MAGNETIC FLUCTUATIONS AND HEAVY ELECTRON SUPERCONDUCTIVITY

M. R. Norman, Matls. Sci. Div., Argonne Natl. Lab., Argonne, IL 60439 USA

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A magnetic fluctuation self-energy based on neutron scattering data is used to calculate mass renormalizations, and superconducting critical temperatures and order parameters, for various heavy electron metals.

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There is a growing consensus that a magnetic fluctuation-based theory contains the essential physics for describing heavy electron behavior [1,2]. This picture is confirmed by neutron scattering data which reveal strong antiferromagnetic moment fluctuations in many heavy fermion metals, including those that superconduct [3-5]. Although some efforts have been made, it is a difficult problem to calculate the observed magnetic fluctuation spectra from first principles. Therefore, the idea was developed to use the magnetic fluctuation spectra from experiment to construct the appropriate self-energy functions [6]. Evaluation of the normal self-energy reveals that the mass renormalization scales with the susceptibility (as opposed to the logarithm of the susceptibility, which is the result when using a Lindhard function). Moreover, the size of the calculated mass renormalizations are consistent with experiment (5 for CeSn_3 , 17 for UPt_3 , and 90 for UPe_{13}). The mass renormalization also decays with frequency, which in turn implies that the electronic specific heat coefficient (C/T) decreases with temperature. In particular, good agreement was found when comparing the calculated C/T against experiment for UPt_3 [6].

Evaluation of the anomalous self-energy leads to superconducting solutions for both UPt_3 and UPe_{13} . In both these metals, the susceptibility function has double-zone symmetry [3,4], with the susceptibility having a minimum at $q=0$ and a peak at the first reciprocal lattice vector ($\langle 001 \rangle$ direction for UPt_3 , $\langle 111 \rangle$ direction for UPe_{13}). This reflects the antiferromagnetic correlations within the unit cell (there are two U atoms per primitive cell). The resulting gap functions also

have this symmetry, and change sign under translation by the above q vector. This has the effect of removing the repulsive part of the interaction (represented by the average susceptibility), with the superconductivity being due to the oscillatory part of the susceptibility.

The gap function calculated for UPt_3 goes as $\cos(k_z c/2)$ (an anisotropic s-wave gap), which has a line of nodes perpendicular to the c axis for the zone-boundary Fermi surfaces centered at the A point. This nodal structure has been seen experimentally by transverse ultrasound [7], and is also consistent with various thermodynamic properties, such as the specific heat [8]. A Fourier transform of the gap function reveals that $\Delta(r)$ vanishes for $r=0$, where r is the relative separation of the electrons in the Cooper pair, and peaks at the near-neighbor separation (note this happens even for this "s-wave" gap since Δ changes sign under a k_z translation of $2\pi/c$). The gap function for UBe_{13} is found to be either pure d-wave (E_g character) or a mixture of d-wave and s-wave. The d-wave gap supports point nodes along the $\langle 111 \rangle$ directions, consistent with various thermodynamic measurements [9]. An s and d-wave mixture has been used to explain the unusual phase diagram for Th doped UBe_{13} [10]. In both the UPt_3 and UBe_{13} cases, the calculated transition temperature is comparable to experiment.

To develop a more complete theory than the one offered here would require calculating both the dynamic susceptibility itself, and how it couples to the quasiparticle charge degrees of freedom. Calculation of the susceptibility from relativistic band calculations reveals a broad frequency response with weak q dependence (except for UPt_3 , where a peak is found at $(0,0,2\pi/c)$), in general agreement with neutron scattering data [11,12]. Also, the correct moment orientations are obtained. Still, the experimental susceptibility is easiest explained as local moment relaxation modulated by near neighbor interactions [3,13]. In addition, the electronic structure calculations predict large moment states for all U heavy electron superconductors, in clear contradiction with experiment. Recently, though, small moment states (with moments of the order of a few hundredths of a Bohr magneton) have been seen in URu_2Si_2 [5] and UPt_3 [14]. It is tempting to speculate that the Kondo effect is acting to suppress the predicted magnetic moments (this

suppression is lifted by doping or by applying a field, leading to moments in agreement with band calculations [12]). With the static magnetic correlations being suppressed, the metal can gain energy by utilizing the dynamic magnetic fluctuations to undergo a superconducting condensation, as discussed above.

Given the local-moment nature of the dynamic fluctuations, a correlated Kondo approach might be the easiest way to derive the susceptibility function (as opposed to finding some way to appropriately renormalize the band structure susceptibility). This still leaves the problem of how to couple the itinerant charge degrees of freedom via intraband and interband matrix elements to the susceptibility. Matrix elements used when deriving the band susceptibility may be able to give us some guidance in this direction.

In conclusion, a magnetic fluctuation theory appears to be successful in describing a number of observed phenomena in heavy fermion metals, including the large normal state specific heats and their temperature dependences, as well as the observed nodal structure of the superconducting gaps. Moreover, the magnetic fluctuations have the correct energy scale to obtain reasonable superconducting transition temperatures. It is also speculated that the calculated band structure magnetic moments for these superconductors are suppressed by the Kondo effect. This in turn allows the dynamic magnetic fluctuations to induce the observed superconducting states at low temperatures.

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