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Mesoscopic fluctuations in the Fermi-liquid regime of the Kondo problem

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Abstract. We consider the low temperature regime of the mesoscopic Kondo problem, and in particular the relevance of a Fermi-liquid description of this regime. Mesoscopic fluctuations of both the quasiparticle energy levels and the corresponding wavefunctions are large in this case. These mesoscopic fluctuations make the traditional approach to Fermi-liquids impracticable, as it assumes the existence of a limited number of relevant parameters. We show here how this difficulty can be overcome and discuss the relationship between the resulting Fermi-liquid description "*à la Nozières*" and the mean field slave fermion approximation.

The progress made in the control and miniaturization of micro- or nano-structures has renewed interest in the Kondo problem, and in particular made relevant the question of what would happen if the magnetic impurity is connected to a *finite-size* fully-coherent electron bath rather than a bulk piece of material [1–19]. As a first consequence, the finite size of the bath implies a finite mean level spacing Δ, and it becomes meaningful to discuss the individual properties of levels and wave-functions. Lack of translational invariance will furthermore be associated with interference effects, and thus mesoscopic fluctuations of the energy levels and wave-functions. These mesoscopic fluctuations will affect the Kondo physics. They imply for instance fluctuations of the Kondo temperatures [9,10,19–23]. They also impact the low temperature description of the Kondo problem.

In the bulk case, that is in the absence of mesoscopic fluctuations, it is known since Nozières [24,25] that this low temperature regime of the Kondo problem is a Fermi liquid. Furthermore, in that case, symmetries, and the fact that the only energy scale in the *bulk* Kondo problem is the Kondo temperature T_K, make it possible to essentially completely specify the properties of this Fermi liquid: the quasi-particles are characterized by a phase shift $\delta_s(\epsilon_F) = s\pi/2$ at the Fermi energy ($s = \pm 1$ is the sign of the spin), with a variation

$$\delta_s(\epsilon_F + \omega, B) = s\pi/2 + \omega/T_K - s(g\mu_B/2)B/T_K, \quad (1)$$

away from the Fermi energy and with a small magnetic field B (g and μ_B are the corresponding Landé factor and Bohr magneton). In addition to this phase shift, the magnetic impurity generates a weak effective interaction between the electrons of the gas associated with virtual breaking of the Kondo singlet, and thus taking place only locally at the impurity, $V_{\rm eff} = (\pi\nu_0^2 T_K)^{-1}\hat{\Psi}^\dagger_\uparrow(\mathbf{r}_0)\hat{\Psi}_\uparrow(\mathbf{r}_0)\hat{\Psi}^\dagger_\downarrow(\mathbf{r}_0)\hat{\Psi}_\downarrow(\mathbf{r}_0)$.

The physical arguments given by Nozières to justify treating the low temperature regime of the Kondo problem as a Fermi-liquid apply in the mesoscopic case as well as in the traditional bulk case. There is therefore little doubt that for temperature much smaller than T_K the mesoscopic Kondo problem yields a Fermi-liquid too. Given the extraordinary amount of physical insight obtained in the bulk case from the Fermi-liquid description, it is therefore natural to extend it explicitly to the mesoscopic regime.

Obtaining a Fermi-liquid description of a mesoscopic problem is however a priori not a trivial task. Indeed, what usually makes a Fermi liquid description effective is not so much the derivation of its parameters from a microscopic calculation, but rather the fact that because there are only a small number of energy scales at play (and usually a high degree of symmetry), the number of parameters required to fully describe the system is rather small. Taking advantage of the symmetries, and of the fact that the temperatures or energies considered are much smaller than all "natural" energy scales of the problem, one can perform perturbative expansions near the Fermi energy. In this way, the quasi-particles as well as their weak mutual

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interactions can be characterized by a small number of parameters, quite often fixed in practice by measuring a few relevant quantities. From those, the full behavior of the system can be determined. These considerations apply for the Nozières Fermi-liquid as well as more traditional Landau type Fermi-liquids such as the ones describing He^3 or the electron gas.

In the mesoscopic case, however, this approach seems a priori hopeless: one has fluctuations at all scales between the mean level spacing Δ and the scale $E_{\rm fl}$ at which mesoscopic fluctuations set in (typically the Thouless energy for ballistic systems). One, therefore, cannot expect to obtain a parameterization with only a small number of parameters.

The goal of this paper is to show that nevertheless a Fermi-liquid description of the low temperature regime of the mesoscopic Kondo problem can be obtained. We will focus here on the description of the quasi-particle energy levels, *including their mesoscopic fluctuations*. Generalisation to wavefunction properties is relatively straightforward. The approach we follow is similar in spirit to the way a Landau Fermi-liquid description is obtained for a mesoscopic electron liquid, relevant in the context of ballistic or diffusive quantum dots [26]. Indeed in that case as well, the existence of fluctuations at all energy scales between $E_{\rm fl}$ and Δ seems to prevent the description of the problem in terms of a few parameters. This problem has been "solved" using essentially an argument of separation of scales: if the screening length of the Coulomb interaction is much smaller than the size of the dot, the renormalization of the mass and of the interactions (short length scale) are the same as in the bulk, while the confinement effects (large length scale) are obtained from a self-consistent potential derived from a Thomas-Fermi treatment. Note however that this common wisdom way of dealing with a mesoscopic Landau Fermi liquid does not rely on an analytic derivation (see for instance the renormalization group approach proposed in Ref. [26] and the difficulty with that approach discussed in Ref. [27]), but it has been effective in interpreting most experimental data.

This is, then, the approach we would like to follow for the Fermi-liquid description of the mesoscopic Kondo problem. To remain general, we consider a generic Kondo Hamiltonian. In its simplest version, referred to as the *s*-*d* (or simply Kondo) model, this consists in the (local) interaction of a gas of non-interacting fermions with a spin one half. The corresponding Hamiltonian then reads

$$H_{\rm K} = \sum_{\alpha\sigma} \epsilon_\alpha \hat{c}^\dagger_{\alpha\sigma}\hat{c}_{\alpha\sigma} + H_{\rm int} + g\mu_B B S_z, \tag{2}$$

where $\hat{c}^\dagger_{\alpha\sigma}$ creates a particle with energy ϵ_α, spin σ and wave-function $\varphi_\alpha(\mathbf{r})$, and the interaction with the impurity is expressed as:

$$H_{\rm int} = J_0\, \mathbf{S}\cdot\mathbf{s}(\mathbf{r}_0) \tag{3}$$

with $J_0 > 0$ the coupling strength, $\hbar\mathbf{S} = \hbar(S_x, S_y, S_z)$ a quantum spin 1/2 operator (S_i is half of the Pauli matrix σ_i), $\hbar\mathbf{s}(\mathbf{r}_0) = (\hbar/2)\hat{\Psi}^\dagger_\sigma(\mathbf{r}_0)\boldsymbol{\sigma}_{\sigma\sigma'}\hat{\Psi}_\sigma(\mathbf{r}_0)$ the spin density of the electron gas at the impurity position $\mathbf{r}_0$, and $\hat{\Psi}^\dagger_\sigma(\mathbf{r}_0) = \sum_\alpha \varphi_\alpha(\mathbf{r}_0)\hat{c}^\dagger_\alpha$. Finally, with the last term on the right hand side of equation (2), we consider also the possibility that the impurity spin is coupled to a magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$.

We furthermore assume only that, as mentioned above, our mesoscopic system is characterized by the energy scale $E_{\rm fl}$, below which mesoscopic fluctuations take place but above which our electron bath behaves essentially as a bulk system. Thus, smoothing the density of states $\rho_B(\epsilon) \equiv \sum_\alpha \delta(\epsilon - \epsilon_\alpha)$ on the scale $E_{\rm fl}$ gives a "bulk-like" density of states $\rho_0(\epsilon) \equiv \langle\rho_B\rangle_{E_{\rm fl}}$ which shows no mesoscopic fluctuations and has only secular variations on classical scales (e.g. the Fermi energy). In the same way, we assume that a bulk-like wave-function probability $\gamma_0(\epsilon) \equiv \langle|\varphi_\alpha|^2\rangle_{E_{\rm fl}}$ can be defined with variation only on classical scales. To help visualize the problem, one may think of the mesoscopic electron bath as a billiard, thus corresponding to the one particle Schrödinger Hamiltonian $H_0 = -(\hbar^2/2m)\nabla^2$ inside some domain $\mathcal{D}$ of area $\mathcal{A}$ and typical size L. In that case, $\rho_0(\epsilon)$ is the Weyl mean density of states, $\gamma_0(\epsilon) = 1/\mathcal{A}$, and $E_{\rm fl}$ is the Thouless energy $E_{\rm Th} = \hbar/\tau_{\rm fl}$ with $\tau_{\rm fl} \equiv L/v_F$ the time of flight across the system (v_F is the Fermi velocity). We shall not, however, use any specific properties of billiards in what follows and shall furthermore assume that, unlike billiards, our system has a finite bandwidth D (which avoids unessential technical convergence problems and is in any case necessary for a properly defined Kondo problem).

Under the assumption that the Kondo temperature is larger than the Thouless energy, the impurity behaves at the local level as if it were placed in a bulk piece of material characterized by the density of states ρ_0 and the wave-function probability $\gamma_0(\epsilon)$. In this case, the "Kondo cloud" fits entirely within the system, and it is only at longer length scales that the effects of the finiteness of the system are felt. To implement this intuitive idea, let us for a moment consider a localized static potential $U(\mathbf{r}) = U_0\delta(\mathbf{r} - \mathbf{r}_0)$ (with $\mathbf{r}_0$ the location of the impurity). (The divergences associated with a δ-potential are avoided with a finite bandwidth.) Let us furthermore denote by $G_B(\mathbf{r},\mathbf{r}';\omega)$ the Green function of our mesoscopic electron bath, and by $G_0(\mathbf{r},\mathbf{r}';\omega)$ the corresponding "bulk-like" Green function. In particular we have

$$G_B(\mathbf{r}_0,\mathbf{r}_0;\omega) = \sum_\alpha \frac{|\varphi_\alpha(\mathbf{r}_0)|^2}{\omega - \epsilon_\alpha + i\eta} \tag{4}$$

$$G_0(\mathbf{r}_0,\mathbf{r}_0;\omega) = -i\pi\nu_0(\omega) + \Lambda(\omega), \tag{5}$$

with $\nu_0(\omega) \equiv \gamma_0(\omega)\rho_0(\omega)$ the local density of states, and

$$\Lambda(\omega) = \gamma_0(\omega)\mathcal{P}\int d\epsilon \frac{\rho_0(\epsilon)}{\omega - \epsilon}. \tag{6}$$

The T-matrix of the static impurity in the bulk-like system is then given by:

$$\begin{aligned} t(\omega) &= U + UG_0U + UG_0UG_0U + \cdots \\ &= U\frac{1}{1 - G_0U}, \end{aligned} \tag{7}$$

while for the genuine mesoscopic system one has similarly

$$T(\omega) = U + UG_BU + UG_BUG_BU + \cdots = U\frac{1}{1-G_BU}. \quad (8)$$

Since U_0, $t(\omega)$, and $T(\omega)$ as well as $G_0(\mathbf{r}_0, \mathbf{r}_0)$ and $G_B(\mathbf{r}_0, \mathbf{r}_0)$ are just numbers, simple algebra leads to:

$$T(\omega) = \frac{t(\omega)}{1-\delta G(\omega)t(\omega)}, \quad (9)$$

with $\delta G \equiv G_B(\mathbf{r}_0, \mathbf{r}_0) - G_0(\mathbf{r}_0, \mathbf{r}_0)$ the fluctuating part of the Green function. From this equation the full Green function G_B^{tot} including both the confinement and the impurity potential is given by:

$$G_B^{\mathrm{tot}}(\mathbf{r}, \mathbf{r}'; \omega) = G_B(\mathbf{r}, \mathbf{r}'; \omega) + G_B(\mathbf{r}, \mathbf{r}_0; \omega)T(\omega)G_B(\mathbf{r}_0, \mathbf{r}'; \omega). \quad (10)$$

We argue that equations (9) and (10) can be used to characterize the quasi-particles in the Fermi liquid description of the mesoscopic Kondo problem. Indeed, here the Green function G_B contains all the required information about the confinement properties ("long range"), and the Kondo physics ("short range") is implemented by the T-matrix $t(\omega)$. At energies ω sufficiently small compared to T_K so that inelastic processes are negligible, $t(\omega)$ is related to the phase shift equation (1) through

$$t(\omega) = -\frac{1}{2i\pi\nu_0}\left[\exp(2i\delta_s(\omega)) - 1\right]. \quad (11)$$

The full Green function of the quasi-particles is, therefore, entirely determined through equation (10). In particular, the quasi-particles energies λ_β of the Fermi liquid are given by the poles of the T-matrix (9), and therefore fulfill the equation

$$G_B(\mathbf{r}_0, \mathbf{r}_0; \lambda) - G_0(\mathbf{r}_0, \mathbf{r}_0; \lambda) = 1/t(\lambda). \quad (12)$$

Noting that $\mathrm{Im}[1/t(\omega)] = \pi\nu_0$ and, thus, that away from the energies ϵ_α of the unperturbed problem the imaginary part of equation (12) is automatically fulfilled, we see that the λ's are therefore given as the solutions of

$$\sum_\alpha \frac{|\varphi_\alpha(\mathbf{r}_0)|^2}{\lambda - \epsilon_\alpha} - \Lambda(\lambda) = -\frac{\pi\nu_0 \sin(2\delta_s)}{1-\cos(2\delta_s)} \simeq \frac{\pi\nu_0}{T_K}\left(\lambda - s\frac{g\mu_B}{2}B\right), \quad (13)$$

where in the last equality we have inserted the expression (1) for the phase shift and, to remain consistent, expanded to first order in $1/T_K$. Equation (13) is the main result of this work; it is the extension to the mesoscopic Kondo problem of the Fermi-liquid result equation (1) valid for the traditional bulk case. For a given realization of the eigenlevels and eigenfunctions of the mesoscopic electron gas, it completely specifies the energies of the Landau quasi-particles of the corresponding mesoscopic Kondo problem when in the low temperature regime.

At this point, it is interesting to compare equation (13) to the analogous equation derived previously [17–19] in the framework of the slave bosons/fermions mean field approximation:

$$\sum_{\alpha=1}^{N} \frac{|\varphi_\alpha(\mathbf{r}_0)|^2}{\lambda - \epsilon_\alpha} = \frac{\pi\nu_0}{\tilde{T}_K^{\mathrm{MF}}}\left(\lambda - sg\mu_B B/2\right), \quad (14)$$

whose derivation is briefly sketched in the Appendix. Comparing equations (13) and (14), we see that they have the same structure, and basically contain the same qualitative content. Quantitatively they differ in two respects. First, the true Kondo temperature T_K in equation (13) is replaced in equation (14) by $\tilde{T}_K^{\mathrm{MF}}$, which is properly speaking the resonance width of the mean field resonant level, or up to the factor $a_k \simeq 1.133\ldots$ the mean field approximation of the Kondo temperature (see Appendix). Second, the term $\Lambda(\lambda)$ in equation (13) is absent from (14). If the Fermi energy is in the middle of the band, this is of little importance as then $\Lambda \sim 0$. If this is not the case, however, $\Lambda(\lambda)$ compensates the effect of states far from the Fermi energy, and its absence in (14) is certainly a limitation of the mean field approach.

We, thus, see that the mean field and the Fermi liquid approaches have the same physical content as far as the spectrum of the quasi-particles is concerned. In particular, analysis of spectral correlations such as was done in references [18] and [19] could be performed following essentially the same lines and would yield essentially the same results. The mean field result has however some shortcomings, such as the fact that only the mean field approximation to the Kondo temperature can enter, which are naturally cured in the more correct Fermi liquid approach. These differences are of a quantitative nature and would in particular be relevant in a comparison with an exact computation of the quasi-particle energies for some specific realisation of the mesoscopic Kondo problem – that is, for a particular choice of a mesocopic electron gas coupled to a Kondo impurity. Such an exact computation could be obtained for instance from a numerical renormalisation group calculation [2,28], which however implies the development of rather non-trivial codes and is, therefore, left for future work.

Finally, we can roughly estimate the range of energies for which the above neglect of inelastic processes is applicable. It is known that at low energy and temperature, the rate of inelastic processes in the Kondo problem grows as the square of the deviation from the Fermi energy. This is the expected Fermi liquid result; it has been shown, for instance, that the imaginary part of the self-energy of the quasi-particles goes to zero as ω^2, $\Im\{\Sigma(\omega)\} \propto \omega^2/T_K$ [29]. To extract the quasi-particle energies via the procedure outlined here, this inelastic rate must be much smaller than the level spacing, $\omega^2/T_K \ll \Delta$. Thus, the number of quasi-particle energy levels that are accurately treated by our argument, $N \equiv \omega/\Delta$, is roughly given by $N \sim \sqrt{T_K/\Delta}$. Since we are in any case assuming $T_K \gg \Delta$, this means that only levels near the center of the Kondo resonance can be captured.

To conclude, we have shown that the basic equation (13) can be derived directly from a Fermi-liquid treatment "*à la Nozières*" and that, as in the bulk, the slave boson mean field approach gives for the mesoscopic Kondo problem a description which in the low temperature regime is equivalent to the Fermi liquid description. More precisely, limiting our discussion here to the quasi-particle energy levels, we have seen that if the chemical potential is in the middle of the band, both approaches give the same result for those energies, except that the true Kondo temperature is replaced in the mean field approach by its mean field approximation (which is of course the best the mean field can provide). The Fermi liquid approach proposed here corrects in certain respects the description of the low energy quasi-particle spectra obtain earlier through the mean field approach.

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Appendix: Slave boson mean field

We summarize here briefly the principle of the mean field approximation scheme [30]. Starting from the Hamiltonian H_K equations (2)–(3), one introduces a representation of the spin $\mathbf{S}$ in terms of Abrikosov fermions $\hat{f}_\sigma^\dagger$ with spin $\sigma =\uparrow,\downarrow$ and writes the Kondo part of the Hamiltonian as:

$$H_{\rm int} = \frac{J_0}{2}\sum_{\sigma\sigma'} f_\sigma^\dagger f_{\sigma'} \hat{\Psi}_{\sigma'}^\dagger(\mathbf{r}_0)\hat{\Psi}_\sigma(\mathbf{r}_0) - \frac{J_0}{4}\sum_\sigma \hat{\Psi}_\sigma^\dagger(\mathbf{r}_0)\hat{\Psi}_\sigma(\mathbf{r}_0). \tag{A.1}$$

One furthermore needs to impose the constraint

$$\hat{f}_\uparrow^\dagger \hat{f}_\uparrow + \hat{f}_\downarrow^\dagger \hat{f}_\downarrow = 1, \tag{A.2}$$

which is done through a Lagrange multiplier ϵ_0 in the action and amounts in practice to the substitution

$$H_{\rm imp} \mapsto H_{\rm imp} + \epsilon_0 \sum_\sigma \hat{f}_\sigma^\dagger \hat{f}_\sigma.$$

This fermionic representation is exact. The mean field approximation consists in replacing the quartic part of the Kondo term by an effective quadratic term

$$\sum_{\sigma\sigma'} \hat{f}_\sigma^\dagger \hat{f}_{\sigma'} \hat{\Psi}_\sigma^\dagger(\mathbf{r}_0)\hat{\Psi}_\sigma(\mathbf{r}_0) \mapsto \sum_{\sigma\sigma'} [\hat{f}_\sigma^\dagger \hat{\Psi}_\sigma(\mathbf{r}_0)\langle \hat{\Psi}_{\sigma'}^\dagger(\mathbf{r}_0)\hat{f}_{\sigma'}\rangle + \text{h.c.}],$$

where the mean value $\langle\cdots\rangle$ is computed self consistently. The mean field Hamiltonian obtained in this way is a resonant level model:

$$H_{\rm MF} = \sum_\sigma \Bigg[\left(\sum_\alpha \epsilon_\alpha \hat{c}_{\alpha\sigma}^\dagger \hat{c}_{\alpha\sigma}\right) + \epsilon_{0\sigma}\hat{f}_\sigma^\dagger \hat{f}_\sigma + \left(v^* \hat{f}_\sigma^\dagger \hat{\Psi}_\sigma(\mathbf{r}_0) + v\hat{\Psi}_\sigma^\dagger(\mathbf{r}_0)\hat{f}_\sigma\right)\Bigg] \tag{A.3}$$

where we define $\epsilon_{0\sigma} \equiv \epsilon_o + sg\mu_B B/2$. To fix the parameters of the resonant level model, there are two self-consistency conditions,

$$v = \frac{J_0}{2}\sum_\sigma \langle \hat{f}_\sigma^\dagger \hat{\Psi}_\sigma(\mathbf{r}_0)\rangle, \tag{A.4}$$

$$1 = \sum_\sigma \langle \hat{f}_\sigma^\dagger \hat{f}_\sigma\rangle\ ; \tag{A.5}$$

note that the second one consists in treating the constraint equation (A.2) only on average. This mean field treatment has been used to study the mesoscopic Kondo problem in references [17–19].

Under our assumption that the Kondo temperature is larger than the scale $E_{\rm fl}$ below which mesoscopic fluctuations occur, we expect that the parameters v and ϵ_0 are the same as for the bulk analogue of our system. A detailed analysis of the fluctuations of the mean field parameters shows indeed that their relative variance goes to zero as T_K becomes much larger than the mean level spacing Δ [9,19,23]. Therefore, in the low temperature regime, ϵ_0 is fixed at the Fermi energy μ (taken equal to zero), and the low temperature limit of the resonance width $\Gamma(T) \equiv \pi\nu_0|v|^2$ can be interpreted as the Kondo temperature. More precisely, $\Gamma(0) = a_k T_K^{\rm MF} = \frac{1}{2}T_K^{\text{1-loop}}$ ($a_k \simeq 1.133\ldots$), where $T_K^{\rm MF}$ and $T_K^{\text{1-loop}}$ are, respectively, the mean field and one-loop approximations to the Kondo temperature. Now as can be easily shown (see, e.g., Ref. [19]) the eigenenergies $\lambda_{\beta\sigma}$ of the resonant level are the solutions of the equation

$$\sum_\alpha \frac{|\varphi_\alpha(\mathbf{r}_0)|^2}{\lambda - \epsilon_\alpha} = \frac{\lambda - \epsilon_{0\sigma}}{|v|^2}, \tag{A.6}$$

which is equivalent to equation (14).

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