Title: Incommensurate Spin Resonance in URu2Si2

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Incommensurate spin resonance in URu$_2$Si$_2$.

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I. INTRODUCTION

The problem of the nature of the hidden order below $T_{HO} = 17K$ and the superconducting order below $T_c = 1.5K$ in URu$_2$Si$_2$ has perplexed the condensed matter physics community for over two decades.

The heavy-fermion (HF) superconductor URu$_2$Si$_2$ exhibits an order of an unknown origin which sets in at $T_{HO} = 17.5K$. Thermodynamic measurements revealed a rather large jump of approximately 300 mJ/mol-K$^2$ in the linear specific heat coefficient $\gamma$ at 17.5 K. This material contains a linear specific heat coefficient $\gamma$ measured at 70-180 mJ/mol-K$^2$, placing it as a moderately HF material. Below $T_{HO}$, the specific heat follows an exponentially activated behavior $\exp(-\Delta/T)$ with $\Delta$ estimated at 110 K. This gap also appears in optical measurements and vacuum tunneling and is comparable to that observed in inelastic neutron scattering experiments. Anomalies in the DC resistivity, Hall coefficient, thermal expansion and linear and nonlinear susceptibilities are also seen at $T_{HO}$, suggesting a substantial reordering of the conduction electrons. Neutron-scattering experiments found an antiferromagnetic order below 17.5 K but with a staggered magnetization of only 0.03 $\mu_B$ per U atom, which is far too small to account for the observed specific heat anomaly. This anomaly corresponds to an unobserved order which is therefore termed "hidden". Yet there are physical fields that clearly destroy hidden order. It is believed to be destroyed by an applied magnetic field of $\sim 40$ T, suggesting a possible magnetic origin, but in $^5$ it was shown that there are two distinct field-independent energy scales, with opposite tendencies with magnetic field. Therefore, any magnetic origin of this order must not couple directly to field in the same manner as the small AFM order. The application of pressure and Rh doping also suppress the $HO$.

Concomitant with the determination of the experimental facts, there have been many theoretical attempts to understand this hidden order. Theories proposed include spin density waves of either unconventional or higher angular momentum character, orbital antiferromagnetism, staggered quadrupolar order and Jahn-Teller distortions, multispin correlated order, AFM states with anomalous g factors, valence admixture, octupole order and helicity order. Determining the hidden order is complicated by possible phase separation into a magnetic moment phase and regions of hidden order, as argued by $. To date no theory has shown conclusive agreement with the above experimental facts, and there exists no consensus as to the origin of the hidden order.

Recently, Wiebe et al conducted an inelastic neutron scattering (INS) study of URu$_2$Si$_2$, in conjunction with specific heat measurements above and below the 17.5 K onset temperature. Wiebe et al found that above the ordering temperature $T_{HO}$, gapless (with velocity $\sim v_F$) spin wave excitations centered on incommensurate wavevectors $Q' = (1 \pm 0.4, 0, 0)$ appeared but that below this temperature these excitations were gapped, with an approximate gap at 1.5 K of 4-6 meV. Wiebe also estimated the specific heat coefficient of these gapless excitations and found a fair agreement with the experimental value. It was concluded that the reduction in specific heat below $T_{HO}$ resulted from the gapping of these spin-wave excitations; however, the order parameter responsible for this gapping remained indeterminate.

The effect of opening a HO gap on spin excitations appears remarkably similar to the phenomenon of spin resonance in INS, seen in the superconducting state in cuprate materials, in Sr$_2$RuO$_4$, and in the CeCoIn$_5$ superconductor. For example, in the cuprates this resonance in the susceptibility is centered at the commensurate wavevector $q_c=(\pi, \pi)$, and can be interpreted as a bosonic mode transferring weight from the neutron to the Cooper pair. One might therefore expect that a similar effect of gapping on the spin excitations can occur in a state with hidden order, even if the exact nature of HO is not yet settled.

In this paper we propose that URu$_2$Si$_2$ should exhibit an incommensurate spin resonance based on an analogy with the inelastic neutron scattering resonance observed at 41 meV in the cuprates. We argue that

1) The observation by Wiebe et al of the substantial changes of spin susceptibility below and above $T_{HO}$ at an incommensurate momentum is indicative of the gapping of spin excitations due to the gapping of the electronic spectrum below $T_{HO}$. We estimate the energy of the spin resonance to be in the range $\omega_{res} = 4 - 6$ meV and the momentum to be $Q' = (1 \pm 0.4, 0, 0)$. We interpret the changes in spin susceptibility as due to HO gap $\Delta_{Q'}$. 

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Given the mean field character of the gap opening as seen in the specific heat data we predict that the intensity of the resonance scales as $|\Delta Q^*|^2 \sim (T_{HO} - T)^2$ below $T_{HO}$.

2) The experimental observations are consistent with a particle-hole order that has a finite incommensurate momentum $Q^* = (1 \pm 0.4, 0, 0)$ (and related by $k_x \rightarrow -k_y$ permutation) and leads to a gap in the spectrum $\Delta Q^*$. The exact nature of this hidden order is likely a hybridization gap $\Delta Q^*$ that opens up due to the nesting of different parts of Fermi surface separated by $Q^*$. For our analysis of the spin susceptibility we focus on terms of second order in $\Delta Q^*$ that would contribute to the spin susceptibility and therefore we do not need to know the exact details of the HO. Nevertheless our conclusion is that the data on INS and specific heat are consistent with the particle hole excitation being gapped below $T_{HO}$. Recent neutron scattering work by Janik et.al.\textsuperscript{22} does point to the nesting phenomenon as a possible source of HO and is consistent with our proposal.

3) The HO leads to spectral weight changes that produce a peak in the spin susceptibility which we call a spin resonance with energy $\omega_{res} = 4 - 6meV$ at momentum $Q^*$. In the previous cases where a resonance peak has been seen in the ordered state, opening up a partial gap at the Fermi surface, this resonance peak has been observed at commensurate momenta. Here we propose that the resonance peak in $URu_2Si_2$ occurs at the incommensurate momentum $Q^*$.

To support our claim about fermion spectrum gapping we will provide fits to the specific heat based on a mean field gap $\Delta Q^*$ that gives a reasonably good fit to the data. We also address the density of states that can be measured by a scanning probe as another observable that might reveal the existence of an energy feature at $\omega_{res}$.

The plan of this paper is as follows. First we present arguments that naturally lead to the prediction of the spin resonance in $URu_2Si_2$ in Sec II. Then we discuss observables such as the specific heat and the local density of states due to this resonance in Sec III. We conclude with a discussion section.

II. SPIN RESONANCE IN $URu_2Si_2$

First let us discuss the previously established cases where resonance peaks have been seen. In the cuprates, this resonance in the susceptibility $\chi(q, \omega)$ is centered at the commensurate wavevector $q=(\pi, \pi)$, and can be interpreted\textsuperscript{17} as a bosonic mode transferring $q=(\pi, \pi)$ from the neutron to the Cooper pair. The energy of this resonance is independent of temperature, while its intensity depends strongly on temperature and vanishes at $T_c$. Within the SO(5) theory\textsuperscript{17} linking superconductivity and magnetism in the cuprates, an excitation bearing these properties can arise naturally in the particle-particle superconducting channel, and leads to a resonant susceptibility $\chi(q=(\pi, \pi), \omega) \propto \Delta^2/(\omega - \omega_{res} + i\Gamma)$, where $\Delta$ is the superconducting order parameter and $\Gamma$ is a damping constant. This resonance peak appears only below $T_c$ because it is only below this temperature that the mixing of electrons and holes that occurs in the superconducting state allows coupling of magnetic excitations via particle-hole and particle-particle channel coupling. In the cuprates, this interaction is active within the superconducting particle-particle channel, but as we shall see it can be extended under suitable conditions to the particle-hole channel, leading to a similar result. In this case, however, the resonance occurs at an incommensurate wavevector, putting constraints on the origin of this resonance.

In a more recently investigated case of CeCoIn$_5$, a similar resonance\textsuperscript{19} is seen at $(\pi, \pi, \pi)$ and has been interpreted as evidence for d-wave symmetry.

We point here that conflicting opinions on the possible origin of resonance peak exist. In particular alternative explanations of resonance peak, including nonsuperconducting and purely magnetic commensurate response of incommensurate magnets also have been discussed\textsuperscript{20,21}. Relevance for the present discussion is that we do not see a need to have a superconducting reference state as a prerequisite for spin resonance. Gapping of spectrum is essential but the gap does not have to be superconducting. This is an important difference we stress: most of the cases of spin resonance were discussed in superconductors. We do not imply here that $URu_2Si_2$ has superconducting correlations in the HO phase.

A. Spin Susceptibility

The suggestions of the previous section quickly lead to another option for connecting the formation of the hidden order with the spin dynamics. We propose a relatively simple explanation, consistent with the spin/hidden order coexistence, namely that a resonance peak in the susceptibility $\chi(Q^*, \omega = \omega_{res})$ appears as a result of the appearance of a particle-hole condensate, although more complex than the usual density-wave condensate. In particular, we will argue below that the Fermi surface geometry, as depicted in Figure 1, is such as to allow an incommensurate nesting between the central $\Gamma$ Fermi surface pocket and the pocket.

We start with the calculation of spin-spin susceptibility, assuming that the particle hole ordering gaps the FS, which is nested with momentum $Q^*$. Assuming that the gap opens up below $T_{HO}$ we will argue that the change in susceptibility will have a term that is proportional to $\Delta Q^*$. As such this second order correction will occur regardless of the detailed nature of the HO. Similar second order terms in spin susceptibility for superconducting gap were argued for in earlier work\textsuperscript{17}.

We begin with the spin-spin susceptibility of itinerant electrons in $URu_2Si_2$ at $T=0$ $\chi^{ss}(Q^*, \omega) = \langle \sigma^z(Q^*, t) \sigma^z(-Q^*, 0) \rangle$ (in paramagnetic phase\textsuperscript{22} and
FIG. 1: A depiction of the calculated Fermi surface geometry of URu2Si2, taken from 22, with potential Q* nesting vectors indicated entered at the corner of the Brillouin zone. However, this nesting is between two bands of substantially different character, as indicated by LDA calculations, so that there is little or no diagonal signal and the order is "hidden".

\[ \chi^{zz}(Q^*, \omega) = -i \sum_{kk'} \int \frac{\Delta_{Q^*}}{\omega^2 - E_{k, Q^*}^2 + i\delta} \delta_{\omega} \delta_{\omega'} \frac{1}{\sqrt{E^2 - \Delta_{Q^*}^2}} \frac{1}{\omega^2 - 4E^2} dE + \text{smooth terms} \]

The integral in \( \chi(Q^*, \omega) \) can be written as,

\[ \chi(Q^*, \omega) = \Delta_{Q^*} \Delta_{-Q^*} \sum_k \frac{1}{2E_{k, Q^*}} \left( E_{k, Q^*} + \omega \right)^2 - E_{k, Q^*}^2 \]

\[ + \Delta_{Q^*} \Delta_{-Q^*} \sum_k \frac{1}{2E_{k, Q^*}} \left( -\omega + E_{k, Q^*} \right)^2 - E_{k, Q^*}^2 \]

\[ = \Delta_{Q^*} \Delta_{-Q^*} \sum_k \frac{1}{2E_{k, Q^*}} \omega^2 - 4E_{k, Q^*}^2 \]

We took (see below) \( N(E) = N(0) \frac{E}{\sqrt{E^2 - \Delta_{Q^*}^2}} \) as appropriate for a gapped spectrum, then

\[ \chi(Q^*, \omega) = |\Delta_{Q^*}|^2 \int \frac{1}{\sqrt{E^2 - \Delta_{Q^*}^2}} \frac{1}{\omega^2 - 4E^2} dE + \text{smooth terms} \]

Thus susceptibility indeed acquires a term that scales quadratically with HO gap. The details of the integral over energy in Eq(9) depends on the band structure. For any density of states that is smooth, simple analysis shows that for \( \omega << \Delta, \chi(Q^*, \omega) \propto |\Delta_{Q^*}|^2 \omega^2 \), and for \( \omega >> \Delta_{Q^*} \), \( \chi(Q^*, \omega) \propto \frac{|\Delta_{Q^*}|^2}{\omega^2} \), with the crossover at \( \omega \sim |\Delta_{Q^*}| \). We therefore immediately conclude that there is a resonance contribution to spin susceptibility \( \sim \Delta_{Q^*}^2 \), and that contribution will have a peak at \( \omega \sim \Delta_{Q^*} \). We thus proved the points 1) and 2) we made in the Introduction.

### III. EXPERIMENTAL CONSEQUENCES

We now focus on experimental predictions that can be used to test the prediction of resonance peak in URu2Si2.

#### A. Inelastic Neutron Scattering

We expect a resonance peak with \( \omega_{res} = 4 - 6 \text{meV} \) should appear in INS below \( T_{HO} \), and, as in prior work \(^{17}\), the intensity of this peak should increase quasilinearly

\[ \delta \chi^{zz}(q = Q^*, \omega = \omega_{res}, T) \sim \Delta_{Q^*}^2 \sim |T - T_{HO}| \]

with decreasing temperature before saturating at low temperature \( (< 0.6 \ T_{HO}) \). This peak should be centered at the incommensurate wavevectors \( (1 \pm 0.4, 0, 0) \),

\[ \delta \chi^{zz}(q, \omega = \omega_{res}, T << T_{HO}) \sim \frac{\Delta_{Q^*}^2}{(q - Q^*)^2 + \xi^2} \]

FIG. 2: (Color online) a) The Spin susceptibility at the resonance momentum $Q^*$ and at the resonance energy $\omega_{\text{res}}$ is plotted as a function of temperature normalized to the hidden order transition temperature, $T_{\text{HO}}$. The temperature dependence is shown to be determined by the temperature dependence of the "hidden-order" order parameter. b) The intensity plot of spin susceptibility near $Q^*$ and $\omega_{\text{res}}$ is shown. It is clearly seen that the spectral weight of the susceptibility is transferred to the resonance momentum and the resonance energy. The spin susceptibility c) at the resonance energy as a function of the momentum and d) at the resonance momentum as a function of the energy are shown.

Energy, momentum and temperature dependence of the resonance peak is illustrated in Fig(2) with a width $1/\xi$ depending on the microscopic details of the theory. We make quantitative predictions for the temperature dependence of the width of this peak (in energy space).

**B. Specific Heat**

Finally, the gapping of the Fermi surface directly results in the loss of entropy observed below $T_{\text{HO}}$, and we will demonstrate an excellent quantitative fit to the experimental specific heat data.

In Figure 3 we plot the specific heat data of Wiebe, and our fit, assuming a $\Delta Q/(T_{\text{HO}})$ ratio of 2.5 and a "strong-coupling" temperature dependence of $\Delta Q(T)$. We work by analogy with the BCS theory of superconductivity, which shares many of the same expressions with this gapping of the Fermi surface. In particular, the specific heat of the gapped portion of the system is given by

$$C(T) = 2k_B\alpha \beta^2 \sum_k f_k (1 - f_k) \left( E_k^2 + \beta \frac{d \Delta^2}{d \beta} \right)$$  \hspace{1cm} (12)

where $E_k$ is the quasiparticle energy in the gapped state given by

$$E_k = \sqrt{\epsilon_k^2 + \Delta^2_Q}.$$  \hspace{1cm} (13)

$\epsilon_k$ is the normal state dispersion, $\beta = 1/k_BT$, and $\alpha$ is the gapped fraction of the Fermi surface. The jump in the specific heat at $T_{\text{HO}}$ is caused by the second term of the above equation. The effect of this term is enhanced both by the $\Delta Q/(T_{\text{HO}})$ value of 2.5 exceeding the BCS weak-coupling value of 1.76 and by the assumed "strong-coupling" form of $\Delta Q(T)$, in which the quasiparticle gap develops more rapidly below $T_c$ than in standard BCS theory. Such a rapid gap opening is well-known from studies of the cuprates, and can occur due to the rapid suppression of bosonic excitations below $T_{\text{HO}}$. The gap still retains a square-root singularity at $T_{\text{HO}}$, and hence a mean-field, second-order phase transition at this temperature.

To the gapped specific heat must be added a term from the ungapped portion of the Fermi surface, given simply by $C_n = (1 - \alpha)\gamma T$, with $\gamma$ the Sommerfeld specific heat coefficient. For this calculation approximately 60 percent of the Fermi surface was assumed to be gapped.

We have not included in the calculation the effects of the phonon specific heat or of the apparently correlation-induced rise in $C/T$ at very low temperature; these effects have opposite temperature dependencies and are of comparable magnitude, so that the overall effect on the fit of neglecting these effects is expected to be small.

![Data of Wiebe](image)

**FIG. 3:** (Color online) Shown are the results of a calculation of the electronic specific heat of URu2Si2 assuming that the Fermi surface is split into a gapped and ungapped region, with the order parameter taken at $T=0$ as $2.3T_{\text{HO}} \approx 3.76\text{meV}$. For this calculation a temperature dependence of $\Delta Q(T)$ was assumed in which the gap develops below $T_{\text{HO}}$ more rapidly (inset, dashed line) than in canonical BCS theory (inset, solid line), as is often observed in strong-coupling superconductivity, but still maintaining mean-field character. The gap $\Delta_{\text{HO}}$ used in the fit is assumed to be a FS averaged HO gap.
C. Local density of states

Here we present a simple qualitative argument that shows how the Local Density of States (LDOS) can be used to reveal the resonance peak. The energy of the resonance makes its observation relatively simple with a Scanning Tunneling Microscope (STM). The main feature that we focus is the LDOS at the tunneling bias that reveals the energy gap in the electron spectrum in the range 2 - 4 meV. We begin by assuming a typical ordered state self-energy

$$\Sigma(k, \omega) = \frac{|\Delta Q|^2}{\omega - \epsilon_k - \omega}$$  \hspace{1cm}(14)

which can then be combined with Dyson's equation:

$$G(\omega, k) = \frac{1}{\omega - \epsilon_k - \Sigma(k, \omega) + i\delta}$$ \hspace{1cm}(15)

Solving for the poles of the Green's function gives the quasiparticle dispersion relation as

$$\omega = \epsilon_k + \epsilon_{k+Q^*} \pm \sqrt{(\epsilon_k - \epsilon_{k+Q^*})^2 + 4|\Delta Q|^2} \hspace{1cm}(16)$$

which is the dispersion for a density-wave nested at $Q^*$. In particular, if $k$ and $k + Q^*$ are on the gapped portion of the Fermi surface, we obtain a simple gapped spectrum

$$\omega = \pm |\Delta Q|$$ \hspace{1cm}(17)

The local density of states will depend to a certain extent on the details of the dispersion, which we have not attempted to model here. For example summation over the whole Fermi Surface will lead to the finite DOS $N(\omega = 0)$. In general LDOS will contain a feature at $E = \pm |\Delta Q|$ from the usual density-of-states relationship of a gapped spectrum,

$$N(\omega) = N_0 \frac{\omega}{\sqrt{\omega^2 - |\Delta Q|^2}}$$ \hspace{1cm}(18)

Such a feature should be readily observable by low-temperature STM for $E = 2 - 4$ meV, although the effects of impurities and inhomogeneities will tend to broaden this peak.

DAVID, WE MIGHT TRY TO SEE HOW IT COMES OUT.

SASHA

IV. DISCUSSION AND CONCLUSION

In conclusion, we propose to search for the spin resonance in $U\text{Ru}_2\text{Si}_2$ at $\omega_{\text{res}} = 4 - 6$ meV at the incommensurate wavevector $Q^* = (1 \pm 0.4, 0, 0)$. We expect that this spin resonance will set in at temperatures below HO transition and the intensity of this peak will scale as $\sim \Delta_{\text{HO}} \sim (T_{\text{HO}} - T)$.

The resonance peak is known to occur in the states with superconducting gap and results in the gapping of the electronic spectrum $\pm \omega$. In the case of HO the gap $\Delta_{\text{HO}}$ results in the partially gapped electron spectrum. That appears to be a sufficient condition, as shown by Wiebe et al.\(^7\) to produce a gap in spin excitation spectrum. In addition, we predict a peak in the spin excitation spectrum, as spectral weight redistribution produces the resonance feature. To the best of our knowledge, if the predicted resonance indeed occurs, it would be the first case where the spin resonance occurs at an incommensurate vector $Q^*$.

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