Nonuniversality in the Kondo Effect

M. Naghashpour and S. E. Barnes
Department of Physics, University of Miami, Coral Gables, Florida 33124
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We have analytically evaluated, up to fourth order, all logarithmic terms in the perturbation expansion of the magnetization $\mathcal{M}$ for the Kondo model. All nonlogarithmic terms have been evaluated up to third order. When these results are compared with the claimed universal function $\mathcal{M}(H/T_H)$ calculated with the Bethe ansatz, we find that the two cannot be made to agree whatever the form of T_H. We conclude that such universal functions *do not* exist.

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Although to many the Kondo problem appears highly esoteric, it remains a basic test bed for theoretical methods which would claim to handle infrared-divergent problems of which there exist many in both condensed matter and elementary particle physics. And while it is reasonable to claim that the Kondo problem was solved *in principle* by Anderson and co-workers [1], it is Wilson [2] who provided the first detailed solution using numerical methods. Some time later the same problem was solved [3,4] analytically using the Bethe ansatz and there exists a claim by one of the present authors [5] that exact results can also be obtained using a certain special self-consistent parquet approximation.

What is of interest here is an oft repeated claim, which seems to have been first made by Wilson [2], that the important properties associated with the model exhibit universal behavior. Specifically studied in the work presented here is the universality of the magnetization $\mathcal{M}$ at zero temperature. Universality implies that

$$\mathcal{M}\equiv\mathcal{M}(H/T_H)\,, \tag{1}$$

where H is the magnetic field and $T_H\sim D|\rho J|^{1/2}\times\exp\{-1/|\rho J|\}$ is a characteristic scale or Kondo temperature, both specified in energy units; i.e., universality implies that $M(x)$ is the same function for all reasonable variants of the Kondo model. All differences between models are to be accommodated in the scale energy T_H. There *are* a couple of important caveats. The coupling constant $|\rho J|\ll 1$ and the characteristic energy of the measurement, H for this example, must be much less than the effective band cutoff D. In fact H should be sufficiently small that within the region $\pm H$ of the Fermi energy ϵ_F, the density of states is flat.

It is also to be recognized, for the comparison made here, that there is a nonanalytic relationship between the coupling constants for the versions of the model solved by the Bethe ansatz [3] and by Wilson [2]. There is a special notation [3]; the Bethe approach implies a cutoff scheme, denoted D, in which the *interacting* states are cut off outside a certain energy region, while in the $\mathcal{D}$ scheme, it is the *noninteracting* states which must lie within an energy D on either side of the Fermi energy ϵ_F (=0 here). Andrei, Furuya, and Lowenstein [3] have shown that the leading orders of the perturbation expansions agree *if* the coupling constant $2g/\pi$ ($\equiv|\rho J|$ above) in the D scheme is related to the similar quantity $2g/\pi$ in the $\mathcal{D}$ scheme by

$$\frac{2g}{\pi}\to\frac{2g}{\pi}-\frac{1}{2}\left[\frac{2g}{\pi}\right]^2\ln\frac{2g}{\pi}+O(g^2)\,. \tag{2}$$

However, despite this nonanalytic relationship between the coupling constants, it is claimed by the authors [3] of the Bethe solution that their result is of the same universality class as the Wilson version of the model, i.e., that the only real effect of this nonanalytic relationship is the absence of the factor of $(2g/\pi)^{1/2}$ or $(|\rho J|^{1/2})$ in their definition of T_H.

We have tested this universality hypothesis by performing very careful perturbation expansions using standard perturbation theory for the $\mathcal{D}$ scheme and comparing this with the corresponding terms generated by an expansion of the Bethe expression for the high-field regime.

We have taken the analytic expressions for the Bethe approach as a definition of the function $M(x)$. With some choice of T_H this universal $M(x)$ should, when expanded, generate any valid perturbation expansion to all orders. We have calculated *all* logarithmic terms in such an expansion for the usual $\mathcal{D}$ scheme up to $O(g^4)$ and all nonlogarithmic terms up to $O(g^3)$. The relevant form for the scale, which enters $M(H/T_H)$, is

$$T_H=\mathcal{D}\left(\frac{2g}{\pi}\right)^{1/2}e^{-(\pi/2g)+\alpha(g)}\,, \tag{3}$$

where $\alpha(g)=b_1(2g/\pi)+b_2(2g/\pi)^2+\cdots$, i.e., is an expansion in the coupling constant $2g/\pi$ ($\equiv|\rho J|$). The coefficients b_1 and b_2 are determined by nonlogarithmic terms which first occur in $O(g^2)$ and $O(g^3)$. Such coefficients correspond to next-to-leading and next-to-next-leading logarithmic quantities. Once a coefficient is determined, it, in turn, determines the coefficient of *all* the similarly logarithmic divergent terms in all orders of perturbation theory. Specifically, the first coefficient is determined by the nonlogarithmic terms in $O(g^2)$ and *in fact* is confirmed by next-to-leading logarithmic terms in both $O(g^3)$, *and* by our new detailed calculations for

$O(g^4)$. However, the second coefficient, corresponding to a nonlogarithmic term in $O(g^3)$, first generates logarithmic terms in $O(g^4)$; this coefficient *is not* confirmed by this least divergent logarithmic term in $O(g^4)$. We are led to the conclusion that the Bethe ansatz and Wilson solution *do not* belong to the same universality class. In fact we suspect that the universality class is very much smaller than suggested by Wilson; i.e., not only is the Bethe solution not in the same class but also $\mathcal{D}$ scheme models with different densities of states distant from the Fermi surface correspond to different functions $M(x)$, etc.

These contentions may appear surprising in view of one of the present authors' claim [5] to be able to obtain exact results for the same Kondo problem with what amounts to a self-consistent parquet approximation. Such an approach can only claim to be good to next-to-leading logarithmic accuracy. Specifically it is claimed that such a method yields the exact result for the so-called Wilson "crossover ratio" $W'=2\pi(n/2e)^{n/2}/\Gamma(n/2)$, for the compensated case when $n=2S$. What the present authors believe to be true is that W' *is* a universal constant, and as is required by Ward identities [6] the Wilson ratio $R=n/(n-1)$, even though there do not exist universal functions such as $M(x)$, or the resistivity $\rho(x)$, etc. That is, the large-energy-scale perturbative *and* low-energy so-called strong-coupling results, when $H,T<T_K$, are both determined by the self-consistent parquet approximation. In fact, it is suggested that the label "strong coupling" is more appropriate to the intermediate regime when $H,T\sim T_K$, and when all orders in perturbation theory *are* required to determine most physical quantities such as $M(x)$, $\rho(x)$, and $C_V(x)$. It seems likely that all modifications to the model which can change the relationship between the coefficients of next-to-leading and next-to-next-leading order logarithmic terms change the form of the would-be universal functions, e.g., $M(x)$, $\rho(x)$, and $C_V(x)$, without (usually) changing W' and R.

Despite the fact that there exist any number of computer programs which when given a set of, e.g., Feynman, rules can numerically sum perturbation series, the work described here involves the *analytic* evaluation of all contributions to fourth order. We chose to perform analytic calculations since, first, easy to make estimates readily indicate that very high precision is needed to pick out the sought for coefficient of the next-to-next-leading logarithmic term in fourth order. The difficulty of such a numerical approach is best illustrated by Wilson [2] who *did* perform such calculations. Unfortunately his results cannot be used for the present purpose since he did not evaluate his modified $\tilde{D}(\rho J)$ within his scheme. [In effect, he did not evaluate the constant term in $O(g^3)$.] Second, analytic calculations are more transparent and easier to confirm by others. Full details of the calculations of the fourth-order terms are prohibitively long to be reproduced here; a fairly complete presentation *is* available [7].

The method and notation used correspond to an appendix of Ref. [3], in particular we will use the notation $2g/\pi$ for the magnitude of the coupling constant when evaluating our perturbation expression in the $\mathcal{D}$ (non-Bethe) scheme. We have evaluated the necessary additional terms in the expansion of the Bethe $M(x)$ and obtain

$$\mathcal{M}_i(H>T_H)=S\left[1-\frac{1}{2}z+\frac{1}{4}(\ln 2)z^2-\frac{1}{8}\left(\ln^2 2+\ln 2-1+\frac{2\pi^2}{3}-\frac{4\pi^2S^2}{3}\right)z^3+\cdots\right], \tag{4}$$

where the invariant charge z is defined by

$$\frac{1}{z}-\frac{1}{2}\ln z=\ln\frac{H}{T_H}. \tag{5}$$

With

$$T_H=\frac{1}{2}\mathcal{D}\exp\left[-\frac{\pi}{2g}+\frac{1}{2}\ln\left(\frac{2g}{\pi}\right)+b_0+b_1\left(\frac{2g}{\pi}\right)+b_2\left(\frac{2g}{\pi}\right)^2\right], \tag{6}$$

this set of equations defines the universal $M(x)$ to sufficient accuracy for the present purposes.

Following the appendix of Ref. [3], a standard perturbation expansion is made for the free energy, i.e., written as

$$\mathcal{F}=-T\ln Z=-T\left\{\ln Z_0+\frac{Z_1}{Z_0}+\left[\frac{Z_2}{Z_0}-\frac{1}{2}\left(\frac{Z_1}{Z_0}\right)^2\right]+\left[\frac{Z_3}{Z_0}-\left(\frac{Z_1}{Z_0}\right)\left(\frac{Z_2}{Z_0}\right)+\frac{1}{3}\left(\frac{Z_1}{Z_0}\right)^3\right]\right.$$
$$\left.+\left[\frac{Z_4}{Z_0}-\left(\frac{Z_1}{Z_0}\right)\left(\frac{Z_3}{Z_0}\right)-\frac{1}{2}\left(\frac{Z_2}{Z_0}\right)^2+\left(\frac{Z_1}{Z_0}\right)^2\left(\frac{Z_2}{Z_0}\right)-\frac{1}{4}\left(\frac{Z_1}{Z_0}\right)^4\right]+\cdots\right\}, \tag{7}$$

where Z_n corresponds to the nth-order term in the perturbation expansion for the partition function Z. The magnetization is obtained by evaluating the derivative $\partial/\partial H|_{H\to 0}$, whence the well-known second-order term is, in the present notation,

$$\mathcal{M}_i^{(2)}=(2g/\pi)^2S[\ln(H/D)+\ln 2], \tag{8}$$

while the third-order term becomes

$$\mathcal{M}_i^{(3)} = -\left(\frac{2g}{\pi}\right)^3 \left\{ S\left[\ln^2\left(\frac{H}{D}\right) + \frac{1}{2}\ln\left(\frac{H}{D}\right) + 2\ln 2\ln\left(\frac{H}{D}\right) + \frac{1}{4} + \ln 2 + \ln^2 2 + \frac{\pi^2}{12}\right] + S^2\left(\frac{\pi^2}{4}\right) + S^3\left(\frac{\pi^2}{24}\right)\right\}. \tag{9}$$

We are not aware of any existing calculation with which to compare the constant term in this expression. The final result for the fourth-order expression is

$$\mathcal{M}_i^{(4)} = \left(\frac{2g}{\pi}\right)^4 \left\{ S\left[\ln^3\left(\frac{H}{D}\right) + \frac{5}{4}\ln^2\left(\frac{H}{D}\right) + 3\ln 2\ln^2\left(\frac{H}{D}\right) + \frac{1}{2}\ln\left(\frac{H}{D}\right) + \frac{7}{2}\ln 2\ln\left(\frac{H}{D}\right) + \frac{11}{4}\ln^2 2\ln\left(\frac{H}{D}\right) + \frac{7\pi^2}{24}\ln\left(\frac{H}{D}\right)\right] + S^2\left[\frac{\pi^2}{2}\ln\left(\frac{H}{D}\right)\right] + S^3\left[\frac{1}{4}\ln^2 2\ln\left(\frac{H}{D}\right) - \frac{7\pi^2}{24}\ln\left(\frac{H}{D}\right)\right]\right\}. \tag{10}$$

We have *not* evaluated the constant in this order. [It is to be emphasized, again, that neither of the above results may be compared with the numerical evaluation of this series by Wilson, since an expression for his $\tilde{D}(\rho J)$ is needed, and anyway his "onion" scheme implies a different cutoff procedure.] We were initially concerned by the presence of even terms in the spin magnitude S since we expected that the transformation $S \rightarrow -S$ corresponds to $H \rightarrow -H$ and should reverse the sign of M. However, it is observed that, e.g., the effective cutoff D, when expanded in g, might contain the invariant $S(S+1)$ which can generate terms even in S. We have confidence in this result since all but the next-to-next-leading logarithms have the coefficient expected if $M(x)$ were to be universal and it is these same coefficients which also determine that of the weakest divergence of interest. Also essentially the same method of evaluating these weakly divergent terms was used to evaluate the next-to-leading terms in the third order; again these terms conform with the expectations of universality.

The first constant

$$b_0 = -\tfrac{1}{2}\ln 2 \tag{11}$$

in T_H has already been determined. The second constant

$$b_1 = -\frac{1}{2}\ln 2 - \frac{1}{2} + \frac{\pi^2}{12} - \frac{3\pi^2}{8}S^2 - \frac{\pi^2}{4}S \tag{12}$$

is therefore our principal result. When substituted into the Bethe expansion for $M(x)$, we obtain the fourth-order term,

$$\mathcal{M}_i^{(4)} = \left(\frac{2g}{\pi}\right)^4 S\left\{\ln^3\left(\frac{H}{D}\right) + \frac{5}{4}\ln^2\left(\frac{H}{D}\right) + \frac{1}{2}\ln\left(\frac{H}{D}\right) + 3\ln^2 2\ln\left(\frac{H}{D}\right) + 3\ln 2\ln^2\left(\frac{H}{D}\right) + 4\ln 2\ln\left(\frac{H}{D}\right) + \frac{\pi^2}{3}\ln\left(\frac{H}{D}\right) + \frac{\pi^2}{2}S\ln\left(\frac{H}{D}\right) - \frac{\pi^2}{4}S^2\ln\left(\frac{H}{D}\right) + \text{const}\right\}, \tag{13}$$

which clearly does not correspond to our direct perturbation calculations in this order.

We conclude that, at least, the Bethe and Wilson solutions for the compensated case of the Kondo model do *not* belong to the same universality class.

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