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THE KONDO BOSON THEORY OF THE DYNAMIC SUSCEPTIBILITY OF HEAVY FERMIONS

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We apply the Kondo-boson – $1/N$ expansion to the microscopic Anderson lattice model, properly generalized to include the effects of spin–orbit coupling. We compute the imaginary susceptibility for a generic cubic band structure including the effects of the leading order Fermi liquid interactions. We show that the antiferromagnetic correlations (at the zone boundary) which occur at frequencies of the order of the Kondo temperature, arise naturally as a consequence of transitions across the hybridization gap or the Fermi surface. Finite frequency structure at the zone center derives from f-spin non conserving interactions mediated by exchange of Kondo boson propagators. We discuss alternate "interacting impurities" approaches in light of the experimental evidence for coherence and a sharp Fermi surface at low temperatures.

Much attention has been given to the neutron scattering measurements of several heavy fermion compounds [1, 2, 3]. In order to infer from the observed spin fluctuations about the mechanisms leading to superconductivity and/or antiferromagnetism, their microscopic origin needs to be understood. First we survey the following common features of the dynamical susceptibility $\chi(\boldsymbol{q}, \omega)$ which have been observed at temperatures in the coherent (low resistivity) regime:

1) $\chi''(\boldsymbol{q}, \omega) \equiv \mathrm{Im}\, \chi$ peaks at low frequencies $\omega_{\max}(\boldsymbol{q})$ (of order 5 and 0.2 meV in UPt_3 and $CeCu_6$ respectively).

2) These peaks are generally maximized at the reduced momentum $\boldsymbol{q} = \pi/a^*$ (zone boundary ZB), where a^* is the inter rare earth separation in the $\hat{q}$ direction. By transforming χ'' into real space one can conclude that antiferromagnetic correlations between f-spins at neighboring rare earth sites are observed. Also, $\chi''(\boldsymbol{q} = 0)$ peaks at a comparable frequency in apparent contradiction to a spin conserving Fermi liquid theory, where the f-sum rule [4] requires that

$$\int_0^\infty \mathrm{d}\omega\, \omega \chi'' \propto |\boldsymbol{q}|^2 ,$$

The theoretical interpretations of these observations have been divided into two main schools of thought: (I) Interacting Kondo impurities [1, 5], and (II) Quasiparticles of hybridized bands [6].

Approach (I) is based on the results of the Single Kondo Impurity (SI) model at zero temperature, for which

$$\chi_{\mathrm{SI}} = \chi^{\mathrm{r}} \frac{T_{\mathrm{K}}}{\mathrm{i}\omega + T_{\mathrm{K}}} , \tag{1}$$

where χ^{r} is the real static susceptibility, and T_{K} is the Kondo temperature. Effects of intersite correlations and coherence are included only in allowing momentum dependence in the parameters $\chi^{\mathrm{r}}(\boldsymbol{q})$ and $T_{\mathrm{K}}(\boldsymbol{q})$. Although, phenomenologically, this generalization of eq. 1 seems to work reasonably well in fitting some of the data, it leaves serious conceptual difficulties in understanding the compatibility of the neutron data with much of the bulk thermodynamic and transport properties. It is unlikely that the *itinerant* Fermi liquid properties at low temperatures (most strikingly the De Haas–Van Alphen [7] measurements, and the low temperature T^2 resistivity) can be understood in terms of localized incoherent spin fluctuations.

On the other hand, approach (II), which we shall support here, explains the neutron data using a quasiparticle picture in which two hybridized bands are within the small energy range of

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T_K near the Fermi energy. The resulting susceptibility at large $\boldsymbol{q}$ is thus dominated by extraordinarily low frequency interband transitions $\omega \approx T_K$ between the two bands and across the Fermi surface.

Here we shall address features 1 and 2 of the data, by following a $1/N$ Kondo boson analysis [8, 9] of the large U Anderson lattice model properly generalized to include the effects of spin–orbit coupling and crystal fields. We assume that the emerging small Kondo energy scale T_K is much smaller than the lowest crystal field splitting, thus reducing the f-degeneracy N to 2, and quenching its orbital moment [10]. We compute the imaginary susceptibility χ'' for a generic cubic band structure including effects of leading order Fermi liquid interactions.

As previously shown by several authors (see references in ref. [8]), the mean field Kondo Boson theory ($N \rightarrow \infty$) results in an effectively non-interacting quasiparticle band structure with dispersion:

$$E_{\boldsymbol{k}}^{\pm} = \tfrac{1}{2}(\varepsilon_f + \varepsilon_{\boldsymbol{k}}) \pm \sqrt{\tfrac{1}{2}(\varepsilon_{\boldsymbol{k}} - \varepsilon_f)^2 + \bar{V}^2}\,, \tag{2}$$

where $\bar{V}$ and ε_f are the renormalized hybridization and f-level energies respectively. $\varepsilon_{\boldsymbol{k}}$ is the conduction band of "bare" width D (of order eV). The mean field equations yield the small Kondo energy given by

$$T_K = \varepsilon_f - E_F \approx D \exp(-1/J)\,. \tag{3}$$

E_F is the renormalized Fermi energy and J is the small Kondo coupling constant. The mean field susceptibility (shown in fig. 1a) is

$$\chi_{MF}(\omega, \boldsymbol{q}) = -\sum_{kQ\alpha\alpha'} \mathrm{Tr}[(\mu_{\boldsymbol{k},\boldsymbol{k}+\boldsymbol{q}}^{\alpha\alpha'})^2] \times \frac{f(E_{\boldsymbol{k}}^{\alpha}) - f(E_{\boldsymbol{k}+\boldsymbol{q}+Q}^{\alpha'})}{E_{\boldsymbol{k}}^{\alpha} - E_{\boldsymbol{k}+\boldsymbol{q}+Q}^{\alpha'} + \omega + \mathrm{i}\eta}\,, \tag{4}$$

where Q are reciprocal lattice vectors and $\mu_{\boldsymbol{k},\boldsymbol{k}+\boldsymbol{q}}$ is the f-electron magnetic moment operator transformed to the quasiparticle basis.

We have numerically evaluated eq. 4 for some typical cubic band structures, and observed that the features shown in fig. 2 for spherical dispersions, are common to Fermi surfaces with large $K_F \gg \pi/2a^*$. Similar features are observed for small $K_F \ll \pi/2a^*$, where intraband transitions across the small Fermi surface dominate χ''. The following general properties are noted:

1) The peaks are antiferromagnetic, i.e. occur at the ZB $\boldsymbol{q} = \pi/a^*$. We find, however, that they are suppressed when the fermi surface has substantial necks in that direction and $K_F \simeq \pi/2a^*$. Three-dimensionality and umklapp processes play an important role in "hiding" the Fermi wave vector.

2) At temperatures $T \geq 0.5T_K$, the large $\boldsymbol{q}$ peaks can be fitted by the Kondo impurity Lorentzian eq. 1, but at $T = 0$ and for $K_F \gg \pi/2a$ (dashed line) a shifted Lorentzian would do bet-

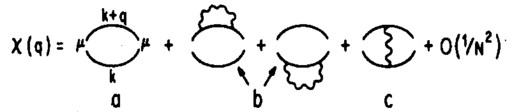

Fig. 1. Leading order diagrams for the dynamical susceptibility. (a) is the mean field term (eq. 4), (b) and (c) are the $1/N$ self energy and vertex contributions (eq. 5) respectively. Solid and wiggly lines are mean field Greens functions and 2×2 boson propagator matrix D respectively. See text and ref. [8] for notations.

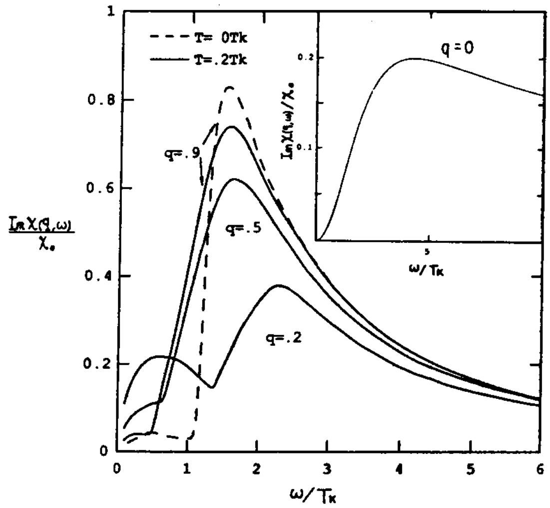

Fig. 2. Dynamic susceptibility calculated for a cubic heavy fermion model with a spherical Fermi surface, at $T = 0.2T_K$ and $K_F = \pi/a^*$, for different momenta $\boldsymbol{q} = (0, q, q)\pi/a^*$. Dashed line shows $T = 0$ behavior which fits a shifted Lorentzian. Inset: Im $\chi(\boldsymbol{q} = 0, \omega)$, (eq. 6) at $T = 0$, for spin–orbit parameter $\bar{\mu}$ set equal to $\sqrt{\chi_0/\gamma}$.

ter. This is consistent with experimental observation [2] in $CeCu_6$. Both effects 1 and 2 are expected to be less pronounced in the presence of complicated surface topology, and anisotropy of the Fermi velocity.

3) The spin fluctuation energy, (determined by the maxima at $q = \pi/a^*$), scales with the Kondo temperature [11] T_K. This would be interesting to verify experimentally (e.g. via pressure dependence). In case Fermi surface nesting occurs, antiferromagnetism in the direction of the nesting vector can be expected. The energy scale of fluctuations in that direction would not be universal and should not be expected to scale with T_K.

From eq. (4) it can be seen that the mean field susceptibility contains no finite frequency contribution at the zone center $\boldsymbol{q} = 0$. Following ref. [7] we integrate out the gaussian fluctuations of the Bose fields to obtain the $\mathcal{O}(1/N)$ correction to the susceptibility, given diagramatically in figs. 1b and c:

$$\Delta\chi_{1/N} = \frac{1}{N}\,(\chi_{1b} + \chi_{1c})\,. \tag{5}$$

After some algebra, which will be presented elsewhere [12], we can reduce the integrals involved in calculating the diagrams to yield the low ω and T result:

$$\Delta\chi''_{1/N}(0, \omega) = \frac{2}{N}\sum_{\boldsymbol{q}} \int_0^{\omega} \frac{d\omega'}{\pi\omega^2} \sum_{r,r'} \bar{\Pi}''_{rr'}(\boldsymbol{q}, \omega') \times D''_{rr'}(\boldsymbol{q}, \omega - \omega')]\,, \tag{6}$$

where

$$\bar{\Pi}''_{rr'} = \mathrm{Im}\Big\{-\sum_{k\alpha\alpha'} \mathrm{Tr}[(\mu^{\alpha,\alpha}_{kk} - \mu^{\alpha',\alpha'}_{k+qk+q})^2] \times \frac{f(E^{\alpha}_{k}) - f(E^{\alpha'}_{k+q})}{E^{\alpha}_{k} - E^{\alpha'}_{k+q+Q} + \omega + i\eta}\, C^{\alpha\alpha'}_{r} C^{\alpha'\alpha}_{r}\Big\} \approx \bar{\mu}^2(1 - e^{-q^2/\bar{q}^2})\Pi''\,. \tag{7}$$

Here $D_{rr'}$, $\Pi_{rr'}$, and C_r, $rr' = 1, 2$, are the boson propagator, Lindhard functions and coherence factors respectively, all previously defined [8]. Eq. 6 is our main result. It is clear from eq. 7 that the susceptibility would vanish, as expected from the sum rule eq. 2, whenever spin is a good quantum number for excitations and $\mu^{\alpha\alpha}_{kk}$ is independent on $\boldsymbol{k}$, α. Thus $\bar{\mu}$ parameterizes the spin–orbit and crystal field effects and determines the scale of the zone center contribution. By fitting to the numerical results we arrive at an analytic approximation to $\Delta\chi_{1/N}$ which can be used to fit the data:

$$\Delta\chi_{1/N} = 0.3a\chi^{r}\,\frac{(\omega/T_0)^2}{1 + (\omega/T_0)^{\eta+2}}\,, \tag{8}$$

where $\eta \approx \frac{1}{2}$ is the fall-off exponent, the characteristic frequency scale is $T_0 \approx 2.5T_K$, and $a = \bar{\mu}^2\rho/\chi^{r}$ (ρ is the renormalized density of states). We point out that the $\boldsymbol{q} = 0$ susceptibility is also accessible to polarized ligh scattering [13].

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