Hidden spin liquid in an antiferromagnet: Applications to FeCrAs

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The recently studied material FeCrAs exhibits a surprising combination of experimental signatures, with metallic, Fermi liquid like specific heat but resistivity showing strong non-metallic character. The Cr sublattice possesses local magnetic moments, in the form of stacked (distorted) Kagome lattices. Despite the high degree of magnetic frustration, anti-ferromagnetic order develops below \( T_N \approx 125 K \) suggesting the non-magnetic Fe sublattice may play a role in stabilizing the ordering. From the material properties we propose a microscopic Hamiltonian for the low energy degrees of freedom, including the non-magnetic Fe sublattice, and study its properties using slave-rotor mean field theory. Using this approach we find a spin liquid phase on the Fe sublattice, which survives even in the presence of the magnetic Cr sublattice. Finally, we suggest that the features of FeCrAs can be qualitatively explained by critical fluctuations in the non-magnetic sublattice Fe due to proximity to a metal-insulator transition.

I. INTRODUCTION

The ubiquity of Landau’s Fermi liquid is a testament to universality in the solid state. As such, departures from these classic experimental signatures in metallic systems act as a guide to novel and interesting physics. Non-Fermi liquid behaviour appears in many strongly correlated materials such as unconventional superconductors,\(^4\)\(^5\) heavy fermion materials,\(^6\)\(^7\) and near quantum phase transitions.\(^8\)\(^9\) Some routes to realize this behaviour include coupling itinerant electronic systems to localized magnetic moments and through intermediate strong electron-electron interactions. These mechanisms can give rise to characteristics and experimental signatures that do not fit neatly in the Fermi liquid paradigm.

A recently re-examined compound, FeCrAs,\(^10\)\(^11\) provides a direct example of a material that does not fit completely within Fermi liquid theory and combines aspects of the mechanisms discussed above. The unit cell of FeCrAs shown in Fig. 1 shows Cr and Fe form alternating two dimensional lattices along what we will denote the \( ab \) axis. Cr forms layers with the structure of a distorted Kagome lattice where the Cr – Cr distances are approximately constant. The Fe layers have a more complicated structure, forming a triangular lattice of three atom units which we will call trimers as shown in Fig. 2.

The As is interspersed throughout both the Fe and Cr layers, as well as in between. Most of the known experimental data is nicely presented in Wu et al.\(^10\) which we summarize below.

The specific heat exhibits Fermi liquid behaviour at low temperatures, i.e. \( C \sim \gamma T \) where the slope \( \gamma \) is sample dependent.\(^11\) The measured linear range is roughly \( T \sim 3 K - 10 K \). Resistivity measurements show insulating behaviour at low and high temperatures. In plane \((ab)\) and out of plane \((c)\) resistivities are of the same order over the entire temperature range considered. The resistivity monotonically decreases (that is \( d\rho/dT < 0 \)) as \( T \) is raised from \( 5K \) up to \( \sim 800 K \) except for a small peak in the \( c \) axis resistivity around \( T \sim 125 K \). A low temperature power law \( \rho \sim \rho_0 - AT^\alpha \) is observed for \( T \sim 80 mK - 5 K \) in both \( ab \) planes and \( c \) axis resistivity with \( \alpha \approx 0.6 - 0.7 \).

There is a peak in the susceptibility at \( T_N \approx 125 K \) indicating a magnetic transition with a lack of hysteresis pointing to anti-ferromagnetic ordering. Below \( T_N \) the susceptibility is anisotropic, differing between the \( ab \) plane and the \( c \) axis. Elastic neutron scattering\(^12\) done deep in the magnetic phase, at \( T = 2.8 K \), is consistent with the anti-ferromagnetic order inferred from the susceptibility, signaling an ordering vector at \( \vec{Q} = (1/3, 1/3, 0) \), indicating ferromagnetic (stacked) order along the \( c \)-axis, but with a tripped unit cell in the \( ab \) plane. While measurements of the specific heat give a result consis-
tent with a metallic Fermi liquid, transport is unusual
and deviates strongly from the classic Fermi liquid result
for metals, while being distinct from the expected result
for strong insulators. Furthermore, this material has a
frustrated magnetic sublattice that nonetheless orders at
low temperatures, while the remaining sublattices show
either small or no magnetic moment.\(^{[10,12]}\) The magnetic
sublattice takes the form of a distorted Kagome lattice,
where even classical Heisenberg models fail to order mag-
netically for both the stacked\(^{[13,14]}\) and purely two di-
mensioinal case.\(^{[15,16]}\) Very few experiments have been carried
out on FeCrAs, so theoretical models are not completely
restricted. Regardless, there are a number of questions
that need to be addressed, such as the nature of the stabi-
lization of magnetic order, the cause of the very different
thermodynamic and transport signals and the role of the
non-magnetic sublattice.

The nature of the magnetic order has been recently
addressed by Redpath et al.\(^{[20]}\) where a minimal model
was proposed which suffices to explain the experimentally
observed stabilization of a particular magnetic ordering
vector. However, transport and thermodynamic behavior
remains to be explained along with the role of the
non-magnetic, Fe sublattice. In this paper, we elaborate
a microscopic route to an effective model for the com-
ound FeCrAs, taking into account the Fe sublattice, and
present a scenario to address the incongruities between
the conflicting metallic, Fermi liquid specific heat and
insulating like transport signals. This model consists of
interacting electrons of the non-magnetic sublattice cou-
pled to magnetic moments of the magnetic, Cr sublattice.
Here we do not address the detailed nature of the mo-
mements themselves, treating them classically,\(^{[23]}\) with the
non-Fermi liquid physics arising from strong charge fluc-
tuations occurring at intermediate Hubbard coupling in
the Fe sublattice. In this picture we are excluding any
Kondo physics, a view supported by the experimental re-
results. Our emphasis is on the interplay between strong
charge fluctuations near the metal-insulator transition on
the Fe sublattice and the magnetic order of the Cr sub-
lattice. For this we turn to the slave-rotor method which
allows access to the intermediate coupling regime and
metal-insulator transition.

The structure of the paper is as follows: in Section II
we present an argument to pass from the atomic limit
through to an effective model of the electronic degrees of
freedom in FeCrAs. In Section III, we discuss the local-
ized moments and magnetic interactions and we present
the effective Hamiltonian relevant for FeCrAs. We pro-
ced to review the slave-rotor method in Section IV and
the assumptions and implementation of our mean field
theory in Section V. In Section VI, we comment on the
application of our results to FeCrAs and summarize con-
clusions in Section VII.
and Cr, we include the term Hund’s coupling as \( J \)

atom at site \( i \) where \( n \)

potential as \( \Delta \), the intra-orbital repulsion as \( \alpha \)

for the Cr site \( e \). Integrating out all of the high energy degrees of freedom on the Cr atom, the ground state for sufficiently large \( J \) is given by the doubly occupied, \( S = 1 \) triplet states which we denote by \( |t_{ja}\rangle \) with \( a = 0, \pm \). Noting that \( H_{\text{Cr-Fe}} \) does not connect triplet to triplet states, as it changes the electron number on the Cr atom we can formulate the effective Hamiltonian following

\[
H_{\text{eff}} = P_1 H_{\text{Cr-Fe}} (E_0 - H_{\text{Cr}})^{-1} H_{\text{Cr-Fe}} P_1, \tag{3}
\]

where \( E_0 \) is the triplet energy and \( P_1 = \sum_{ja} |t_{ja}\rangle \langle t_{ja}| \) projects onto the triplet subspace. Carrying out the expansion of the effective Hamiltonian, denoting the spin operators on the Fe and Cr atoms as \( \vec{S}_i \) and \( \frac{1}{2} \sigma_i \) respectively, our full effective Hamiltonian is given by

\[
H_{\text{eff}} = -\sum_{ijl} \frac{1}{W} \left( \sum_{\alpha} t_{ijl}^\alpha (t_{ijl}^\alpha)^* \right) d_i^\dagger \left( 1 - \vec{\sigma} \cdot \vec{S}_j \right) d_j, \tag{4}
\]

where

\[
\frac{1}{W} = \frac{U + \frac{5J}{2}}{\Delta^2 + \left( \frac{5J}{2} \right)^2 + U(\frac{5J}{4} - \Delta)} > 0. \tag{5}
\]

For \( i = l \) this represents an anti-ferromagnetic exchange between the Fe and Cr atoms, while \( i \neq l \) presents a spin-dependent hopping term, non-zero for both intra-trimer and inter-trimer hopping paths. Based on overlap of the orbital wavefunctions, we assume that the hopping \( \sum_\alpha |t_{ijl}^\alpha|^2 \) is dominant for \( i = l \) and independent of the orbitals, leading to the effective exchange Hamiltonian

\[
H_{\text{exch}}^{\text{eff}} = \sum_{ij} \frac{1}{W} \left( \sum_{\alpha} |t_{ijl}^\alpha|^2 \right) d_i^\dagger (\sigma \cdot \vec{S}_j) d_j, \tag{6}
\]

up to a shift of the chemical potential. For future use, we will denote the effective exchange as

\[
J_K = \frac{1}{W} \sum_{\alpha} |t_{ijl}^\alpha|^2 > 0. \tag{7}
\]

C. Trimer Approximation for Fe

From the inter-atomic distances we expect that the Fe-Cr atoms in the trimer structure are tightly coupled. We can take advantage of this by grouping the degrees of freedom in the trimer into a single unit and formulating the rest of our theory in terms of these variables. This process is similar to the treatment of the pairs of molecules as the effective degrees of freedom, frequently employed in studies of organic superconductors. This assumes the energy scales for interactions and inter-trimer hopping matrix elements are small relative to the intra-trimer hoppings. In addition, we need that the tetrahedral crystal field splitting be much larger than our intra-orbital interactions (this is the low spin assumption) and both the intra- and inter-trimer hopping elements.
Cr spins are denoted as $c$ where the low energy degrees of freedom on the trimers

This gives a pair of decoupled three site chains with hop-

Considering the $C_3$ freedom of a trimer, keeping only the three site cluster.

For the degeneracies of the two lowest levels, leading to

With this in mind, let us find the low energy degrees of

The gross magnetic structure of FeCrAs is captured by

D. Effective Hamiltonian and magnetic interactions

The gross magnetic structure of FeCrAs is captured by a classical model of localized moments interacting with the Fe sublattice via a simple exchange\cite{20}. The utility of the classical model for the moments is also supported by the fact that Kondo-like signatures are absent in the experimental data. Futhermore, due to the uniform character of the relevant trimer states and the assumption of equal exchanges between Cr and different Fe orbitals, the effective exchange between the Cr and the trimers will be equal and between all of the Cr in the surrounding hexagons in the layers above and below. We thus take our Hamiltonian to have the form

afforded hoppings $t$ and $t'$ which originate from direct overlaps between trimers (or indirectly via Cr or As) in the $ab$ planes and along the $c$ axis respectively. Here we
denote sites on the Fe sublattice as \( i \) and \( j \), while sites on the Cr sublattice are denoted as \( a \) and \( b \). The notation \( a \in \mathcal{O}_i \) indicates that the sum on the Cr sublattice is over sites in the hexagon that surround the trimer at \( i \) on the Fe sublattice. Furthermore \( \langle ij \rangle \in ab, c \) denotes bonds in the \( ab \) or \( c \) planes respectively. The interactions are given as follows: \( U \) is the intra-trimer repulsion, inherited from the Fe atoms, \( J_K \) is the Fe–Cr exchange and \( J_H \) is the Cr–Cr exchange. In this Hamiltonian the Cr spins appear as an effective magnetic field for the trimers, which we will denote as \( \vec{h}_i = \sum_{\mathcal{O}_i} \vec{S}_a \).

In the large \( U \) limit, where \( U \gg t \) and \( t^2/J \ll U \), this model should reproduce the model studied in Ref. [20], and thus their classical results provide a useful point of comparison for our large \( U/t \) behaviour. To attack the intermediate \( U/t \) regime we will use a slave-rotor approach, reviewed in the following section.

## III. SLAVE ROTORS

For completeness and standardization of notation, we review the general properties of two dimensional rotors and follow with a discussion of the slave particle representation that bears their name.[22]

A rotor in two dimensions is an object that possesses only angular momentum, prototypically of the form \( H \propto L^2 \) where \( L \) is the angular momentum operator about some axis, say the \( \hat{z} \) axis. We classify states by the eigenstates of the \( L \) operator, \( L|n\rangle = n|n\rangle \) where \( n \) is an integer. Raising and lowering operators are defined as

\[
U^\dagger |n\rangle = |n+1\rangle, \quad U |n\rangle = |n-1\rangle,
\]

where \( U \) is a unitary operator. From this definition it is simple to show that \( L \) and \( U \) satisfy the commutation relations,

\[
[L,U] = U, \quad [L,U^\dagger] = -U^\dagger.
\]

Since \( U \) is unitary it can be written as \( U = \exp(-i\theta) \) where \( \theta^\dagger = \theta \) and one can show that this implies the canonical commutation relation \( [\theta,L] = i \), showing that \( L \) and \( \theta \) are canonically conjugate variables.

To use these rotors as a slave-particle we associate the local electron basis with the product of the states of slave fermion and the states of an \( O(2) \) rotor,

\[
|0\rangle = |0\rangle_f |+\rangle_\theta, \\
|\uparrow\rangle = |\uparrow\rangle_f |0\rangle_\theta, \\
|\downarrow\rangle = |\downarrow\rangle_f |0\rangle_\theta, \\
|\uparrow\downarrow\rangle = |\uparrow\downarrow\rangle_f |-\rangle_\theta.
\]

The slave fermion is called a spinon and spinon states are denoted by an \( f \) subscript. The slave-rotor will be referred to as a rotor and a \( \theta \) subscript will be used to denote rotor states. The natural interpretation is to have the spinon to be neutral and the rotor to carry the charge of the electron, thus explicitly separating the spin and charge degrees of freedom. Having expanded our local Hilbert space, a constraint is required to remove the unphysical states. The four physical states above are characterized by

\[
L_i + \sum_{\sigma} n^f_{i\sigma} = 1,
\]

where \( L_i \) is the rotor angular momentum operator and \( n^f_{i\sigma} \) is the spinon number operator. This is the Hilbert space constraint. The electron operators can therefore be expressed as

\[
c_{i\sigma} = f_{i\sigma} \exp(i\theta_i),
\]

where \( \exp(-i\theta_i) \) is the rotor lowering operator and \( f_{i\sigma} \), \( f^\dagger_{i\sigma} \) are the fermionic spinon operators. Using this representation the electronic Hamiltonian for the trimers [14] is written as

\[
H = -t \sum_{\langle ij \rangle \in ab} f^\dagger_{i\sigma} f_{j\sigma} e^{-i(\theta_i - \theta_j)} -t' \sum_{\langle ij \rangle \in c} f^\dagger_{i\sigma} f_{j\sigma} e^{-i(\theta_i - \theta_j)} + U/2 \sum_i L_i(L_i - 1) + J_K \sum_{i,a \in \mathcal{O}_i} \left( f^\dagger_{i\alpha} f_{i\beta} \right) \cdot \vec{S}_a.
\]

The Hubbard term is now a kinetic term for the rotors, so the complexity of the Hubbard interaction has been moved to the hopping term and the constraint. We note that the Fe–Cr coupling term only involves the spinon degrees of freedom.

## IV. MEAN FIELD THEORY

We approach this problem using mean field theory. For simplicity we take the perspective of Florens and Georges[22] first decoupling the hopping term into

\[
f^\dagger_{i\sigma} f_{j\sigma} e^{-i(\theta_i - \theta_j)} \approx \chi_{ij} e^{-i(\theta_i - \theta_j)} + B_{ij} f^\dagger_{i\sigma} f_{j\sigma} - \chi_{ij} B_{ij},
\]

where we have introduced the mean fields \( \chi_{ij} = \frac{1}{2} \sum_{\sigma} \langle f^\dagger_{i\sigma} f_{j\sigma} \rangle \) and \( B_{ij} = \langle e^{-i(\theta_i - \theta_j)} \rangle \). Note that we have assumed that \( \chi_{ij} \) is independent of spin. To handle the constraint we treat it both on average in space and on average in our states. For the case of half-filling this leads to the two conditions,

\[
\sum_i \langle L_i \rangle = 0, \quad \sum_{i\sigma} \langle n^f_{i\sigma} \rangle = 1.
\]

Note that applying this on average in space prohibits us from considering charge ordering in our calculations. To enforce these constraints we introduce chemical potentials for the rotors and for the spinons, \( \mu_L \) and \( \mu_f \) respectively. This leads to two independent Hamiltonians.
which only talk to each other through the mean fields $\chi_{ij}$ and $B_{ij}$,
\begin{equation}
H_f = -\sum_{\langle ij \rangle} (t_{ij} B_{ij} + \mu_f \delta_{ij}) f_i^\dagger f_j^\sigma + \frac{J_K}{2} \sum_{i,a \in O_i} (f_i^\dagger \sigma f_i) \cdot \vec{S}_a,
\end{equation}
\begin{equation}
H_L = -2t \sum_{\langle ij \rangle} \chi_{ij} e^{-i \theta} e^{i \phi} + \frac{U}{2} \sum_i (L_i^2 - \mu_L \chi_{ii}),
\end{equation}
where we’ve introduced $t_{ij}$ which is equal to $t$ on the in-plane triangular bonds and equal to $t'$ on the out of plane bonds. While the spinon Hamiltonian can be treated using mean field theory, the rotor Hamiltonian needs a different strategy.

Two approaches for the rotor Hamiltonian have been used in the literature: a self-consistent cluster approach$^{23}$ and a bosonic approach$^{23}$, taking the bosonic approach, which is most simply tackled using a path-integral formulation, the imaginary time action takes the form,
\begin{equation}
S(\theta, L) = \int_0^\beta d\tau \left[ \sum_i \left( i L_i \partial_\tau \theta_i + \frac{U}{2} L_i^2 \right) - 2 \sum_{ij} t_{ij} \chi_{ij} e^{-i \theta} e^{i \phi} \right],
\end{equation}
where $\mu_L$ is chosen to eliminate the linear terms in $S$. Due to the symmetry of the action this guarantees that $\langle L_i \rangle = 0$. Next, we integrate out $L$ to get the following action,
\begin{equation}
S(\theta, \phi, \lambda) = \int_0^\beta d\tau \left[ \frac{1}{2U} (\partial_\tau \theta_i)^2 - 2 \sum_{ij} t_{ij} \chi_{ij} e^{-i \theta} e^{i \phi} \right].
\end{equation}
We write this using a bosonic variable $\phi_i = e^{i \phi}$ subject to the constraint that $|\phi_i|^2 = 1$, giving
\begin{equation}
S(\tilde{\phi}, \phi, \lambda) = \int_0^\beta d\tau \left[ \frac{1}{2U} \sum_i (\partial_\tau \phi_i)^2 - \sum_i \lambda_i \right]
+ \sum_{ij} (i \lambda_i \delta_{ij} - 2t_{ij} \chi_{ij}) \tilde{\phi}_i \phi_j,
\end{equation}
where $\lambda$ is an auxiliary field introduced to enforce the constraint. Treating this new constraint in saddle point approximation, the solution of the bosonic part of the Hamiltonian is reduced to solving this saddle point equation and a free bosonic problem. These saddle point equations simply fix the boson number at each site to one.

We assume a uniform state on the Fe sublattice, by considering $\chi_{ij} \equiv \chi$ and $B_{ij} \equiv B$ in plane, with $\chi_{ij} = \alpha \chi$ and $B_{ij} = \alpha B$ out of plane, where $\alpha$ is chosen so that we smoothly match the non-interacting limit$^{23}$. For the Cr spins it is natural to assume that the periodicity is that found by experiment$^{19,20}$ and previous classical calculations$^{20}$, with wavevector of $(1/3, 1/3, 0)$. Within this space of magnetic states, we consider only canted classical ground states, that is states where the inplane components in each triangle are at $120^\circ$ but they are tilted out of plane by a canting angle $\psi$. These states interpolate between a subset of the ground states for $J_H \gg J_K$ at $\psi = 0$ and the ferrimagnetic state valid for $J_K \gg J_H$ with $\psi = \pi/2$. Among these states one can see that only those with a finite moment, as one sums around a hexagon in the Kugome lattice, will be favoured due to the $J_K$ interaction. With these constraints we only have a single set of magnetic states to consider parametrized by the canting angle $\psi$. Under these assumptions the trimer feels the following effective magnetic field (defined as $\vec{h}_i = \sum_{a \in O_i} \vec{S}_a$) after summing around the hexagon
\begin{equation}
\vec{h}_i = 6S \cos \psi \left[ \cos (\vec{Q} \cdot \vec{r}_i) \hat{x} + \sin (\vec{Q} \cdot \vec{r}_i) \hat{y} \right] + 12S \sin \psi \hat{z},
\end{equation}
where $\vec{Q} = (1/3, 1/3, 0)$ and $S$ is the magnitude of the Cr moment. Note the factor of 2 between the in-plane and out-plane components due to the partial cancellation as we sum around the hexagon. The phase diagram for $J_H/t = 0.4$ is shown in Fig. 7 and demonstrates the full range of phases.

There are three distinct phases shown in these phase diagrams. At low $J_K/t$ and $U/t$ we find a metallic phase on the Fe sublattice with zero canting angle (i.e. in plane, $120^\circ$ ordering) on the Cr sublattice. This metallic state is characterized by condensation of the bosonic degree of freedom ($\langle \phi \rangle \neq 0$) and a uniform, real $\chi_{ij} = |\chi|$ implying the existence of an electron Fermi surface and gapless charge excitations. Furthermore, the Fe trimers have an induced moment (anti-ferromagnetically) following the Cr moment. This moment scales with $J_K/t$, and is thus will be small so long as $J_K/t$ is. As we increase $U/t$ and keep $J_K/t$ small, we find a metal insulator transition near $U_c/t \approx 3.5$ into a uniform, $U(1)$ spin liquid (SL) phase. The metal-insulator boundary is very flat, as seen in Fig. 7, since under the mean field ansatz we have employed the critical $U$ is only a function of $\chi$ which changes only by a small amount as we increase $J_K$ (below the jump into the paramagnet phase). This SL phase is also characterized by a uniform, real $\chi_{ij}$ but gapped bosons ($\langle \phi \rangle = 0$), meaning the existence of a spinon Fermi surface but gapped charge excitations. This insulating phase carries the induced moment as in the metallic phase, with the magnitude also being proportional to $J_K/t$. In both the metallic and insulating phases as $J_K/t$ is increased (but remains small) the $\chi$ order parameter decreases towards zero.

From the spin only model of Ref. 20 (accounting for the differing normalizations) one expects that for large $U/t$ the canting angle will become non-zero at $J_K = 2J_H$ and saturate at $J_K = 4J_H$ as one sees in Fig. 7. We find that the uniform spin liquid does not support a non-zero canting angle. By this we mean that as $J_K/t$ is increased the canting angle remains zero until some critical $J_K/t$,
wherein the spin liquid is replaced by the canted AF with \( \chi = B = 0 \). The converse is not true, as can be seen in Fig. 7. We see that the spin liquid phase can be destroyed before the onset of the canted magnetic state, leaving a window where we have a simple insulating, in-plane antiferromagnet. Once inside this canted AF phase with \( \chi = B = 0 \), the canted angle increases with \( J_K/t \) until it becomes saturated and we enter a ferrimagnetic phase, with a net magnetic moment. The key feature of the phase diagrams we want to emphasize is that for a variety of values of \( J_H \) and for small \( J_K \) this spin liquid state is stable and does not coexist with a finite canting.

V. DISCUSSION

To discuss the applications of this to FeCrAs the effects of fluctuations must be taken into account near the metal insulator transition. These include both charge and gauge degrees of freedom and are treated in detail in the work of Podolsky et al.\(^{21}\) In this work it is found that there are two relevant temperature scales \( T^* \) and \( T^{**} \) that determine the qualitative features of the thermodynamic and transport properties. These temperature scales vanish as one approaches the critical point separating the metal and insulator. At temperatures above these scales the specific heat has weak logarithmic corrections

\[
C \sim T \ln \ln(1/T),
\]

while the conductivity has a strong temperature dependence. Specifically, writing \( \sigma = \sigma_f + \sigma_b \) where \( \sigma_f \) is the spinon conductivity and \( \sigma_b \) is boson conductivity, under the assumption of weak disorder we have \( \sigma_f \sim \sigma_b^{\text{imp}} \) due to impurity scattering and

\[
\sigma_b \sim T \ln^2(1/T).
\]  

This implies that the effects of the fluctuations on the specific heat are much more difficult to discern experimentally than the effect on the resistivity, which will be a monotonically decreasing function of \( T \), as seen in the experiments on FeCrAs. This is possible scenario for FeCrAs where a nearly linear specific is observed, as these logarithmic corrections would only be visible over long temperature ranges, where other contributions would begin to dominate and wash out the signature. This is also consistent with the magneto-resistance measurements\(^{10}\) where no change is seen in the low temperature resistivity under magnetic fields up to 8T, as the magnetic field would only couple weakly to the rotor fluctuations.

A method to test this hypothesis experimentally would be a study of the pressure dependence of the transport and thermodynamic properties. Naively one expects that the application of pressure should drive the material through the metal-insulator transition, into the quantum critical metal and eventually into a Fermi liquid phase. Under our scenario, this could in principle be visible as the development of a maximum in the resistivity at low temperatures as the pressure is increased. Furthermore, the specific heat should be relatively unaffected, still only being renormalized by a logarithmic term.

The limitations of the current study deserve some discussion as they lead to future directions. Due to the natural ansatz used in the slave-rotor study, a number of non-trivial spin-liquid states have been excluded from the analysis, such as those with a non-trivial phase structure or that break translational symmetry\(^{22} \). A full exploration of the possible phases in this model could yield useful insights for FeCrAs. Another aspect of this problem that requires future work is the inclusion quantum effects in the description of Cr, leading to a Kondo-Heisenberg model with strong interactions for the conduction electrons. While the addition of frustrating interactions for the Kondo spins has attracted attention recently\(^{23,24} \), the inclusion of electronic interactions is largely undressed (particularly with frustration on the conduction electrons) and is an interesting, but highly non-trivial, question for future study.

VI. SUMMARY

In this paper we have presented and motivated a minimal model for the low energy degrees of freedom in the compound FeCrAs. Starting from the crystal structure and using the experimental facts, we have argued that the magnetic degrees of freedom are well described by a set of classical, localized moments and the electronic degrees of freedom take the form of a half-filled Hubbard model on the trimer sublattice. The coupling between these two subsystems stabilizes a definite magnetic order on the localized moments despite the high degree frustration. To
explain the thermodynamic and transport properties of this material at low temperatures we propose that the electrons residing on the Fe trimers could be close to a quantum critical point separating metallic and insulating phase. The charge fluctuations associated with the critical point strongly renormalize the transport properties but provide only small corrections to the thermodynamic point strongly renormalize the transport properties but provide only small corrections to the thermodynamic.

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Appendix A: Hopping integrals

We first consider direct hopping between the Fe atoms in a trimer. The $t_2$ level is composed of $xz$, $yz$ and $xy$ orbitals with respect to the canonical choice of tetrahedron axes. Rotating these into the axes of a tetrahedron in a trimer, the orbitals are oriented as shown in Fig. 8.

![Orbitals](image)

FIG. 8: (Color Online) The orbitals of the $t_2$ level, rotated along the local axes of an As tetrahedron.

From Fig. 8 one can estimate that the only significant hoppings would be between $xy - xy$, $xz - yz$ and $yz - xz$. One can approach this more quantitatively using the ideas of Slater-Koster[28] theory to compute the orbitals overlaps in terms of rotation matrices and irreducible overlaps. We identify the vector connecting two sites in a trimer $\hat{a}$ as $(\hat{x} + \sqrt{3}\hat{y})/2$, giving the (Euler) representation $R = R_z(0)R_y(-\frac{\pi}{2})R_z(-\frac{\pi}{3})$. The rotation that takes our tetrahedron into the proper axes is given as $R_T = R_z(-\frac{\pi}{2})R_y(\frac{\pi}{2})R_z(\frac{\pi}{3})$ giving the transformation to local axes $R_T$ and $R_z(\frac{\pi}{3})R_T$ for the neighbouring tetrahedron in the trimer. This reduces the number of parameters to three, given by overlaps of $l = 2$, $m = 0, \pm 1, \pm 2$ orbitals displaced along the $\hat{z}$ direction which we will denote as $t_\alpha, t_\beta$ and $t_\delta$ respectively. The hopping matrix in the basis of $xz, yz$ and $xy$ is then given by

$$
\frac{1}{32} \begin{bmatrix}
 t_\alpha - 8t_\beta - 9t_\alpha & 7t_\alpha - 16t_\beta + 9t_\alpha & \sqrt{2}(7t_\alpha - 4t_\beta + 3t_\alpha) \\
 7t_\beta - 16t_\alpha + 9t_\alpha & t_\beta - 8t_\alpha - 9t_\beta & \sqrt{2}(7t_\beta - 4t_\alpha + 3t_\beta) \\
 \sqrt{2}(7t_\alpha + 4t_\beta - 3t_\alpha) & \sqrt{2}(7t_\beta + 4t_\alpha - 3t_\beta) & \frac{1}{2}(49t_\alpha - 12t_\beta + 3t_\alpha)
\end{bmatrix}.
$$

Considering the orbitals at atomic separations, we expect $t_\alpha$ and $t_\delta$ to be positive with $t_\beta$ negative. The simplest ansatz to try is $t_\alpha = t_\delta = -t_\beta \equiv t$. This gives:

$$
t = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},
$$

as one might guess by looking at the orbital overlaps in the rotated axes. Varying the numerical values for the irreducible hopping parameters around this point gives qualitatively the same picture as this simple case, justifying our naive guess.

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29 More general ansatzes could be employed while maintaining uniformity, such as varying the phases of $\chi$ and $B$ over the tripled unit cell or include spin-dependent $\chi$. For simplicity we leave these considerations for future work.