are other data that suggest unusual correlated electron behavior (magnetic fluctuations, presumably) for MnSi. The field dependence of the muon spin relaxation rate reported by Gat-Malureau et al.\(^12\) requires an unconventional explanation. In addition, the optical conductivity even at ambient pressure is strongly non-Drude-like, with the behavior having been represented by Mena et al.\(^13\) in terms of a frequency-dependent effective mass.\(^13\) The measured complex low frequency optical conductivity has been modeled by the form \(\sqrt{\gamma(T)+i\omega}\), where \(\gamma(T)\) is the \(T\)-dependent relaxation rate. The antisymmetric part of the magnetic susceptibility that appears due to the non-centrosymmetric space group has recently been measured by Roessli et al.\(^14\) The fluctuations well above \(T_c\) are incommensurate with the lattice, and furthermore are chiral in nature, meaning that the fluctuation spectrum depends on the sign of the polarization with respect to the momentum transfer \((\vec{P}_{\text{ps}}\cdot\vec{Q})\).

As mentioned above, MnSi shares the B20 crystal structure with FeSi, but contains one electron less per formula
unit. In spite of the strong interest in this unique compound, there has been no thorough study of its electronic and magnetic structure in general, and in particular how it relates to the B20 crystal structure. The paramagnetic bands and density of states were presented in a short report by Nakaniishi et al. Taillefer and collaborators applied the linear muffin-tin orbital method with band shifting to model the Fermi surfaces, but did not report the general electronic structure and magnetic behavior. Trend studies of several transition metal monosilicides using a planewave pseudopotential method were reported by Imai et al. Yamada and coworkers have reported studies of the volume dependence of the magnetic moment using the linear muffin-tin orbital method in the atomic sphere approximation.

In this paper we present a detailed investigation of the electronic structure and magnetization of MnSi within the local density approximation (LDA) using self-consistent full potential methods. We address specifically the connection of the electronic and magnetic structure to the unusual coordination of the Mn atom and to the nonsymmorphic B20 space group which has no inversion operation. We find that “band sticking” around the faces of the Brillouin zone have consequences for the electronic structure and Fermi surfaces that should be recognized when interpreting data. The LDA minimum of energy occurs for a ferromagnetic moment of almost $1\mu_B$/Mn, considerably higher than the experimental value of 0.4$\mu_B$ and also quite different from the value of 0.25$\mu_B$ reported earlier by Taillefer, Lonzarich, and Strange with a more approximate method of calculation. Fixing the moment at the observed value, we report the resulting Fermi surfaces. In the minority band, considerable potential for nesting arises. The manner in which these features may influence the observed properties of MnSi are discussed. The equation of state was calculated earlier by Lerch and Jarlborg.

II. THE B20 CRYSTAL STRUCTURE

One view of the MnSi B20 structure is shown in Fig. 1. There are four MnSi formula units in the cubic primitive cell. MH have described in detail how the local coordination of an individual Mn or Si atom can be pictured in terms of an atomic sphere approximation. 18,19

Starting from the rocksalt idealization, one considers a dimerizing-type distortion involving displacement of Mn or Si atoms along [111] directions, whose primary effect is to transform rocksalt Mn-Si neighbors along [111] directions into MnSi nearest neighbors. These distortions are large (1.6 eV energy gain per molecule calculated by MH), and strongly distort the space-group symmetry from $Fm\bar{3}m$ to $P2_13$, a primitive lattice generated by a screw axis $2_1$ and a threefold axis (3). The Bravais lattice remains simple cubic but the point symmetry is reduced to four threefold axes. The space group consists of threefold rotations around one specific (111) direction, three screw axes consisting of a 180° rotation around a cubic axis followed by a $(\frac{1}{2},\frac{1}{2},0)$ type nonprimitive translation, and combinations of these.

Both the Mn and Si atoms are located at the 4(a)-type sites in the simple-cubic unit cell, with position coordinates at $(u,u,u), (\frac{1}{2}+u, \frac{1}{2}-u,-u), (-u, \frac{1}{2}+u, \frac{1}{2}-u)$, and $(\frac{1}{2}-u, -u, \frac{1}{2}+u)$. The corresponding values for the internal atom-position parameters are $u_{\text{Mn}}=0.137$ and $u_{\text{Si}}=0.845$. Given the MnSi lattice parameter is $a=4.558$ Å, 15 the local coordination of Mn consists of one Si neighbor at 2.11 Å (lying along a [111] direction, three neighbors at 2.35 Å and three neighbors at 2.69 Å). The point symmetry at the Mn and Si sites is $C_3$. Taking into account time-reversal symmetry (when nonmagnetic) with the twelve space group operations, the reducible Brillouin zone (BZ) is 1/24 of the full zone.

Another way to picture the B20 structure has been discussed by Vočadlo et al. in terms of an “ideal B20” structure with $u_{\text{Mn}}=1/4(\tau)=0.1545, u_{\text{Si}}=1-1/4(\tau)=0.8455$, where $\tau=(1+\sqrt{5})/2$ is the golden ratio. The nearest neighbor coordination of each atom then is seven equidistant atoms of the opposite kind, at a distance $a\sqrt{3}/(2\tau)$. These seven atomic sites lie on seven of the twenty vertices of a pentagonal dodecahedron centered on the atom. This sevenfold coordination also supports the interpretation of Dmitrienko that the B20 structure can be viewed as a crystalline approximation to an icosahedral quasicrystal. To our knowledge, there has been no clear interpretation in terms of chemical bonding of why MnSi (and CrSi, FeSi, CoSi) prefer the B20 structure. Vočadlo et al. have calculated the equation of state for FeSi in the B20, NaCl, CsCl, NiAs, and inverse-NiAs structures using the VASP planewave code. They find that under pressure the internal coordinates move closer to...
IMPLICATIONS OF THE B20 CRYSTAL STRUCTURE

...their ideal values discussed above, and that a transformation to the CsCl structure is predicted at 13 GPa, far above the quantum critical point where magnetism vanishes.

III. METHOD OF CALCULATIONS

We have used the full-potential nonorthogonal local-orbital (FPLO) method\textsuperscript{24} within the local density approximation (LDA).\textsuperscript{25} Mn 3s, 3p, 4s, 4p, 3d states and Si 3s, 3p, 3d were included as valence states. All lower states were treated as core states. The inclusion of the relatively extended 3s, 3p semicore states as band states was done because of the considerable overlap of these states on nearest neighbors. This overlap would otherwise be neglected in the FPLO scheme. Si 3d states were added to increase the quality of the basis set. The spatial extension of the basis orbitals, controlled by a confining potential \((r/r_0)^3\), was optimized to minimize the total energy. The self-consistent potentials were carried out on a \(20 \times 20 \times 20\) uniform mesh in the Brillouin zone, which corresponds to 700k points in the irreducible part for \(P2_13\).

IV. RESULTS AND DISCUSSIONS

A. Paramagnetic bands

Considering the B20 structure as derived from the rocksalt structure, the MnSi bands look very similar to those presented by MH for FeSi, in both the primitive cell and for the unit cube in which the \(X\) points are folded back to the \(\Gamma\) point. As noted by MH, there is no reason to expect any Fermi surface driven instability of the rocksalt structure, because several transition metal monosilicides with different band fillings have the same structure. We calculate the B20 structure to be 1.5 eV per formula unit lower in energy than the rocksalt structure. Because of some symmetry-related peculiarities of the band dispersion, we compare the paramagnetic band structure of MnSi with those of rocksalt MnSi as well as to those of the Mn skeleton itself.

\textit{Full bands of MnSi}. We first show the full bands of MnSi in the valence-conduction region in Fig. 2. It is this PM band structure (at slightly reduced volume) that becomes relevant at the quantum critical point. Since Si contributes four, and Mn contributes seven, valence electrons, there are enough electrons to fill \(11 \times 4\) molecules/2 spins=22 bands. With the four 3s, 3p states of Si and the five 3d states of Mn, there are 36 bands valence-conduction bands. The lowest four bands in the range \(-6.5\) to \(-11\) eV (see Fig. 2) are Si 3s bands. Mn 3d character is confined primarily to the \(-3\) to \(+1\) eV region, nevertheless these bands are strongly affected by the mixing with Si (see below). As a result of the Mn \(d\)-Si \(p\) interaction, the Si 3p character is repelled strongly to the region \(-3\) to \(-6\) eV in the valence bands, and above 1 eV in the conduction bands.

A very narrow indirect gap of 0.1 eV lies just above the Fermi level, as reported earlier by Nakanishi \textit{et al}.\textsuperscript{15} This gap, which is the fundamental gap in semiconducting FeSi, occurs above the MnSi Fermi level since this system contains four fewer valence electrons per unit cell. This gap acquires some significance in establishing the stability of the FM state, at least within LDA (see below).

\(\text{Mn}\square\). To give an impression of Mn bands undisturbed by Si \(p\) states, and therefore an indication of direct Mn \(d\)-\(d\) coupling, we show in Fig. 3 the bands of Mn\square=MnSi with the Si atoms missing. The 3d bands are about 2 eV wide at \(k\) =0 (the density of states extends over 2.5 eV). As is the case also for MnSi itself (Fig. 2), bands “stick together” in pairs along the BZ edges \(R-X-M-R\). This symmetry-dictated band-sticking (discussed more fully below) and hybridization make the dispersion appear small along the BZ faces, but the bands emanating radially (along \(\Gamma-X\) and \(\Gamma-R\) directions) reflect the actual dispersion. At \(\Gamma\) the twenty states (four atoms \(\times\) five 3d states) break up into a single nondegenerate state, two twofold degenerate, and five threefold degenerate states. At the zone corner \(R\) point, all bands show unusual fourfold degeneracy, again a consequence of the nonsymmorphic nature of the B20 space group.

The zone-edge bands show one other unusual feature. The twenty bands break up into a single sticking pair at the bot-
sticking can be found in the recent papers of König and Mermin. 26,27 Band degeneracy at a wave vector \( \vec{k} \) is associated with the little group of \( \bar{k} \), which is the subgroup of the point group operations \( \{g\} \) that bring \( \vec{k} \) back to itself, each modulo a reciprocal lattice vector \( \bar{G}_g \). General (nonsymmetric) points on the face of the BZ of the \( P2_13 \) space group have a little group containing only the identity. To obtain the full symmetry of the actual band structure, we have to augment the symmetry considerations to include time reversal \( T \), whose effect is \( T\psi_g(r) = \psi_g(-r) \), i.e., its effect is to invert the wave vector \( \vec{T}k = -\vec{k} \) just as would an inversion operation (which is missing from \( P2_13 \)). Thus in the operations on \( \vec{k} \), we include \( T \) together with the actual point group operations. Consider a point on the BZ face \( K = (\pi, k_y, k_z) \) (taking unit lattice constant). Now the little group of \( \bar{K} \) consists of the identity \( I = g_1 \) and the product \( TS = g_2 \), where \( S \) is the 180° rotation around the \( \bar{x} \) axis \((x, y, z) \rightarrow (\bar{x}, \bar{y}, \bar{z})\). When combined with the nonsymmetric translation \( \tau = (1/2, 1/2, 0) \), it forms the screw axis space group operation \( S = [S; \tau_5] \). With two members in the little group together with the phase factor introduced by \( \tau \) for the \( g_2 \) operation, the analysis of König and Mermin indicates band sticking over the entire \( k_x = \pi \) face (and thus all faces) of the BZ. Explicit calculation confirms the band sticking. The extensive fourfold degeneracy at \( \bar{R} \) that was pointed out in the previous subsection arises already in the rocksalt supercell of Fig.4. Extra degeneracies are expected when a supercell (nonprimitive cell) is chosen; it is a consequence of the \( P2_13 \) symmetry that these degeneracies remain after the rocksalt \( \rightarrow B20 \) internal distortion.

At the zone corner \( R \) point, the little group consists of all space group operations, often referred to as “full symmetry of the \( \Gamma \) point.” In fact, most of the little group members of the \( R \) point are associated with nonzero reciprocal lattice vectors \( \bar{G}_g \) (unlike the \( \Gamma \) point case), and associated sticking leads to more degeneracy than occurs at the \( \Gamma \) point.

C. Ferromagnetic phase

Since the long wavelength helical magnetic structure can be considered to be locally FM and a field of only 6 kOe is sufficient to drive the heliomagnetic structure to FM order, it is relevant to consider a simple FM ordering. Since spin-orbit coupling is small in 3d magnets, we neglect it, so the direction of magnetic polarization is not coupled to the lattice. Within LDA, a FM state with moment almost at the half metallic value of \( 1 \mu_B/\text{Mn} \) is obtained: the Fermi level in the minority bands lies just at the bottom of the gap in the majority bands. The four holes compared to FeSi lie entirely in the minority states. This result is substantially different from experimental moment of 0.4 \( \mu_B/\text{Mn} \), and overestimate that is not uncommon for weak ferromagnets near the quantum critical point. It does, however, mean that analyzing the LDA minimum is unfruitful.

To reveal the electronic and magnetic structure of MnSi as fully as possible, we have constrained the moment to the experimental value of 0.4 \( \mu_B/\text{Mn} \). The bands in the 3d region

FIG. 4. Band structure for nonmagnetic MnSi in the simple cubic four-molecule nonprimitive cell of the reference rocksalt structure MnSi. Actually, both Mn and Si have been displaced by \( \Delta u = 0.0025 \) to the B20 structure to illustrate lifting of degeneracies (the tiny band splittings, especially at \( \Gamma \) and \( M \)) by the crystal symmetry breaking. Note that there is no splitting whatsoever at the zone corner \( R \) point, while fourfold degeneracies at \( X \) and \( M \) are broken into “sticking” pairs.
Fermi surface, which includes a situation represents the point of change in topology of the length in the high temperature superconductors, and the of possible consequences which have been discussed at.

\[ R \text{ has vanishing velocity at } k = 0, \text{ a threefold level lies precisely at } E_F. \]  

The FM bands are nearly uniformly split versions of the paramagnetic bands. The notable feature is the coincidence of two complexes of degenerate bands at high symmetry points that lie essentially at the Fermi level. (Since the magnetization has not been determined to any more accuracy than “$0.4 \mu_B$/Mn” there is an uncertainty of several tens of meV of band placements.) At $k=0$, a threefold level lies precisely at $E_F$. The middle of these three bands approaches $k=0$ with vanishing slope, while the other two have nonvanishing (equal and opposite in sign) velocities of 1.25 x 10^7 cm/s. At the zone corner $R$ point, a fourfold level lies extremely near $E_F$ (about 15 meV above). These bands all have vanishing velocity at $R$.

The occurrence of a vanishing velocity at $E_F$ has a variety of possible consequences which have been discussed at length in the high temperature superconductors and the associated van Hove singularities have great general importance. The most well known case is the half-filled square lattice with only nearest neighbor hopping, where a van Hove singularity occurs at the zone edge $X = (\pi/\alpha, \pi/\alpha)$ point in two dimensions. In addition to causing the van Hove nonanalyticity (and peak) in the DOS, this situation represents the point of change in topology of the Fermi surface, which includes a “Lifshitz anomaly of order 21/2” in thermodynamic properties at low temperature.

**D. Fermi surfaces**

The Fermi surfaces for a magnetization of 0.4 $\mu_B$/Mn are shown in Figs. 6–8 for majority and minority spins, respectively. The majority surfaces consist of a $\Gamma$-centered rounded octahedron and a pair of open jungle gym type surfaces. These latter two surfaces illustrate two consequences of the unusual B20 space group of MnSi. First, although the Bravais lattice is simple cubic, the lack of a fourfold rotation around the cubic axes is reflected in the elliptical (rather than circular) intersection of the arms with the zone faces. The orientation of the major axis of this ellipse rotates from face to face in a way that preserves the threefold rotation symmetry around (111) axes.

More difficult to accommodate with our conception of periodic cells (whether in real or reciprocal space) is the recognition that these jungle gym arms do not intersect the zone faces perpendicularly. The periodicity of the total Fermi surface is restored by the fact that there are two touching Fermi surfaces on these zone faces (in this case, the two jungle gyms) guaranteed by the sticking together of bands discussed in the previous section. At a given point on the Fermi surface at a zone face, one surface intersects the face at an angle $\pi/2 - \theta$ and the other at an angle $\pi/2 + \theta$; each Fermi surface connects smoothly to the other Fermi surface in the neighboring zone. As a result, the open magneto-oscillation orbits on these surfaces may have behavior different from what is expected from the reciprocal lattice periodicity. In addition, extremal orbit ends do not automatically encircle the $X$ point as is commonly the case (see Fig. 6).

The minority Fermi surfaces, shown in Fig. 7 consist of $\Gamma$-centered cube and two jungle gyms (again, stuck together along the zone faces) and appear to be direct analogs of the majority surfaces. There are also two small $R$-centered ellip-
soids that are not well resolved in Fig. 7. The resemblance of the jungle gyms to those of the majority band (Fig. 6) is largely accidental. As mentioned in the previous section, the spin splitting is nearly uniform at 0.4 eV, so the Fermi level produces a cut in two different regions, which are ±0.2 eV from the paramagnetic Fermi level. The intersections of the jungle gym surfaces with the zone faces can be seen to arise from majority and minority bands which have, apparently accidentally, nearly the same shape along \( M-X-R \) in Fig. 5.

The similarity in shape of the jungle gym surfaces (for either spin direction) may be understood simply by the fact that they are required by symmetry to “stick” along each of the zone faces, and they do not extend too far away from the faces.

The minority surfaces in particular present a great deal of potential for nesting, as represented, for example, in the quantity

\[
\xi(\vec{q}) = \sum_{\vec{k}} \delta(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_f) \delta(\varepsilon_{\vec{k}} - \varepsilon_f)
\]

that measures the number of transitions on the Fermi surface involving momentum transfer \( \vec{q} \). Taken together, the cube and the more jungle gym in the center panel of Fig. 7 arise from a set of parallel flat ribbons oriented along each of the three Cartesian directions to form intersecting square tubes (somewhat rounded). The dimension across the tube, hence the nesting wave vector, is \( Q = 0.4(2\pi/\alpha) \). Due to the flat nature of the surfaces, nesting vectors are of the general form \( \vec{q} = (q_x, Q, 0) \) and \( \vec{q} = (q_x, 0, Q) \) for arbitrary \( q_x \), and others related by cubic symmetry. [We say cubic symmetry rather than the strictly correct “B20 symmetry” because the departure of the shapes of the minority surface from cubic symmetry seems to be less than for the majority jungle gyms.]

We leave a more detailed study of nesting and \( q \) dependence of scattering processes for subsequent work. A few other possibilities can be noted, however. The majority octahedron may provide some nesting across the octahedron “faces,” that is, for \( q \) along the \( \langle 111 \rangle \) directions, but they do not appear to be extremely flat. In addition, the sticking together of the jungle gym surfaces all over the zone faces provides substantially larger phase space for \( q \to 0 \) transitions than for conventional Fermi surfaces and deserves further study. [The trivial intraband \( 1/q \) divergence\textsuperscript{35} is a different matter, and is usually killed by intraband matrix elements.]
V. DISCUSSION

The fundamental questions underlying the unusual and perhaps unique characteristics of MnSi center on (1) its unusual bonding and coordination, identical to that of the “Kondo insulator” FeSi, which is related to (2) its low symmetry but still cubic B20 space group in which 75% of the rotations are coupled with a non-primitive translation, and (3) its lack of inversion center (also an integral part of the space group). Frigeri et al. have argued, for example, that lack of inversion symmetry in the MnSi space group acts as a strong inhibition to spin triplet pairing (but does not totally exclude it). Based on prior study of FeSi, many Mn 3d bands near the Fermi level should be expected, together with the occurrence of several valence and conduction band extrema within a few tens of meV of the Fermi level.

We have presented a detailed look at the electronic structure of MnSi both in its paramagnetic phase, which is relevant to the quantum critical point, and also for the FM phase with the observed value of the magnetization. Peculiarities arising from the nonsymmorphic nature of the space group are evident. One peculiarity is the sticking together in pairs of bands over the entire surface of the Brillouin zone. This sticking allows a related uncommon feature: the Fermi surface saddle point is close to \( E_F \). For the FM case, a vanishing velocity at a fourfold degenerate state at \( R \) lies within 30 meV of \( E_F \). Almost exactly at \( E_F \) at the zone center is a threefold level, where the anomalous feature is not the zero velocity (usual at \( k=0 \)) but rather the two nonvanishing velocities. A near (but not exact) occurrence of nonvanishing velocities at \( k=0 \) (which can be interpreted as diverging effective mass) has been studied in the skutterudite materials.\(^{37}\)

Such band features definitely influence the spectrum of low-energy excitations of the system, and may help to account for the observed peculiarities in the normal state properties of MnSi.

The lack of inversion symmetry \textit{per se} has not been implicated in the peculiarities we have located, partly because time-reversal symmetry restores the band symmetry (and band sticking) that “normally” would be provided by inversion. Affects of the lack of inversion will arise in the FM phase when spin-orbit coupling is considered, in which case (1) some of the band sticking will be relieved and (2) there is no longer enough symmetry to enforce \( e_{-k} = e_k \). One important result is that the Fermi surface becomes “lopsided,” restricting the formation of zero-momentum superconducting pairs built from \( k \) and \( -k \). We will pursue this question elsewhere; however, spin-orbit coupling is small in Mn so its importance will have to be assessed.

VI. CONCLUSIONS

MnSi is attracting great attention due to its quantum critical point under modest pressure and to the unusual behavior of several normal state properties in the general vicinity of the quantum critical point. We have provided a detailed analysis of the effects of the B20 crystal structure—both the nonsymmorphic space group without a center of inversion and the unusual coordination—on the band structure of both the paramagnetic and ferromagnetic phases. Several types of unusual occurrences have been identified, and some of them are likely to be implicated in the anomalous normal state behavior and possibly the lack of any superconducting phase in the vicinity of the quantum critical point.

ACKNOWLEDGMENTS

We acknowledge illuminating discussions with J. Kuneš, I. I. Mazin, and C. Pfeifer, and important technical assistance from D. Kasinathan and K.-W. Lee. W.E.P. acknowledges illuminating communication on the band sticking question with J. Kuneš and N. D. Mermin. This work was supported by DOE Grant No. DE-FG03-01ER45876.

7C. Pfeifer, G. J. McMullan, S. R. Julian, and G. G. Lonzarich,