Incommensurate spin resonance in URu_2Si_2

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The nature of the hidden order (HO) in URu_2Si_2 below T_{HO}=17.5 K has been a puzzle for a long time. Neutron-scattering studies of this material reveal a rich spin dynamics. We focus on the inelastic neutron scattering in URu_2Si_2 and argue that the observed gap in the fermion spectrum naturally leads to the spin feature observed at energies ω_{res}=4–6 meV at momenta at $\mathbf{Q}^*=(\mathbf{1}\pm\mathbf{0.4},\mathbf{0},\mathbf{0})$. We discuss how spin features seen in URu_2Si_2 can indeed be thought of in terms of the *spin resonance* that develops in HO state and is *not related* to the superconducting transition at 1.5 K. In our analysis, we assume that the HO gap is due to a particle-hole condensate that connects nested parts of the Fermi surface with nesting vector $\mathbf{Q}^*$. Within this approach, we can predict the behavior of the spin susceptibility at $\mathbf{Q}^*$ and find it to be strikingly similar to the phenomenology of resonance peaks in high T_c and heavy fermion superconductors. The energy of the resonance peak scales with T_{HO} $\omega_{res}\simeq 4k_BT_{HO}$. We discuss observable consequences that spin resonance will have on neutron scattering and local density of states. Moreover, we argue how the establishment of spin resonance in URu_2Si_2 and better characterization of susceptibility, temperature, pressure, and Rh-doping dependence would elucidate the nature of the HO.

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I. INTRODUCTION

The problem of the nature of the hidden order (HO) below T_{HO}=17 K and the superconducting order below T_c =1.5 K in URu_2Si_2 has perplexed the condensed-matter physics community for over two decades.[1]

The heavy-fermion (HF) superconductor URu_2Si_2 exhibits an order of an unknown origin which sets in at T_{HO} =17.5 K. Thermodynamic measurements[2] revealed a rather large jump of approximately 300 mJ/mol K^2 in the linear specific-heat coefficient γ at 17.5 K. This material contains a linear specific-heat coefficient γ 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 Δ estimated at 148 K. This gap also appears in optical measurements and vacuum tunneling and is comparable to that observed in inelastic neutron-scattering (INS) 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[2,3] found an antiferromagnetic (AFM) order below 17.5 K but with a staggered magnetization of only 0.03μ_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 ~40 T, suggesting a possible magnetic origin; but in Ref. 4 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[5] and Rh doping also suppress the HO.[5,6]

Along with the determination of the experimental facts, there have been many theoretical attempts to understand this hidden order. Theories that were proposed include spin-density waves of either unconventional or higher angular momentum character,[7,8] orbital antiferromagnetism,[9] staggered quadrupolar order,[10] Jahn-Teller distortions,[11] multispin-correlated order,[12] AFM states with anomalous g factors,[8,13] valence admixture,[14] octupole order,[15] and helicity order.[16] Determining the hidden order is complicated by the possible phase separation into a magnetic-moment phase and regions of hidden order, as argued by Amitsuka *et al.*[5] 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,[17] Wiebe *et al.* conducted an INS study of URu_2Si_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 wave vectors $\mathbf{Q}^*=(1\pm 0.4,0,0)$ appear. But below this temperature, these excitations were gapped, with an approximate gap at 1.5 K of 4–6 meV. Wiebe *et al.* 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,[18] and in the $CeCoIn_5$ superconductor.[19] For example, in the cuprates this resonance in the susceptibility $\chi(\mathbf{q},\omega)$ is centered at the commensurate wave vector $\mathbf{q}$ $=(\pi,\pi)$ and can be interpreted[18] as a bosonic mode transferring $\mathbf{q}=(\pi,\pi)$ from the neutron to the Cooper pair. For completeness of the discussion, we also point the case of Sr_2RuO_4 where resonance was predicted but not observed to date.[20] 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_2Si_2 should exhibit an *incommensurate* spin resonance based on an analogy with the inelastic neutron-scattering resonance observed at 41 meV in the cuprates.[18] We argue that (1) the observation by Wiebe *et al.*[17] of the substantial changes in 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 have developed a microscopic theory of the spin susceptibility outlined below. This theory is based on the estimate of changes in susceptibility due to the gap in the fermionic spectrum. We estimate the gap in spin susceptibility to be twice as large as a gap in the single spin excitation as explained below. As a result, we estimate $\omega_{\mathrm{res}} \simeq 4k_B T_{\mathrm{HO}}$ opening that allows us to estimate the energy of the spin resonance to be in the range of $\omega_{\mathrm{res}}=4-6$ meV and the momentum to be $\mathbf{Q}^*=(1\pm 0.4,0,0)$. Changes in the spin susceptibility due to the HO gap Δ_{Q^*} will naturally change the spin excitation spectrum. Given the mean-field character of the HO gap opening as seen in the specific-heat data, we expect that the intensity of the resonance scales as $|\Delta_{\mathbf{Q}^*}|^2 \sim (T_{\mathrm{HO}}-T)$ below T_{HO}. (2) Multiple orders were proposed as an explanation of HO. We argue that the experimental observations are consistent with a specific particle-hole order that has a finite incommensurate momentum $\mathbf{Q}^*=(1\pm 0.4,0,0)$ (and related by $k_x \leftrightarrow k_y$ permutation) and leads to a gap in the spectrum $\Delta_{\mathbf{Q}^*}$. The exact nature of this hidden order is likely be a hybridization gap $\Delta_{\mathbf{Q}^*}$ that opens up due to the nesting of different parts of Fermi surface (FS) separated by $\mathbf{Q}^*$. For our analysis of the spin susceptibility, we focus on terms of the second order in $\Delta_{\mathbf{Q}^*}$ 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.*[21] and theory proposal by Oppeneer and co-workers[22] did 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 $\omega_{\mathrm{res}}=4-6$ meV at momentum $\mathbf{Q}^*$. 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. We point that complicated spin dynamics that is affected by the HO, in addition to the already established spin gapping, should exhibit a phenomena of spin resonance *peak* in URu_2Si_2. The main difference with respect to the previous discussion on spin resonance is that this resonance occurs at the incommensurate momentum $\mathbf{Q}^*$ in the nonsuperconducting state.

To support our claim about the fermion spectrum gapping, we will provide fits to the specific heat based on a mean-field gap in the spectrum with the ratio $\Delta_{\mathbf{Q}^*}/k_b T_c=2.5$ that give a reasonably good fit to the data. We also address the density of states (DOS) that can be measured by a scanning probe as another observable that might reveal the existence of an energy feature at ω_{res}.

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 DOS (LDOS) due to this resonance in Sec. III. We conclude with a discussion section.

II. SPIN RESONANCE IN URu_2Si_2

In the cuprates, the resonance in the susceptibility $\chi(\mathbf{q},\omega)$ is centered at the commensurate wave vector $\mathbf{q}=(\pi,\pi)$ and can be interpreted[18] as a bosonic mode transferring $\mathbf{q}=(\pi,\pi)$ 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[18] 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 $\chi[(\mathbf{q}=\pi,\pi),\omega] \propto \Delta^2/(\omega-\omega_{\mathrm{res}}+i\Gamma)$, where Δ is the superconducting order parameter and Γ 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 couplings. 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 wave vector, putting constraints on the origin of this resonance.

In a more recently investigated case of $CeCoIn_5$, a similar resonance[19] is seen at (π,π,π) and has been interpreted as an evidence for *d*-wave symmetry. On the other hand, a spin resonance has been observed in the pnictide superconductor $Ba_{0.6}K_{0.4}Fe_2As_2$, where the pairing symmetry could be different.[23]

We point out here that conflicting opinions on the possible origin of resonance peak exist. In particular, alternative explanations of the resonance peak, including nonsuperconducting and purely magnetic commensurate response of incommensurate magnets, have also been discussed.[24,25] The 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. The gapping of the 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 with regard to superconductors. We do not imply here that URu_2Si_2 has superconducting correlations in the HO phase.

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 $\chi(\mathbf{Q}^*, \omega=\omega_{\mathrm{res}})$ appears as a result of the appearance of a particle-hole condensate, although more complex than the usual density-wave condensate. In particular, we argue that the Fermi surface geometry, as depicted in Fig. 1, is such as to allow an incommensurate nesting between the central Γ Fermi surface pocket and the pocket separated by $\mathbf{Q}^*$. This nesting is not complete and would require a strong interaction to produce an instability. This fact is in accord with our observation that we need to use a strong-coupling version of the mean-field specific heat to fit specific-heat data (see below).

We start with the calculation of the spin-spin susceptibility, assuming that the particle-hole ordering gaps the FS, which is nested with momentum $\mathbf{Q}^*$. 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 $\Delta^2_{\mathbf{Q}^*}$. As such, this second-order correction will occur regardless of the detailed nature of the HO. Similar second-order terms in the spin susceptibility for superconducting gap were argued for in earlier work.[18]

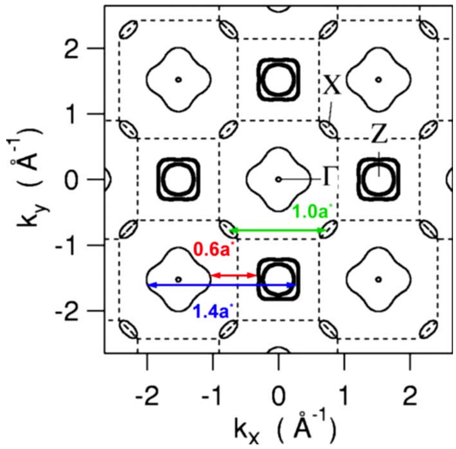

FIG. 1. (Color online) A depiction of the calculated Fermi surface geometry of URu_2Si_2 taken from Ref. 21 with potential $\mathbf{Q}^*$ nesting vectors indicated entered at the corner of the Brillouin zone. However, this nesting is between two bands of the same spin so that there is little or no magnetic signal and the order is hidden.

We begin with the spin-spin susceptibility of itinerant electrons in URu_2Si_2 at $T=0$ signatures are seen in zz component $\chi^{zz}(\mathbf{Q}^*,t)=i\langle TS^z(\mathbf{Q}^*,t)S^z(-\mathbf{Q}^*,0)\rangle$,

$$\begin{aligned}\chi^{zz}(Q^*,\omega) &= i\sum_{\mathbf{kk}'}\int \langle Tc^\dagger_{\mathbf{k}'+\mathbf{Q}^*,\mu}(t)\sigma^z_{\mu,\nu}c_{\mathbf{k}',\nu}(t)c^\dagger_{\mathbf{k}-\mathbf{Q}^*,\alpha}(0)\sigma^z_{\alpha\beta}c_{\mathbf{k},\beta}(0)\rangle e^{i\omega t}dt\\ &= -i\sum_{\mathbf{kk}'}\int \langle Tc^\dagger_{\mathbf{k}'+\mathbf{Q}^*,\mu}(t)c_{\mathbf{k},\beta}(0)\rangle\langle Tc^\dagger_{\mathbf{k}-\mathbf{Q}^*,\alpha}(0)c_{\mathbf{k}',\nu}(t)\rangle e^{i\omega t}\sigma^{\mu\nu}\sigma^z_{\alpha\beta}dt. \qquad (1)\end{aligned}$$

To make the next step, we introduce the anomalous Green's functions that capture the appearance of an incommensurate order at $\mathbf{Q}^*$,

$$F_{\mathbf{k},\mathbf{Q}^*}(\omega_1) = i\langle Tc^\dagger_{\mathbf{k}-\mathbf{Q}^*,\alpha}(0)c_{\mathbf{k},\nu}(t)\rangle\delta_{\alpha\nu} = \frac{\Delta_{\mathbf{Q}^*}}{\omega_1^2 - E^2_{\mathbf{k},\mathbf{Q}^*} + i\delta}, \qquad (2)$$

function F describes the particle-hole density order that represents HO and is *nonmagnetic*. This order partially gaps excitations at the Fermi surface. F relates regions of the Fermi surface that are connected by the nesting vector $\mathbf{Q}^*$. We choose it to have a typical mean-field form. As we have argued, with the focus on second-order terms in $\Delta_{\mathbf{Q}^*}$, the detailed structure of the propagators is not critical. The same conclusions can be drawn from Ginzburg-Landau theory for the HO state. Hereafter, we will ignore smooth terms in the susceptibility. Then the susceptibility related to the appearance of anomalous order is

$$\chi^{zz}(\mathbf{Q}^*,\omega) = -i\sum_{\mathbf{k}}\int F_{\mathbf{k},\mathbf{Q}^*}(\omega_1)F_{-\mathbf{k},-\mathbf{Q}^*}(\omega+\omega_1)d\omega_1, \qquad (3)$$

the integral in $\chi^{zz}(\mathbf{Q}^*,\omega)$ can be written as

$$\chi(\mathbf{Q}^*,\omega) = \Delta_{\mathbf{Q}^*}\Delta_{-\mathbf{Q}^*}\sum_{\mathbf{k}}\frac{1}{2E_{\mathbf{k},\mathbf{Q}^*}}\frac{1}{(E_{\mathbf{k},\mathbf{Q}^*}+\omega)^2 - E^2_{\mathbf{k},\mathbf{Q}^*}} \qquad (4)$$

$$+\Delta_{\mathbf{Q}^*}\Delta_{-\mathbf{Q}^*}\sum_{\mathbf{k}}\frac{1}{2E_{\mathbf{k},\mathbf{Q}^*}}\frac{1}{(-\omega+E_{\mathbf{k},\mathbf{Q}^*})^2 - E^2_{\mathbf{k},\mathbf{Q}^*}} \qquad (5)$$

$$=\Delta_{\mathbf{Q}^*}\Delta_{-\mathbf{Q}^*}\sum_{\mathbf{k}}\frac{1}{E_{\mathbf{k},\mathbf{Q}^*}}\frac{1}{\omega^2 - 4E^2_{\mathbf{k},\mathbf{Q}^*}}. \qquad (6)$$

We took (see below) $N(E)=N(0)\frac{E}{\sqrt{E2-\Delta 2_{\mathbf{Q}^*}}}$ as is appropriate for a gapped spectrum, then

$$\chi^{zz}(\mathbf{Q}^*,\omega) = |\Delta_{\mathbf{Q}^*}|^2\int\frac{1}{\sqrt{E^2-\Delta^2_{\mathbf{Q}^*}}}\frac{1}{\omega^2-4E^2}dE. \qquad (7)$$

Thus, the susceptibility indeed acquires a term that scales quadratically with the HO gap. The details of the integral over energy in Eq. (7) depend on the band structure. For any density of states that is smooth, simple analysis shows that for $\omega \ll \Delta$, $\chi^{zz}(\mathbf{Q}^*,\omega) \propto |\Delta_{\mathbf{Q}^*}|^2\omega^2$ and for $\omega \gg \Delta_{\mathbf{Q}^*}$, $\chi^{zz}(\mathbf{Q}^*,\omega) \propto \frac{|\Delta_{\mathbf{Q}^*}|^2}{\omega^2}$, with the crossover at $\omega \sim |\Delta_{\mathbf{Q}^*}|$. We there-

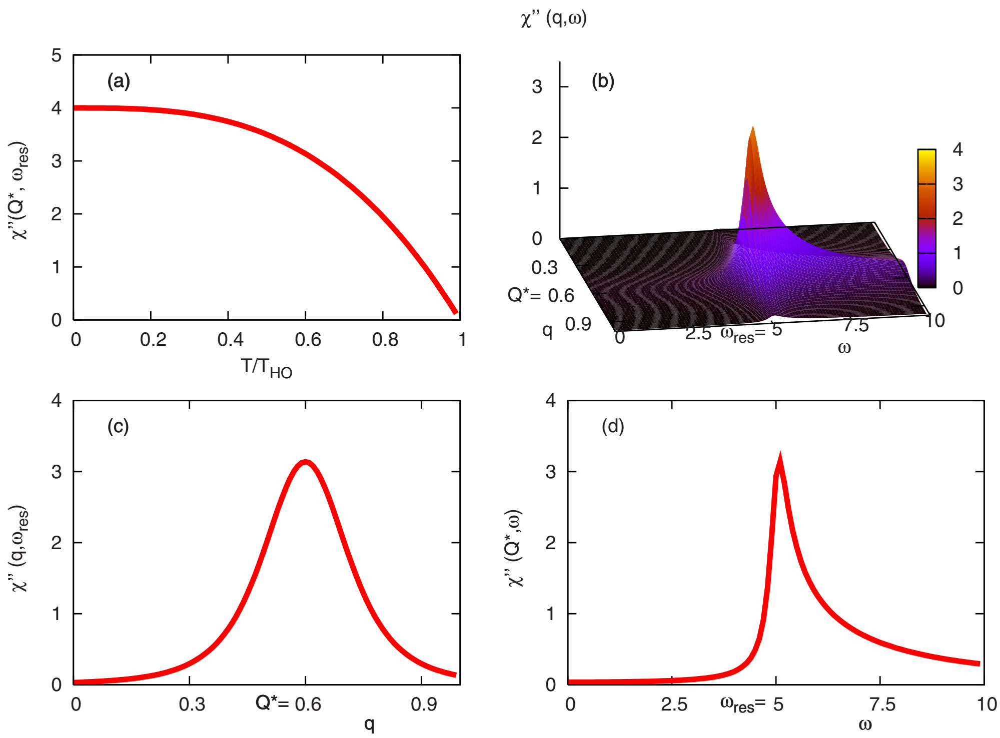

FIG. 2. (Color online) (a) The spin susceptibility at the resonance momentum $\mathbf{Q}^*$ and at the resonance energy $\omega_{\rm res}$ is plotted as a function of temperature normalized to the hidden-order transition temperature $\frac{T}{T_{\rm HO}}$. The temperature dependence is shown to be determined by the temperature dependence of the "hidden-order" order parameter. (b) The intensity plot of spin susceptibility near $\mathbf{Q}^*$ and $\omega_{\rm res}$ 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.

fore immediately conclude that there is a resonance contribution to spin susceptibility $\sim\Delta^2_{\mathbf{Q}^*}$ and that the contribution will have a peak at $\omega\sim\Delta_{\mathbf{Q}^*}$.

Finally, we give an argument on why the spin-resonance energy $\omega_{\rm res}=4k_BT_{\rm HO}\sim 4-6$ meV. For any collective many-body state that develops full or partial gap in the mean-field transition at transition temperature T_c, the single particle gap at low T will be on the order of

$$\Delta_{qp} \geq 1.75 k_B T_c. \tag{8}$$

The single particle gap for any itinerant system would lead to a spin gap on the order of *twice* the single particle gap,

$$\Delta_{\rm spin} = 2\Delta_{qp} = 3.5 k_B T_c. \tag{9}$$

Typical example is the density wave where the gap opening suppresses the low-energy susceptibility and opens up at least a partial spin gap. For materials where strong coupling effects are important, URu_2Si_2 is certainly one of them, the typical single particle gap is larger with respect to the weak-coupling coefficient of 1.75. We therefore would expect that in strong-coupling systems where spin and charge interactions are strong, the coefficient in Eq. (9) will be larger and can reach a value of 4 to 5 and possibly higher. Spin-resonance energy reflects the spin spectral weight redistribution will occur at energies on the order of $\Delta_{\rm spin}$. So the generic relation between $\omega_{\rm res}=4-5k_BT_{\rm HO}$ holds for URu_2Si_2 as well because the transition is demonstrably close to the mean field with single-particle gap. We thus proved the points (1) and (2) we made in the introduction.

III. EXPERIMENTAL CONSEQUENCES

We now focus on the experimental observables that can be used to test the prediction of a resonance peak in URu_2Si_2. We will consider neutron scattering and local density of states features. In addition, we will address electronic specific-heat features due to the HO gap to illustrate that we can achieve a reasonable fit using a simple mean-field description.

A. Inelastic neutron scattering

We expect a resonance peak with $\omega_{\rm res}=4-6$ meV should appear in INS below $T_{\rm HO}$, and the intensity of this peak should increase quasilinearly, as in prior work,[18]

$$\delta\chi^{zz}(\mathbf{q}=\mathbf{Q}^*, \quad \omega=\omega_{\rm res},T) \sim \Delta^2_{\mathbf{Q}^*} \sim |T-T_{\rm HO}|, \tag{10}$$

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

$$\delta\chi^{zz}(\mathbf{q},\omega=\omega_{\rm res}, \quad T\ll T_{\rm HO}) \sim \frac{\Delta^2_{\mathbf{Q}^*}}{(\mathbf{q}-\mathbf{Q}^*)^2+\xi^{-2}}. \tag{11}$$

The energy, momentum, and temperature dependence of the resonance peak are illustrated in Fig. 2 with a width $1/\xi$

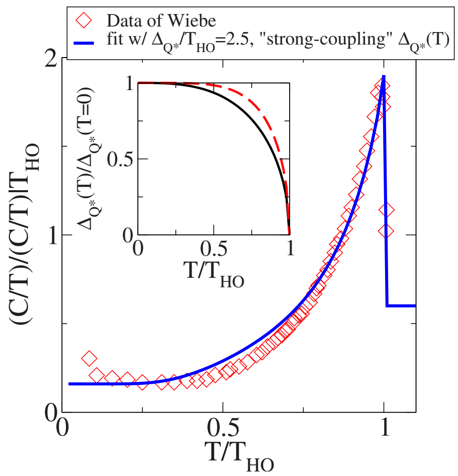

FIG. 3. (Color online) Shown are the results of a calculation of the electronic specific heat of URu_2Si_2 assuming that the Fermi surface is split into a gapped and ungapped region, with the order parameter taken at $T=0$ as $2.5T_{HO} \simeq 3.75$ meV. For this calculation, a temperature dependence of $\Delta_{\mathbf{Q}*}(T)$ was assumed in which the gap develops below T_{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 the mean-field character. The gap Δ_{HO} used in the fit is assumed to be a FS-averaged HO gap.

depending on the microscopic details of the theory. From Ref. 17, we estimate $\xi^{-1} \sim 0.1\frac{\pi}{a}$.

From this analysis, we would expect both intensity and resonance energy be temperature dependent. At temperatures below T_{HO}, resonance energy will evolve with temperature $\omega_{res} \sim \Delta_{Q*}$. In the same region intensity of resonance peak with change as a function of temperature $I(\mathbf{Q}*, \omega_{res}, T) \sim \Delta^2_{Q*}$. Broholm *et al.*.[3] showed that the gap in the neutron-scattering peak at $Q*$ does indeed depend on $T-T_{HO}$ in a mean-field manner. They also argued that the intensity of neutron-scattering feature does increase below T_{HO}. Another mean to test the dependence of resonance on HO gap is to investigate effects of pressure or Rh doping.[5,6] URu_2Si_2 undergoes a first-order transition with increased pressure from HO phase to the large moment antiferromagnetic (LMAF) phase that has a commensurate magnetic order. The key ingredient for the spin resonance is the gapping of quasiparticle spectrum. Spin resonance will persist in LMAF state as long as the gap in fermionic spectrum remains. Resonance peak energy would be suppressed with Rh doping. These estimates can be tested experimentally.

B. Specific heat

The gapping of fermions on the part of the Fermi surface directly results in the loss of entropy observed below T_{HO}, and we will demonstrate an excellent quantitative fit to the experimental specific-heat data. In Fig. 3 we plot the specific-heat data of Wiebe *et al.*[17] and our fit, assuming a $\Delta_{\mathbf{Q}*}/T_c$ ratio of 2.5 and a "strong-coupling" temperature dependence of $\Delta_{\mathbf{Q}*}(T)$. We work by analogy with the BCS theory of superconductivity, which shares many of the same expressions with this gapping of the Fermi surface.[26,27] In particular, the specific heat of the gapped portion of the system is given by

$$C(T) = 2k_B\alpha\beta 2\sum_{\mathbf{k}} f_{\mathbf{k}}(1-f_{\mathbf{k}})\left(E^2_{\mathbf{k}} + \frac{\beta}{2}\frac{d\Delta^2}{d\beta}\right), \quad (12)$$

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

$$E_{\mathbf{k}} = \sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2_{\mathbf{Q}^*}}, \quad (13)$$

$\epsilon_{\mathbf{k}}$ is the normal-state dispersion, $\beta = 1/k_BT$, and α is the gapped fraction of the Fermi surface. The jump in the specific heat at T_{HO} is caused by the second term of the above equation. The effect of this term is enhanced both by the $\Delta_{\mathbf{Q}^*}(0)/T_{HO}$ value of 2.5 exceeding the BCS weak-coupling value of 1.76 and by the assumed strong-coupling form of $\Delta_{\mathbf{Q}^*}(T)$, in which the quasiparticle gap develops more rapidly below T_{HO} than in standard BCS theory. Such a rapid gap opening is well known from studies of the cuprates[28,29] and can occur due to the rapid suppression of bosonic excitations below T_{HO}. The gap still retains a square-root singularity at T_{HO}, and hence a mean-field second-order phase transition at this temperature. Comparing the numbers from the strong-coupling theory with the data, we see a reasonable agreement: $\Delta_{HO} \sim 4-6$ meV, $T_{HO}=17$ K, and $\Delta_{\mathbf{Q}^*}(0)/T_{HO} \sim 2.3$.

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

C. Local density of states

Here we present a simple qualitative argument that shows how the 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 on is the LDOS at the tunneling bias that reveals the energy gap in the electron spectrum in the range 2–4 meV. This feature can be observed with STM and we expect a 2–4 meV LDOS feature which sharpens below the HO transition temperature.

We begin by assuming a typical-ordered-state self-energy

$$\Sigma(\mathbf{k},\omega) = \frac{|\Delta_{\mathbf{Q}^*}|^2}{\omega - \epsilon_{\mathbf{k}+\mathbf{Q}^*}}, \quad (14)$$

which can then be combined with Dyson's equation,

$$G(\omega,\mathbf{k}) = \frac{1}{\omega - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k},\omega) + i\delta}. \quad (15)$$

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

$$\omega = \frac{\epsilon_{\mathbf{k}} + \epsilon_{\mathbf{k+Q*}} \pm \sqrt{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+Q*}})^2 + 4|\Delta_{\mathbf{Q*}}|^2}}{2}, \tag{16}$$

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

$$\omega = \pm \Delta_{\mathbf{Q}^*}. \tag{17}$$

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. A summation over the whole Fermi surface will lead to the finite DOS $N(\omega=0)$. In general, the LDOS will contain a feature at $E=\pm\Delta_{\mathbf{Q}^*}$ from the usual density-of-states relationship of a gapped spectrum,

$$N(\omega) = N_0 \frac{\omega}{\sqrt{\omega^2 - |\Delta_{\mathbf{Q}^*}|^2}}. \tag{18}$$

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

IV. RELATION TO SUPERCONDUCTORS THAT EXHIBIT RESONANCE PEAK

There is an interesting correspondence between the energy of the resonance peak in URu_2Si_2 and in superconductors. Assuming that our prediction about the temperature dependence and the energy of the resonance peak is supported by the experiment, we expect the resonance energy to be in the range $\omega_{res}=4-6$ meV and it to occur below T_{HO}.

The relation between energy and critical temperature for HO phase is remarkably similar to the relation between resonance energy and T_c for unconventional superconductors. For URu_2Si_2 HO state, we find the ratio

$$\hbar\omega_{res} \simeq 4k_B T_{HO}, \tag{19}$$

that is very similar to superconducting relation,

$$\hbar\omega_{res} = 4k_B T_c. \tag{20}$$

We do not know the specific reason for this close correspondence other than the general observation that a gapped spectrum could also produce suppressed spectral weight in the spin susceptibility.

Uemura[30] noticed a universal scaling between resonance energy and critical temperature for unconventional superconductors such as high-T_c cuprates,[18] CeCoIn5 (Ref. 19), where it is seen at (π,π,π), and in the pnictide superconductor $Ba_{0.6}K_{0.4}Fe_2As_2$.[23] He proposed an analogy of resonance mode with rotons in superfluid ^{4}He using a plot shown in Fig. 4. We note that datum for HO phase is remarkably close to relation for superconductors and He, as demonstrated by a new point for URu_2Si_2 added in Fig. 4. This analogy, while appealing, can only go up to a point, since HO state in

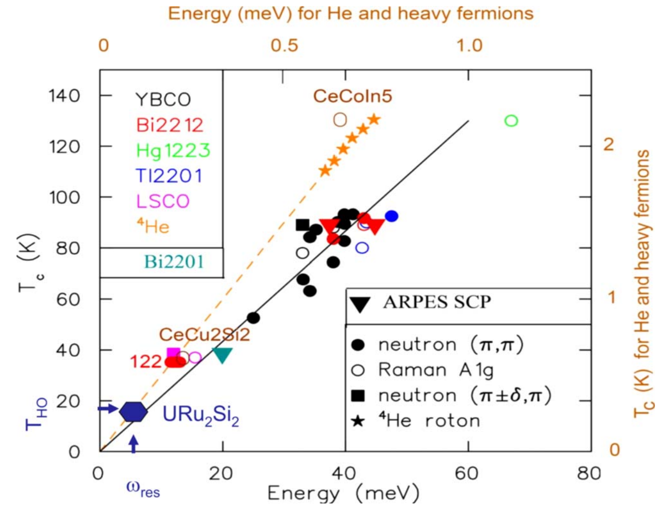

FIG. 4. (Color online) The relation between the resonance energy ω_{res} and T_c is shown for a variety of superconductors in this Uemura roton plot. At a lower left corner, we have added the point indicated by arrows that marks HO relation between expected resonance peak and T_{HO}. The graph for superconductors and superfluid He is taken from Ref. 30.

URu_2Si_2 is nonsuperconducting and resonance feature is incommensurate.

V. DISCUSSION AND CONCLUSION

In conclusion, we propose to search for the spin resonance in URu_2Si_2 at $\omega_{res}=4-6$ meV at the incommensurate *wave vector* $Q^*=(1\pm0.4,0,0)$. We expect that this spin resonance will set in at temperatures below the HO transition and the intensity of this peak will scale as $\sim\Delta_{HO}^2\sim(T_{HO}-T)$.

The resonance peak is known to occur in the states with superconducting gap and results in the gapping of the electronic spectrum.[18,19,23] In the case of the HO, the gap Δ_{HO} results in the partially gapped electron spectrum. That appears to be a sufficient condition, as shown by Wiebe *et al.*,[17] to produce a gap the in spin-excitation spectrum.

There are few ways one can further experimentally test the predicted relation between T_{HO} and resonance energy with temperature, impurity doping, pressure, and magnetic field. Resonance energy $\omega_{res}\sim\Delta_{Q*}$ is a monotonic function of temperature and Rh doping. Similarly, the intensity of resonance peak in critical region will scale as Δ_{Q*}^2. Upon adding Rh and Th into $URu_{2-x}Rh_xSi_2$, one can suppress HO and respective transition temperature and we would expect that the resonance energy ω_{res} would track $T_{HO}(x)$. Similarly, one can measure changes in transition temperature and in resonance energy as a function of pressure and magnetic field, if this is feasible. The resonance discussed here is the case where the spin resonance occurs in a nonsuperconducting state at an incommensurate vector $\mathbf{Q}^*$. We also expect SDW and/or CDW modulation at $\mathbf{Q}'=(0.6,0.6)$ that will be discussed elsewhere.

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