Multi–Channel Kondo Necklace

P. Fazekas* and Hae–Young Kee†

International Centre for Theoretical Physics,
P.O. Box 586, I–34100 Trieste, Italy

Abstract

A multi–channel generalization of Doniach’s Kondo necklace model is formulated, and its phase diagram studied in the mean–field approximation. Our intention is to introduce the possible simplest model which displays some of the features expected from the overscreened Kondo lattice. The $N$ conduction electron channels are represented by $N$ sets of pseudospins $\tau_j$, $j = 1, \ldots, N$, which are all antiferromagnetically coupled to a periodic array of $|S| = 1/2$ spins. Exploiting permutation symmetry in the channel index $j$ allows us to write down the self–consistency equation for general $N$. For $N > 2$, we find that the critical temperature is rising with increasing Kondo interaction; we interpret this effect by pointing out that the Kondo coupling creates the composite pseudospin objects which undergo an ordering transition. The relevance of our findings to the underlying fermionic multi–channel problem is discussed.

*Permanent address: Research Institute for Solid State Physics, P.O.B. 49, Budapest 114, H–1525 Hungary
†Permanent address: Department of Physics Education, Seoul National University, Seoul, 151–742 Korea
1 INTRODUCTION

The essential physics of mixed valent and heavy fermionic systems [1] is habitually described by some suitable version of the periodic Anderson model [2]. In this framework, heavy fermionic systems correspond to the limiting case of nearly integral valence, which permits us to use a Kondo lattice model for the approximate handling of the low–energy, low–temperature behaviour of the Anderson lattice [3]. Though already several steps removed from physical reality, it is widely accepted that the Kondo lattice model incorporates the basic ingredients necessary to understand the competition between two opposing tendencies: the formation and eventual ordering of magnetic moments, and the formation of a heavy Fermi sea. Research has for a long time been focussed on the case where localized spins $S = 1/2$ are compensated by electrons moving in a non–degenerate band

$$H_{KL} = \sum_{k,\sigma} \epsilon(k) c_{k\sigma}^{+} c_{k\sigma} + \frac{J}{2L} \sum_{s} \sum_{k, k'} e^{i(k-k')s} \sum_{\sigma\beta} c_{k\alpha}^{+}\sigma_{\alpha\beta} c_{k'\beta} S$$

where the first term describes a non–degenerate band, and the second the antiferromagnetic ($J > 0$) Kondo coupling at each site $s$. $L$ is the number of lattice sites, and $\sigma$ is the vector of Pauli matrices. $H_{KL}$ is the simplest version of the Kondo lattice hamiltonian; we expect that it shows the same overall features as the $S = N/2$ models, where $N$ is the number of conduction electron channels participating in the Kondo screening process. This special case of exact compensation seems to be the most favourable for the formation of an overall singlet, i.e., a heavy Fermi liquid without any residue of magnetic order. Even these perfectly screened models are, of course, capable of magnetic ordering [3, 4, 5, 6]; but the arising of a completely non–magnetic state can at
least be claimed to be a natural option [7].

In recent years, it has become increasingly clear that considering the underscreened $S > N/2$, and overscreened $S < N/2$, models brings not just additional complications but interesting new physics, and it is also essential to describe many, if not all, of the actual heavy fermionic materials.

The properties of an isolated underscreened, or overscreened, Kondo impurity [8] have been studied in great detail, and for a number of physical quantities, exact results are known [9, 10]. Still, understanding can not yet be considered complete; in particular, we could wish for a clearer physical picture of the low-temperature behaviour of the overscreened model with its intriguing non-integer ground state degeneracy [11, 12].

Much less is known about magnetic ordering in the corresponding periodic models. Just as in the case of perfect screening $S = N/2$, there must be a competition between Kondo screening and intersite interactions; however, the picture is complicated by the fact that the local object which tends to arise from the Kondo effect, has a more intricate internal structure. For the underscreened case, even a very strong Kondo coupling can not do better than to leave a reduced spin $S - N/2$; thus one is led to consider the ordering of the residual magnetic moments. The underscreened Kondo lattice is apparently destined to become magnetic [13], and it was suggested that its study should lead to understanding heavy fermion magnetism in general [14].

The situation is much less clear in the overscreened case. The model which was first introduced as a matter of academic interest [8], was later argued to represent the physical situation for two–level systems interacting with several conduction electron channels [15, 16], and for U–based heavy fermion systems [17]. Subsequent experiments on structurally disordered metallic nanoconstrictions [18], and on the Kondo alloy $Y_{1-x}U_xPd_3$ [19], gave ample confirmation
of the applicability of the overscreened Kondo model. Another remarkable realization of the multi–channel Kondo effect is provided by the transport properties of Pb$_{1-x}$Ge$_x$Te [20].— The solution of the single–impurity problem shows a puzzling mixture of features which one would naively associate either with the absence, or the completion, of spin compensation. The ground state possesses a zero point entropy [10, 11, 12] which, in the limit of an infinite Fermi sea, does not correspond to a half–integer spin, but reduces to ln(2) if the system is finite. The finding of a zero point entropy might lead us to think that the ground state is possessing a residual magnetic moment; however, calculations show [4, 10] that magnetism is quenched as $T \rightarrow 0$, albeit much more slowly than in the $S = N/2$ case. All in all, it turns out to be fairly difficult to form an intuitive picture of the multichannel Kondo system whose behaviour is governed by an intermediate–coupling fixed point. Correspondingly, we have only the haziest idea of what a periodic array of overscreened Kondo centres is supposed to be doing.

In either case, when we undertake the study of the magnetic phases of the periodic models, we have to deal with the ordering of composite spins created by a local Kondo coupling; and the degree to which Kondo compensation can progress is itself limited by the intervention of intersite interactions. Curiously, the effect can go opposite ways in the underscreened, and overscreened, cases. For the underscreened lattice, the resulting total spin is necessarily less than $S$, so the ordering temperature is found [28] to show a decreasing tendency with increasing $J$. In the overscreened case, the Kondo effect is actually building up a screening object which can be ultimately larger than the screened spin $S$. We are going to find this tendency for sufficiently large ($N \geq 3$) numbers of channels.
2 PSEUDOSPIN MODELS: THE KONDO NECKLACE AND ITS GENERALIZATIONS

The fact that the conduction electrons are forming a Fermi sea, with a large number of arbitrarily low–lying excitations, is essential for the appearance of a non–analytic energy scale [the Kondo temperature $T_K \propto B \exp (-1/J \rho(\epsilon_F))$, where $B$ is of the order of the bandwidth, and $\rho(\epsilon_F)$ the density of states at the Fermi level] in the theory of the single–ion Kondo effect. It is, as yet, an open question whether there is a non–analytic energy scale associated with the formation of a non–magnetic ground state of the periodic Kondo model (or, to put it more pointedly, whether there is a Kondo–effect in the Kondo lattice [21]), and if yes, whether the “lattice Kondo temperature” is different from the single–ion $T_K$ [3, 7, 22, 23]. It can be, however, argued [24] that the competition between the Kondo effect, and the interactions opposing it, can be successfully mimicked by just considering the gross effects of different couplings: one can have a crude version of the phase diagram of the Kondo lattice without the “true” Kondo effect. One can then forget about the low–lying electron–hole excitations which can lead to infrared divergencies, and consider the conduction electrons only to the extent that they provide spins which tend to be aligned antiparallel to the localized spins. One can thus reduce the mixed spin–fermion problem to a pure spin problem. This was the rationale behind introducing Doniach’s [25] necklace model

$$H_{KN} = J \sum_m S_m \cdot \tau_m + W \sum_{\langle mn \rangle} (\tau^x_m \tau^x_n + \tau^y_m \tau^y_n)$$ (2)

where the pseudospins $|\tau| = 1/2$ represent the spin degrees of freedom of the conduction electrons, and $W$ is a characteristic amplitude of their propagation.
$H_{KN}$ is the pseudospin version of the $S = 1/2$ lattice model given in eqn. (1); clearly, $W$ is an effective parameter which depends in a complicated manner on the parameters of the underlying electronic model. The mean field treatment of $H_{KN}$ by Doniach [25] led to a ground state phase diagram which looks qualitatively the same as expected from a (still missing) complete treatment of (1), for the case of a half–filled conduction band: the ground state is antiferromagnetic for $J/W < 1$, and non–magnetic (apparently Kondo–compensated) for $J/W > 1$. We conclude that the study of necklace–type pseudospin models is a useful prelude to the investigation of the full fermionic Kondo lattice problems. — We note that recently, Strong and Millis [26] investigated a generalized form of the $S = 1/2$, $N = 1$ necklace model with the ultimate purpose of gaining insight into the behaviour of heavy fermionic systems.

We should emphasize that we use the term “necklace”, as opposed to “lattice”, models to signify that the conduction electron sea has been replaced by a set of pseudospins, and not to mean that the model is necessarily one–dimensional. In (2), the sum over $\langle mn \rangle$ is over nearest–neighbour (nn) pairs in any lattice. In fact, usually we will resort to the mean field approximation (MFA), so lattice dimensionality plays no essential role. The results obtained in the MFA are thought to be a reasonable approximation for the three-dimensional models, but they should serve as a rough guide even in one–dimension [27], except that whenever long–range order is found, it should be interpreted as indication of quasi–long–range order.

Considering the rudimentary stage of the understanding of the underscreened, and quite particularly, the overscreened, periodic Kondo models, we can appreciate the need for any insight to be gained from the study of related simpler models. In [28], we introduced the underscreened, spin–$S$ necklace models, and discussed their properties. The underscreened necklace models
turn out to be inherently antiferromagnetic, with an easy–plane anisotropy; the Kondo coupling merely influences the size of the ordered moment. The relative ease of the solution is thanks to the fact that the dimensionality of the Hilbert space is merely $\propto S$.

In the present work, we perform a similar investigation of a class of overscreened necklace models. We introduce the hamiltonian

$$H = \frac{J}{N} \sum_m S_m \cdot \sum_{j=1}^N \tau_{j,m} + \frac{W}{N} \sum_{(mn)} \sum_{j=1}^N (\tau^x_{j,m} \tau^x_{j,n} + \tau^y_{j,m} \tau^y_{j,n})$$

(3)

where $N$ different kinds of pseudospins $\tau_j$ for $j = 1, \ldots, N$ are meant to represent the $N$ screening channels. The localized moments (in truth, $f$–spins) are taken to be $|S| = 1/2$. The $x – y$ coupling which should correspond to the propagating character of the conduction electron spin degrees of freedom, acts independently in each channel. In order to have a meaningful large–$N$ limit of the model, one has to keep the individual couplings of order $1/N$. We are restricting ourselves to the case when all channels are equivalent; one should be aware, though, that models with inequivalent channels \[30\] should be of great physical interest. The study of some such models is in progress.

A general comment about the necklace replacements of the true Kondo problems should be made here: in the necklace models, the Kondo effect, and the Kondo bound state, become very local. This corresponds to the actual physical situation for very strong Kondo couplings. Thus, the necklace models can be used in good faith for $S \geq k/2$, where the large–$J$ limit is continuously connected to the regime of small $J$’s. The finding of an intermediate coupling fixed point for $S < k/2$ tells us that this is assuredly not the case for an overscreened Kondo impurity. However, we would still like to argue that the study of the lattice model (3) should have relevance for the overscreened peri-
odic Kondo model. It can be generally argued that in Kondo lattice models, especially in the presence of ordering, intersite effects may prevent us from reaching the fixed point of the corresponding single-site models, and so the subtleties of the impurity solution may become irrelevant for the lattice. This argument should apply quite particularly to the overscreened case where the behaviour is known to be extremely sensitive to the presence of external fields \[10, 29\]. It has been pointed out by Andraka and Tsvelik \[31\] that intersite interactions, acting like fields, can be expected to turn the system towards a strong-coupling fixed point. An important piece of corroborative evidence is that for the two-impurity problem, destabilization of the “marginal Fermi liquid” single-impurity behaviour was found by Ingersent, Jones and Wilkins \[32\]. Thus we think it not implausible that in periodic models, ordering of tightly bound objects created by the multichannel Kondo coupling can be taking place, and then our model hamiltonian (3) acquires relevance.

3 MEAN-FIELD THEORY OF THE OVERSCREENED NECKLACE MODEL

The overscreened model presents much larger difficulties than the underscreened one \[28\] because the dimensionality of the Hilbert space is now exponentially large in \(N\). We are, however, aided by the huge symmetry of \(H\): neglecting lattice translations, the symmetry group is \(G = SO(3) \otimes S_N\). \(H\) has full spin-rotational symmetry, as well as invariance under arbitrary permutations of the channel indices \(j\). We will find that symmetry simplifies the appearance of the spectrum to such an extent that at least the single-site mean field problem becomes solvable for general \(N\), without any further approximations.

Assuming a simple magnetic order in which all neighbours of a given site
have their $\tau$-spins polarized in the same direction, we can do the familiar MF decoupling to arrive at the single-site hamiltonian

$$H_{MF} = \frac{J}{N} S \cdot \sum_{j=1}^{N} \tau_j - \frac{\omega}{N} \sum_{j=1}^{N} \tau_j^z$$

(4)

where $\omega = W z \langle \tau \rangle$ is the mean field strength, $z$ being the coordination number. For the sake of solving just the MF problem, we rotated the quantization axis to align up with the mean field; in the sense of the full hamiltonian $H$, this must be an arbitrary direction in the $x-y$ plane. For bipartite lattices, there is no formal difference between ferromagnetic $W < 0$, and antiferromagnetic $W > 0$, intersite couplings; to have a closer correspondence with physical reality, we will have to take $W > 0$.

The Kondo term in $H_{MF}$ has the single-site version of the high symmetry described before: it is invariant under arbitrary rotations of the total spin $\eta = S + \sum_{j=1}^{N} \tau_j$, as well under permutations of the $N$ channels. Switching on the effective field destroys spin rotational invariance, but we will still find it useful to think of the states as derived from splitting the highly degenerate levels of the underlying $SO(3)$-invariant problem. In any case, we have still got the permutational symmetry. Actually, this rests on having chosen a $j$-independent effective field:

$$\langle \tau_1^z \rangle = \ldots = \langle \tau_N^z \rangle = \langle \tau \rangle$$

(5)

In principle, MF solutions breaking the $S_N$ symmetry are imaginable. For small values of $N$, we were exploring this possibility, and found that the symmetrical solution is more advantageous, so we feel confident in using the form of $H_{MF}$.
specified in (4).

In what follows, we set out to classify the eigenstates according to the irreducible representations of $S_N$, by constructing their Young–tableaux [33]. As it turns out, this classification is intimately related to the classification according to the total spin $\eta$, and its $z$–component $\eta^z$, so it is useful to start with the high–symmetry problem $\omega = 0$.

Let us start with the unique $\eta^z = (N + 1)/2$ state

\[ \uparrow \quad \uparrow \quad \ldots \quad \uparrow \]

where $\uparrow$ denotes the $S$–spin, and the $\tau$–spins enter the Young tableau (YT) for the identity representation of $S_N$. Obviously, the $S$–spin cannot be included in the YT because there is no symmetry with respect to interchanging $S$ with one of the $\tau$s. Following custom, we will refer to the $\tau$–part of such a graphical representation as a YT, while the whole picture will be called a “diagram”; since with the inclusion of the $S$–spin, it is not a YT in the conventional sense.

(6) is the $\eta^z = (N + 1)/2$ component of the maximum spin $\eta = (N + 1)/2$ multiplet. Its energy is

\[ \epsilon_0^+ = \frac{J}{4} \]

In the subspace $\eta^z = (N - 1)/2$ we are going to meet several kinds of states. The permutationally symmetrical ones are
As usual, YT represent states fully symmetrized along a row, so it is unequivocal what (8), and (9), stand for. These are not eigenstates of the total Kondo coupling; the actual eigenstates are their properly chosen linear combinations. One of these must be the $\eta^z = (N - 1)/2$ component of the $\eta = (N + 1)/2$ multiplet. The other belongs to a symmetrical $\eta^z = (N - 1)/2$ multiplet, with the energy

$$\epsilon_0 = -\frac{N + 2}{4N} J$$

This is actually the ground state energy of the local Kondo coupling. The corresponding eigenstate can be roughly described by saying that the $S$–spin is pointing antiparallel to an assembly of $\tau$–spins. Actually, it is not quite that: it contains an admixture of states (9) in which a $\tau$–spin is antiparallel to all other spins.

The ground state of the Kondo–term is $N$–fold degenerate. We can inter-

\[ \begin{array}{c c c}
\uparrow & \cdots & \uparrow \\
\downarrow & & \\
\end{array} \] (8)

\[ \begin{array}{c c c}
\uparrow & \cdots & \uparrow \\
\uparrow & & \downarrow \\
\end{array} \] (9)
pret this as a result of an effective ferromagnetic coupling which the common Kondo-coupling to the $S$-spin induces between the $\tau$-spins. This feature is not unlike to that found in rigorous treatments of the overscreened Kondo impurity [10, 29]. — Note, however, that here it leads to ascribing the zero-point entropy $k_B \ln N$ to a Kondo site and thus, as discussed in the Introduction, we fail to recover the subtle features of the single-ion solution of the original overscreened Kondo problem. However, we have the correct features for a strong-coupling solution which may turn out to be of relevance for the lattice case.

$\epsilon_0^+$ and $\epsilon_0^-$ can be seen to result from coupling the $S = 1/2$ spin either parallel, or antiparallel, with a fully polarized $T = |\sum_j \tau_j| = N/2$ set of $\tau$-spins.

All the other $N - 1$ states in the $\eta^z = (N - 1)/2$ subspace belong to the only other Young tableau which can be constructed with one of the $\tau$-spins down:

\begin{equation}
\begin{array}{c}
\uparrow  \\
\uparrow \\
\cdots \\
\downarrow \\
\end{array}
\end{equation}

Antisymmetrizing along the column is effectively the same as putting two $\tau$-spins in a singlet combination, permitting to line up only the residual $N - 1$ spins. The dimensionality of the representation specified by the YT above is just $d_1 = N - 1$, accounting for all the remaining $\eta^z = (N - 1)/2$ states which are thus found to be degenerate. Here we first see the enormous simplification
brought by the $S_N$-symmetry: spin–rotational symmetry alone would permit
the existence of $N$ different levels corresponding to $\eta = (N - 1)/2$ multiplets;
$S_N$-invariance tells us that there are just two levels, corresponding to the two
different possible shapes of Young tableaux. One of these was inherited from
the $\eta^z = (N + 1)/2$ subspace and corresponds to $T = N/2$; the other is the
one in (11), with a down–spin in the second row, for which $T = (N - 2)/2$.
— For our particular problem, which has to do with permutational symmetry
acting within $SU(2)$, all YT have at most two rows.

It is crucial to observe that this scheme holds generally: each time when
we step down $\eta^z$, only one new YT appears, namely the one where one box is
removed from the upper row, and a down–spin box is added to the second row.
This corresponds to a new value of the total $\tau$–spin $T$, which is 1 less than
the previous lowest $T$–value. Though $T = \sum_j \tau_j$ is not a conserved quantity
for the Kondo–term, definite values of $T$ are unambiguously identified with
definite shapes of Young tableaux, $T = (N - 2m)/2$ corresponding to a YT
with $N - m$ boxes in the upper row.

For $\eta^z = (N - 2m + 1)/2$, most of of the states can be represented by turn-
ing down a spin in the first row of a YT which we had seen previously: these
are stepped–down versions of $\eta > \eta^z$ states, corresponding to levels which had
been identified previously. The only new diagrams are

\[
- \begin{array}{c}
\uparrow \\
\downarrow \\
\end{array} 
\begin{array}{c}
\uparrow \\
\downarrow \\
\end{array} 
\begin{array}{c}
\uparrow \\
\downarrow \\
\end{array} 
\begin{array}{c}
\cdots \\
\cdots \\
\end{array} 
\begin{array}{c}
N-m+1 \\
N-m+1 \\
N-m+1 \\
N-m+1 \\
\end{array}
\]

(12)
associated with combining \( T = (N - 2m + 2)/2 \) antiparallel with \( S = 1/2 \), i.e., with \( \eta = (N - 2m + 1)/2 \), and the diagram with the new YT

\[
\begin{array}{c}
\uparrow \\
\cdots \\
\downarrow \\
\end{array}
\]

\( N-m \)

\( m \)

(13)

describing the parallel alignment of \( T = (N - 2m)/2 \) total \( \tau \)-spin with the \( S \)-spin. This also has \( \eta = (N - 2m + 1)/2 \), but belongs to a new representation of \( S_N \), along with the new value of \( T \). The diagram is uniquely associated with the maximum-\( \eta^z \) component of the newly found multiplets which are therefore all degenerate. The degeneracy of the \( T = (N - 2m)/2, \eta^z = (N - 2m + 1)/2 \)

level is

\[
d_m = C_m^N - C_{m-1}^N = C_m^{N+1} \frac{N - 2m + 1}{N + 1} \tag{14}
\]

where the \( C \)s denote binomials.

The energies are simply given by

\[
JT \cdot S = \frac{J}{2}[\eta(\eta + 1) - \frac{3}{4} - T(T + 1)] \tag{15}
\]

The degeneracy of each energy level is the product of the corresponding \( d_m \),

14
and the $SO(3)$–associated multiplicity $2\eta + 1$.

For $N$ even, the procedure finishes with

\[
\begin{array}{c}
\uparrow \\
\uparrow \ldots \uparrow \\
\downarrow \ldots \downarrow \\
\hline
N/2
\end{array}
\]

and a similar diagram with the $S$–spin $\downarrow$. These stand for a $d_{N/2}$–dimensional subspace of $\tau$–singlets, leaving the $S$–spin free to make a disconnected doublet, with energy $\epsilon_{N/2}^\pm = 0$. — For $N$ odd, the last diagram is

\[
\begin{array}{c}
\downarrow \\
\uparrow \ldots \uparrow \uparrow \\
\downarrow \ldots \downarrow \\
\hline
(N-1)/2
\end{array}
\]

signifying an overall singlet $\eta = 0$.

In either case, two energy levels belong to each form of the YT with $0 \leq m \leq [(N + 1)/2] - 1$, and one level goes with $m = [(N + 1)/2]$. The total number of energy levels is $N + 1$.

In the presence of an effective field $\omega \neq 0$, the symmetry is reduced to $S_N$, and $\eta$ is no longer a good quantum number. However, the full spectrum can still be determined, because the eigenvalue problem is easily seen to separate into
a number of two–, and one–dimensional problems, essentially because the
\( S = 1/2 \)–spin can be stepped only once. Permutation symmetry requires that
only states with the same shape of the YT mix. Easiest is the case \( m = 0 \),
with a YT consisting of a single row of \( \uparrow \), and \( \downarrow \)–spins. In the orthonormal
basis

\[
\begin{array}{c}
\uparrow
\end{array}
\begin{array}{c}
\uparrow \quad \cdots \quad \uparrow \quad \downarrow \quad \cdots \quad \downarrow
\end{array}
\begin{array}{c}
\uparrow
\end{array} =
\]

\[
= \frac{1}{\sqrt{C_r^N}} \sum_{j_1 < \cdots < j_r} | \uparrow \rangle | \uparrow \cdots \downarrow \cdots \downarrow \uparrow \rangle
\] (18)

and

\[
\begin{array}{c}
\downarrow
\end{array}
\begin{array}{c}
\uparrow \quad \cdots \quad \uparrow \quad \downarrow \quad \cdots \quad \downarrow \quad \downarrow
\end{array}
\begin{array}{c}
\downarrow
\end{array} =
\]

\[
= \frac{1}{\sqrt{C_{r-1}^N}} \sum_{j_1 < \cdots < j_{r-1}} | \downarrow \rangle | \uparrow \cdots \downarrow \cdots \downarrow \uparrow \rangle
\] (19)

\( H_{MF} \) is represented by the matrix

\[
\begin{pmatrix}
(1/4N)(J - 2\omega)(N - 2r)
&(J/2N)\sqrt{r(N - r + 1)}

(J/2N)\sqrt{r(N - r + 1)}
&-(1/4N)(J + 2\omega)[N - 2(r - 1)]
\end{pmatrix}
\] (20)

The ground state is now non–degenerate, corresponding to \( r = 1 \), and a max-
imum polarization along the effective field. Note that while, in the absence of
an external field term, the pseudospin model gives only a very poor imitation of the highly non–trivial quantum–mechanical ground state of the electronic overscreened model, we have much less reason to doubt the validity of the picture obtained from the necklace model for moderately strong external fields. Since in a lattice, intersite interactions amount to a field acting at any particular Kondo site, herein lies our hope that the multichannel necklace model can give some guidance as to the behaviour of the multichannel Kondo lattice. We have already quoted arguments [31, 32] showing that intersite interactions can make the system turn towards a strong–coupling fixed point: this kind of behaviour can be imitated by a necklace–type model.

Similarly, for states with \( m \downarrow \)–spins in the second row of the YT, the two–dimensional subspace is spanned by

\[
\begin{array}{ccc}
\uparrow & \ldots & \uparrow \\
\downarrow & \ldots & \downarrow \\
\end{array}
\]

(21)

and
The eigenvalue problem is similar to that of \( m = 0 \), only we have to remember that in a YT, the states are antisymmetrized along the columns, so the symmetrization of \( \uparrow \)– and \( \downarrow \)–spins along the first row is not allowed to bring \( \downarrow \)–spins into the first \( m \) boxes. Effectively, in (20), in the off–diagonal elements \( N \) must be replaced by \( N - 2m \), giving the matrix

\[
\begin{pmatrix}
(1/4N)(J - 2\omega)[N - 2(m + r)] & (J/2N)\sqrt{r(N - 2m - r + 1)} \\
(J/2N)\sqrt{r(N - 2m - r + 1)} & -(1/4N)(J + 2\omega)[N - 2(m + r - 1)]
\end{pmatrix}
\]

(23)

The solution of the eigenvalue problem would be trivial to write down, but we do not need the lengthy expressions. First of all, we are interested in the mean field result for the magnetic transition temperature \( T_N \), for which linearized eigenvalues

\[
\lambda_{mr}^+ = \frac{J}{4N}(N - 2m) - \frac{(N - 2m)(N + 1 - 2m - 2r)}{2N(N + 1 - 2m)}\omega
\]

(24)

and
\[ \lambda_{mr}^- = -\frac{J}{4N} (N+2-2m) - \frac{(N+2-2m)(N+1-2m-2r)}{2N(N+1-2m)} \omega \] (25)

are sufficient. We also need \( \langle \tau \rangle \) for the corresponding eigenstates

\[ \tau_{mr}^+ = \frac{(N-2m)(N+1-2m-2r)}{2N(N+1-2m)} - \frac{4r\omega N+1-2m-r}{JN (N+1-2m)^3} \] (26)

and

\[ \tau_{mr}^- = \frac{(N+2-2m)(N+1-2m-2r)}{2N(N+1-2m)} + \frac{4r\omega N+1-2m-r}{JN (N+1-2m)^3} \] (27)

In the linearized self–consistency equation for \( \langle \tau \rangle \), the denominator is just the \( \omega = 0 \) value of the single–site partition function

\[ Z_0 = \sum_{m=0}^{[N+1]-1} d_m \left[ (N-2m+2)e^{-J(N-2m)/JNT} + (N-2m)e^{J(N-2m+2)/4NT} \right] \] (28)

while the numerator is the suitably weighted sum of (26) and (27)

\[ \langle \tau \rangle = \frac{1}{Z_0} \sum_{m=0}^{[N+1]-1} d_m \left[ \sum_{r=1}^{N-2m} e^{-\lambda_{mr}^-/TN} \tau_{mr}^- + \sum_{r=0}^{N-2m+1} e^{-\lambda_{mr}^+/TN} \tau_{mr}^+ \right] \] (29)

Actually, a slight complication has to be dealt with before arriving at (29). In the second \( r \)–sum, the terms \( 1 \leq r \leq N-2m \) arise from the two–dimensional eigenvalue problem (23). However, the state with \( r = 0 \), and \( S \)–spin \( \uparrow \uparrow \), is not coupled to any other state, it presents a one–dimensional eigenvalue problem.
Similarly for \( r = N - 2m + 1 \), and the spin \( \downarrow \). These are actually the \( \eta^z = \pm (N - 2m + 1)/2 \) components of the corresponding \( \eta = (N - 2m + 1)/2 \) multiplets, and are thus eigenstates by construction. It is, however, easy to check that these cases are accounted for by extending the second sum in (29) to include \( r = 0 \), and \( r = N - 2m + 1 \).

Though the \( r \)-sums in (29) are easily done (with the result that \( \langle \tau \rangle \) disappears from the equation), the \( m \)-summation is not, and we did not find any transparent from into which (29) could be cast. Essential simplification can be achieved only for the limiting case \( J/W \to \infty \) when it is sufficient to consider the action of \( H_{MF} \) within the subspace of the \( \eta = (N - 1)/2 \) Kondo ground states associated with the diagrams shown in (8), and (9). From (29), we find

\[
\lim_{J/W \to \infty} T_N = \frac{W (N - 1)(N + 2)^2}{6N^2(N + 1)} \tag{30}
\]

The above result can be easily interpreted by noticing that within the Kondo ground state set of states \( \tau_j \) acts like

\[
\tau_j \Rightarrow \frac{N + 2}{N(N + 1)} \eta
\tag{31}
\]

independently of \( j \). Thus, in the restricted Hilbert space formed by taking the direct product of the Kondo ground state sets for each site, the intersite coupling term in (3) can be exactly represented by the effective hamiltonian

\[
h_{eff} = W \frac{(N + 2)^2}{N(N + 1)^2} \sum_{i,j} [\eta^z_i \eta^z_j + \eta^y_i \eta^y_j] \tag{32}
\]
(30) is just the mean-field solution for (32). Note that it gives 0 for $N = 1$; this is in accordance with Doniach’s finding of a transition to the fully Kondo–compensated state at $J/W = 1$ for the original necklace model.

For general values of $J/W$, we solved (29) numerically. Fig. 1 shows the coupling dependence of $T_N$, for several values of $N$. On the horizontal axis, we have chosen the variable $J/(J+W)$, so as to be able to include the asymptotic regime where (30) becomes valid. (Since in the MFA, the coordination number $z$ enters only through $zW$, we have simply taken $z = 2$).

At $J = 0$, the system separates into $N$ independent channels, disconnected from the $S$–spins. Each set of $\tau$–spins orders at the same mean-field temperature $W/2N$. This point is clearly pathological; our interest lies in the behaviour at intermediate (and in any case, non–zero) values of $J/W$.

First of all, one should note that, with the exception of $N = 2$, all curves show an overall rising tendency with increasing $J/W$: the asymptotic value (30) is lying significantly higher than the low-$J$ value of $T_N$. Remarkably, the Kondo effect does not seem to compete with pseudopsin ordering but rather to assist it! We can understand this tendency by remembering that the ordering is that of composite spins [most clearly seen in the large–$J$ expression (32)] which arise from glueing the $\tau$–spins together. In the starting hamiltonian (3), there is no direct interchannel coupling: the effective ferromagnetic coupling between the channels is done by the Kondo coupling. So, in the multi–channel case, the Kondo coupling is effectively creating the objects which subsequently order.

A subtler feature of our $T_N$ curves is a maximum at some $J/W$ value which appears to increase with $N$. For a better view, we give a blow–up of the relevant region of the phase diagram in Fig. 2. The broad, relatively low
maximum is most discernable for $N = 2$, but it apparently exists (though quickly becoming quite inconspicuous) for any finite $N$.

We have also done the numerical solution of the self–consistency equation at arbitrary temperatures, i.e., at finite effective field strengths. We found that the temperature dependence of the order parameter is of the form usually found in similar mean–field solutions, so we renounce including them here.

In our pseudospin model, the ordering which sets in at $T_N$, is (depending on the sign of $W$), either a ferromagnetic, or a two–sublattice antiferromagnetic, ordering of the $\tau$–spins. Via the Kondo–coupling, this induces a similar, but oppositely polarized, ordering of the $S$–spins. It depends on the nature of the underlying overscreened Kondo model, what the physical meaning of this order is. In Cox’s \cite{17} model of U–compounds, it is primarily the ordering of electric quadrupole moments. The possibility that actual spin magnetization is a secondary order parameter arising from the mixing–in of higher–lying ionic levels, is an attractive possibility to account for the smallness of the ordered magnetic moment of some heavy fermion magnets \cite{24}. It remains an open question whether quadrupolar Kondo effect can assist superconductivity \cite{30}.

4 DISCUSSION AND SUMMARY

The crucial question of the theory of Kondo lattices is to what extent can the results for a single Kondo impurity be taken as a guide for the behaviour of periodic systems? The answer must certainly depend on the size of the localized spin $S$, and the number of conduction electron channels $N$. We are uncertain about the answer even in the relatively simple cases of the underscreened ($S > N/2$), and exactly screened ($S = N/2$), Kondo lattices. The situation is quite obscure for the overscreened ($S < N/2$) Kondo lattice since it is difficult to infer how the subtle, and puzzling, features revealed by the solution
of the single–ion multi–channel Kondo problem should manifest themselves in
the lattice case. The available arguments \[31, 32\] suggest that switching on
intersite interactions must have a drastic effect.

Inspired by the fact that valuable insight into the behaviour of the \(S = 1/2,\)
\(N = 1\) Kondo lattice has been gained from studying the Kondo necklace
model introduced by Doniach \[25\], we set out to define and investigate similar
pseudospin models corresponding to a variety of Kondo lattices. Following our
earlier study of underscreened Kondo necklaces \[28\], here we introduced the \(N–\)
channel, \(S = 1/2,\) overscreened necklace model (3). In the spirit of necklace
models, the \(N\) screening channels of the underlying Kondo lattice problem
are represented by \(N\) sets of pseudospins \(\tau_j\). The low–lying electron–hole
excitations of the Fermi sea, and hence the possibility of a “true” Kondo effect,
are thereby lost. Of the conduction electrons, only their spin degrees of freedom
are retained: the pseudospin model still incorporates the competing tendencies
of a Kondo–like spin compensation, and magnetic ordering. Intersite coupling
is mediated by the propagating character of the pseudospins, described by an
\(x – y\) coupling term in (3).

We studied the phase diagram of the model in the same kind of mean–field
approximation (MFA) as that used by Doniach \[25\]. Setting up the self–
consistency equation requires the diagonalization of the single–site effective
hamiltonian (4) in a \(2^{N+1}\)-dimensional Hilbert space: this is made possible
by exploiting the invariance under permutations of the channel indices. We
found that the low–temperature phase is always ordered; for \(W > 0,\) and
bipartite lattices, this is just the Néel order of the \(\tau\)–spins, accompanied by
the oppositely polarized ordering pattern of the \(S\)–spins. All the channels
are equally polarized (5), corresponding to the well–known tendency that the
Kondo–term mediates an effective ferromagnetic coupling between the different
channels.

The nearly parallel alignment of the pseudospins results in a remarkable effect: for \( N \geq 3 \), the ordering tendency is actually enhanced with increasing Kondo coupling \( J \). This can be understood as arising from the fact that overscreening builds up composite pseudospin objects which are larger than the “naked” original spin \( S \). Their coupling, mediated by the pseudospin \( x-y \) term, turns out to be sufficiently effective to increase the Néel temperature \( T_N \).

In the terms of the model (3), the ordering is of the easy–plane type. This is most clearly born out by the exact form (32) of the effective hamiltonian which becomes valid in the limit of infinite Kondo coupling. Introducing the \( x-y \) form of the intersite \( \tau \)-coupling has destroyed the spin–rotational invariance of the underlying electronic hamiltonian, which is still shown by the isotropic Kondo–coupling. In this sense, the necklace models are in a universality class different from that of the Kondo lattices \[27\], and this has to be kept in mind when trying to transfer results from one class of models to the other.

The low–temperature state of the model can be visualized as the ordering of composite \( |\eta| = (N - 1)/2 \) spins. This apparently corresponds to the strong–coupling behaviour of the overcompensated Kondo–site, and not to its intermediate–coupling fixed point with the strange, quantum–mechanical non–integer zero point degeneracy \[10, 11\]. The conjecture \[12\] that the over–screened lattice might show a corresponding exotic phase is certainly exciting but this is not born out by our study of a drastically simplified model. On the other hand, we can relate our findings to independent arguments \[31, 32\] suggesting that intersite interactions are likely to drive the system towards the strong–coupling regime.

Noting that the multi–channel Kondo problem can be used to model a
variety of systems [15, 17, 19, 20], the physical nature of the predicted order can also be different from case to case. Thinking of potential applications we have, however, primarily the suggested quadrupolar ordering of U–based systems in mind [17, 24].

To summarize, we introduced the \( N \)–channel Kondo necklace model for a preliminary study of the nature of the collective spin state in overscreened Kondo lattices. Our findings indicate that intersite interactions drastically change the state of the Kondo centres, lifting the ground state degeneracy, and inducing (pseudo)spin ordering at low temperatures.

ACKNOWLEDGEMENTS

The authors wish to express their gratitude to the International Centre for Theoretical Physics for financial support, hospitality, and an encouraging scientific atmosphere. P.F. is indebted also to SISSA (Trieste) for the hospitality extended to him. Useful discussions with, and helpful advice from, A. Zawadowski and D.L. Cox are gratefully acknowledged.

References

[1] For comprehensive reviews of the physics of \( f \)–electron systems see, e.g., H.R. Ott: Progr. Low Temp. Phys., Vol. XI, Ed. D.F. Brewer (North–Holland, Amsterdam, 1987) pp. 215–289; and the more recent work by N. Grewe and F. Steglich, in: Handbook on the Physics and Chemistry of the Rare Earths Vol. 14, Ed. K.A. Gschneidner, Jr. and L. Eyring, (North–Holland, Amsterdam, 1991) pp. 434-474.
[2] P.A. Lee, T.M. Rice, J.W. Serene, L.J. Sham and J.W. Wilkins: Comments Cond. Matt. Phys. XII, 99 (1986).

[3] S. Doniach: Phys. Rev. B 35, 1814 (1987). — A recent concise review of Kondo lattice magnetism is given by C. Lacroix: J. Magn. Magn. Mater. 100, 90 (1991).

[4] C. Lacroix and M. Cyrot: Phys. Rev. B 20, 1969 (1979).

[5] P. Fazekas and E. Müller-Hartmann: Z. Physik B85, 285 (1991).

[6] S. Doniach and P. Fazekas: Philos. Mag. B 65, 1171 (1992).

[7] H. Shiba and P. Fazekas: Progr. Theor. Phys. Suppl. No. 101, 403 (1990); P. Fazekas and H. Shiba: Int. J. Modern Phys. B 5, 289 (1991).

[8] Ph. Nozières and A. Blandin: J. Physique 41, 193 (1980).

[9] N. Andrei and C. Destri: Phys. Rev. Lett. 52, 364 (1984).

[10] P.B. Wiegmann and A.M. Tsvelick: Z. Phys. B 54, 201 (1985); A.M. Tsvelick: J. Phys. C 18, 159 (1985).

[11] I. Affleck and A.W.W. Ludwig: Phys. Rev. Lett. 67, 161 (1991).

[12] J. Gan, N. Andrei, and P. Coleman: Phys. Rev. Lett. 70, 686 (1993).

[13] P. Coleman and J. Gan: Physica B171, 3 (1991).

[14] J. Gan, P. Coleman and N. Andrei: Phys. Rev. Lett. 68, 3476 (1992). — For more details, cf. J. Gan: PhD Thesis (1992).
[15] A. Zawadowski: Phys. Rev. Lett. 45, 211 (1980); K. Vladár and A. Zawadowski: Phys. Rev. B 28, 1564 (1983); K. Vladár, G.T. Zimányi, and A. Zawadowski: Phys. Rev. Lett. 56, 286 (1986).

[16] A. Muramatsu and F. Guinea: Phys. Rev. Lett. 57, 2337 (1986).

[17] D.L. Cox: Phys. Rev. Lett. 59, 1240 (1987); J. Magn. Magn. Mater. 76&77, 53 (1988).

[18] D.C. Ralph and R.A. Buhrman: Phys. Rev. Lett. 69, 2118 (1992).

[19] C.L. Seaman, M.B. Maple, B.W. Lee, S. Ghamaty, M.S. Torikachvili, J.-S. Kang, L.Z. Ziu, J.W. Allen, and D.L. Cox: Phys. Rev. Lett. 67, 2882 (1991).

[20] S. Katayama, S. Maekawa, and H. Fukuyama: J. Phys. Soc. Japan 56, 697 (1987).

[21] B. Schuh: Z. Phys. B 34, 37 (1979).

[22] T.M. Rice and K. Ueda: Phys. Rev. B 34, 6420 (1986).

[23] H. Tsunetsugu, Y. Hatsugai, K. Ueda, and M. Sigrist: Phys. Rev. B 46, 3175 (1992).

[24] V.L. Libero and D.L. Cox: preprint.

[25] S. Doniach: Physica B 91, 231 (1977).

[26] S.P. Strong and A.J. Millis: Phys. Rev. Lett. 69, 2419 (1992).

[27] P. Santini and J. Sólyom: Phys. Rev. B 46, 7422 (1992).

[28] P. Fazekas and H.–Y. Kee: Modern Phys. Lett. B 6, 1681 (1992).
[29] P.D. Sacramento and P. Schlottmann: Phys. Rev. B 43, 13294 (1991); J. Phys.: Condens. Matter 3, 9687 (1991).

[30] D.L. Cox: A Unifying Principle for Exotic Superconductors: The Two–Channel Kondo Effect (unpublished).

[31] B. Andraka and A.M. Tsvelik: Phys. Rev. Lett. 67, 2886 (1991).

[32] K. Ingersent, B.A. Jones, and J.W. Wilkins: Phys. Rev. Lett. 69, 2594 (1992).

[33] See, e.g., D.B. Lichtenberg: Unitary Symmetry and Elementary Particles (Academic Press, New York, 1978), and I.G. Kaplan: Symmetry of Many–Electron Systems (Academic Press, New York, 1975).
Figure Captions

Fig. 1 The dependence of the Néel temperature $T_N$ on the dimensionless Kondo coupling $J/W$, for $N=2,3,4,5$, and 10, and $z = 2$. Choosing the variable $J/(J+W)$ on the horizontal axis compresses the half-axis $0 \leq J/W < \infty$ into a finite interval.

Fig. 2 Enlargement of part of Fig. 1 to show more clearly the maxima on the $T_N$ vs $J/(J+W)$ curves. The positions of the maxima are indicated by diamonds. The dotted line is a guide to the eye; it indicates that the maximum shifts to increasingly large values of $J/W$ with increasing $N$. 