Resistivity of the Two-Channel Kondo Lattice Model in Infinite Dimensions

D. L. Cox
Department of Physics, Ohio State University, Columbus, OH 43210

(March 23, 2022)

Analytic results for the resistivity of the two-channel Kondo lattice in a particular infinite dimensional limit (Lorentzian density of states) are presented. It is argued that in the absence of symmetry breaking phase transitions or applied fields there is a residual resistivity at zero temperature due to the spin disorder scattering off of the two-channel screening clouds. This may explain the unusual resistivity of UBe$_{13}$. For the same limit the single channel Kondo lattice is an insulator states at particle hole symmetry and half filling, but metallic away from particle-hole symmetry or in applied magnetic field.

PACS Nos. 74.70.Vy, 74.65.+n, 74.70.Tx
The heavy fermion materials such as UBe$_{13}$, UPt$_3$, and CeCu$_2$Si$_2$ continue to resist comprehensive theoretical understanding. In these intermetallic compounds, strongly correlated 4f/5f orbitals on the rare earth or actinide sites with localized magnetic moments give rise to anomalous properties relative to normal metals. In particular, 100-1000 fold enhancement of the linear coefficient in the electronic specific heat is observed, giant resistivities (of order 100 $\mu - \Omega$-cm) which are non-monotonic in temperature are typical. The three materials above (and several others) exhibit superconducting transitions where the heavy electrons pair.

The simplest model which has been used to understand these complex materials is the Kondo lattice Hamiltonian, given by

$$H_1 = \sum_{\vec{k},\sigma} \epsilon_{\vec{k}} c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} - \frac{J}{N_s} \sum_{\vec{R}} \vec{S}(\vec{R}) \cdot \vec{s}_c(\vec{R})$$  \hspace{1cm} (1)

where $c_{\vec{k}\sigma}$ destroys a spin $\sigma$ conduction electron of momentum $\vec{k}$ and energy $\epsilon_{\vec{k}}$, and the conduction spins interact antiferromagnetically ($J < 0$) with the $S = 1/2$ local moments situated at sites $\{\vec{R}\}$. Here $\vec{S}(\vec{R})$ is a local moment spin operator, and $\vec{s}_c(\vec{R})$ a conduction spin operator.

This model has been extensively studied in one dimension \cite{2}, the related symmetric Anderson model has been studied in infinite dimensions \cite{3}. From these works it is clear that at half filling, for sufficiently large $J$, this model should have an insulating ground state which is readily seen from counting arguments. Away from half filling, the model is metallic in the absence of any symmetry breaking effects.

By comparison, essentially nothing is known about the two-channel Kondo lattice model, in which two degenerate species of itinerant electrons interact with a lattice of local spin 1/2 moments. This model is of considerable interest since in the impurity limit (single local moment) it contains a non-trivial ground state which is critical (possessing infinite range spatial correlations) and a non-Fermi liquid excitation spectrum $\cite{4,7}$. The Hamiltonian is obtained by adding a channel index $\alpha = \pm$ to the conduction creation, annihilation, and spin operators in Eq. (1). In applying this model to describe the heavy fermion materials, the channel index will either be a local orbital index for the magnetic Kondo effect, or a local spin index for the quadrupolar Kondo effect. See Ref. \cite{8} for further details.

Impetus to study the two-channel lattice model is provided by: (i) some properties of heavy electron alloys are described well by two channel Kondo models--Y$_{1-x}$U$_x$Pd\cite{4}, Th$_{1-x}$U$_x$Ru$_2$Si$_2$, \cite{10}, and La$_{1-x}$Ce$_x$Cu$_2$Si$_2$\cite{11}. (ii) UBe$_{13}$ has been proposed as a two-channel Kondo lattice material \cite{12}. It also has an extremely unusual resistivity $\rho(T)$: at the superconducting transition temperature $T_c$, $\rho(T_c)$ is extremely large (order 100 $\mu$-Omega-cm, close to the unitarity limit in which every atom scatters resonantly) and is rapidly suppressed in applied magnetic field \cite{13,14} and applied pressure \cite{15}. The latter fact makes it unlikely that the resistivity is due to any ordinary dirt.

In this paper, new results are presented for the form of resistivity of the two-channel Kondo lattice model in a certain infinite dimensional limit (Lorentzian bare density of states [DOS] for itinerant electrons). For the paramagnetic state that the lattice behaves as an incoherent metal, with finite residual resistivity in the absence of applied or spontaneous symmetry breaking fields. Application of a magnetic field or channel spin field induces a cross-over to a Fermi liquid at low temperatures, below which the resistivity should be described by a universal scaling function. Since the Lorentzian DOS is pathological in possessing only one non-vanishing moment, I control these results by demonstrating that reasonable physics emerges in applying the same method to the one-channel Kondo lattice. In that case the model gives (in the absence of applied or spontaneous symmetry breaking fields) an insulating ground state at half filling and a metallic ground state away from half-filling as anticipated from general considerations and from studies of the Anderson lattice model in infinite dimensions \cite{3}.

All results follow from the asymptotic low energy, low temperature forms of the one particle $T$-matrices for scat-
tering off one spin 1/2 impurity by either one or two
canals of conduction electrons. The infinite dimension
limit is then obtained by self-consistently embedding
the impurity in a manner prescribed below. I normalize the
$T$-matrices by multiplying by the number of sites.

For the one-channel Kondo model, at particle-hole
symmetry, the zero temperature retarded one-particle $T$-
matrix, denoted as $t(\omega, T)$ is given by

$$t(\omega, T = 0) \approx -\frac{i}{2\pi N(0)} \left[ 1 - \tilde{a}(1 + \text{sgn}(\omega)) \frac{\omega}{k_B T_K} + \ldots \right]$$

(2)

where $N(0)$ is the Fermi level density of states, $T_K$ is the
Kondo temperature, $\tilde{a}$ is a (universal) pure number whose
value is unimportant for our purposes, and $b = 0.104$.[8]

The Kondo scale is related to the exchange coupling $J$
according to $k_B T_K \approx D(N(0), J)^{1/2} \exp(1/N(0)J)$
where $D$ is the conduction bandwidth. The scattering strength
at the Fermi energy for the above $T$-matrix is at the
unitarity limit with a maximal, resonant phase shift of
$\delta = \pi/2$; the effective single particle picture at $T = 0$
follows from the singlet formation below $T_K$ which lifts the
spin degeneracy. The linear energy dependence in $\text{Ret}$
describes the large effective mass imparted to the con-
spin degeneracy. The linear energy dependence in $\text{Ret}$
is therefore controlled by $T_K$.

The scattering strength at the Fermi energy
the above $T$-matrix is at the
unitarity limit with a maximal, resonant phase shift of
$\delta = \pi/2$; the effective single particle picture at $T = 0$
follows from the singlet formation below $T_K$ which lifts the
spin degeneracy. The linear energy dependence in $\text{Ret}$
describes the large effective mass imparted to the con-
spin degeneracy. The linear energy dependence in $\text{Ret}$
is therefore controlled by $T_K$.

To proceed to the lattice, a relation of the $T$-matrix to
the local self energy $\Sigma(\omega, T)$ is needed. Using the defining
relation for the $T$-matrix and Dyson’s equation gives

\[ \Sigma(\omega, T) = \frac{t(\omega, T)}{1 + G_0(\omega)t(\omega, T)} \]

(4)

where $G_0(\omega)$ is the non-interacting on-site Green’s
function.

The infinite dimensional limit renders the conduction
electron self energy purely local.[8] This simplifies the
problem greatly: one must solve self consistently the “im-
 purity” problem for one site removed from the lattice in
which all other sites feel the impurity self energy cor-
responding to the removed site. The self-consistency is
implicit in the equation relating the local electronic propagator
$G(\omega, T)$ to the momentum space one, which is

\[ G(\omega, T) = \frac{1}{N_s} \sum_k \frac{1}{\omega - \epsilon_k - \Sigma(\omega, T)} \]

(5)

where the electrons have single particle energy $\epsilon_k$
measured with respect to the Fermi energy and live on an
$N_s$-site lattice.

The Lorentzian DOS corresponds to a peculiar lim-
iting large $d$-lattice with infinite range oscillatory hopping
along each of the hypercubic principal directions[19]. The simplifying feature of the Lorentzian DOS is
that self consistency in Eq. (5) is automatic[19]. To
see this, first take the non-interacting density of states
$N_0(\epsilon) = D/\pi(\epsilon^2 + D^2)$ to obtain $G_0(\omega) = 1/(\omega + iD)$.
Converting sum to integral in Eq. (5) gives $G(\omega, T) = 1/(\omega + iD - \Sigma(\omega, T))$ which clearly satisfies Dyson’s equation.

To proceed to the lattice, a relation of the $T$-matrix to
the local self energy $\Sigma(\omega, T)$ is needed. Using the defining
relation for the $T$-matrix and Dyson’s equation gives

\[ \Sigma(\omega, T) = \frac{t(\omega, T)}{1 + G_0(\omega)t(\omega, T)} \]

(4)

where $G_0(\omega)$ is the non-interacting on-site Green’s
function.

The infinite dimensional limit renders the conduction
electron self energy purely local.[8] This simplifies the
problem greatly: one must solve self consistently the “im-
 purity” problem for one site removed from the lattice in
which all other sites feel the impurity self energy cor-
responding to the removed site. The self-consistency is
implicit in the equation relating the local electronic propagator
$G(\omega, T)$ to the momentum space one, which is

\[ G(\omega, T) = \frac{1}{N_s} \sum_k \frac{1}{\omega - \epsilon_k - \Sigma(\omega, T)} \]

(5)

where the electrons have single particle energy $\epsilon_k$
measured with respect to the Fermi energy and live on an
$N_s$-site lattice.

The Lorentzian DOS corresponds to a peculiar lim-
iting large $d$-lattice with infinite range oscillatory hopping
along each of the hypercubic principal directions[19]. The simplifying feature of the Lorentzian DOS is
that self consistency in Eq. (5) is automatic[19]. To
see this, first take the non-interacting density of states
$N_0(\epsilon) = D/\pi(\epsilon^2 + D^2)$ to obtain $G_0(\omega) = 1/(\omega + iD)$.
Converting sum to integral in Eq. (5) gives $G(\omega, T) = 1/(\omega + iD - \Sigma(\omega, T))$ which clearly satisfies Dyson’s equation.

Hence, solving the problem on the lattice for a
Lorentzian DOS means you can just plug in the impu-
irty results for the corresponding DOS provided there is
no significant shift of the electronic chemical potential[19]. For particle-hole symmetry, this last point is safely
ensured.

For the one channel model with the Lorentzian bare
DOS, it follows that the resulting renormalized one par-
ticle DOS in the presence of the interactions vanishes
quadratically in $\omega, T$ for low frequency,temperature in
the case of particle hole symmetry. Explicitly,

\[ N(\omega) = -\frac{1}{\pi} \text{Im} G(\omega + i0^+, T) \approx \frac{b}{\pi D}(\omega^2 + \pi^2 T^2) \]

(6)

As a corollary, the resistivity diverges like $T^{-2}$. The rea-
son for this is two fold. First, the imaginary part of the
self energy may be seen by similar analysis to that of
Eq. (3) to diverge as $-\text{Im} \Sigma(0, T) \approx D/\pi \omega^2 T^2$. Second, there are no conductivity vertex corrections in infinite
dimension due to the locality of the interacting vertex[20]. Hence, $\rho(T) \sim 1 < -\text{Im} \Sigma(\omega, T) >_S$ where the an-
gular brackets denote the usual Fermi surface transport
average[21]. Thus, at particle hole symmetry the single
channel Kondo lattice is an insulator for this Lorentzian
bare DOS with a “soft gap” (power law vanishing of the
density of states).
Modifying the Fermi level phase shift for the single channel case to $\delta \neq \pi/2$ allows us to go away from particle hole symmetry. The real part of the Fermi level self energy is then given by $\Sigma(0,0) = D \tau \alpha(\delta)$, while the imaginary part $\Sigma(\omega, T)$ now vanishes as $\omega^2 + \pi^2 T^2$. Thus, away from particle hole symmetry the Lorentzian bare DOS gives a metallic behavior at the Fermi energy. This also simulates the effect of doping which tunes the available screening charge from unity and thus modifies the phase shift according to the Friedel sum rule. The application of a magnetic field $H$ will modify the $\pi/2$ zero field phase shift in the $\pm$ spin channel to $[\pi/2 - c(\mu_{\text{eff}} H/k_B T)^2 + ...]$ for low fields, and thus will produce a continuous metal-insulator transition for this Lorentzian bare DOS. In this case, the height of the Fermi level renormalized DOS will grow quadratically in the applied field strength. As in previous average $T$ matrix calculations (which are exact in infinite dimensions for a Lorentzian bare DOS [22]), I anticipate that the high temperature behavior of the resistivity will be little different from the impurity limit. These results for a non-particle-hole symmetric scattering and applied magnetic field agree qualitatively with previous calculations for Kondo lattice materials [23,24]. Differences in detail are due to the anomalous tails of the Lorentzian DOS.

In the case of the two-channel model, using Eq. [8] it is straightforward to see that the self energy at zero temperature and low frequency goes as $-i \text{Im} \Sigma(\omega, 0) \approx D[1 - 2\bar{a}[\omega/k_B T_K + ...]$ so that the resistivity at zero temperature will be at the unitarity limit (scattering rate $1/\tau = 2D/h$) and the lattice is an incoherent metal in the absence of any symmetry breaking. Concomitantly, the one electron density of states at the Fermi energy will exhibit a square root cusp at $E_F$.

The physical interpretation of this remarkable result is straightforward: in the two channel case the degeneracy of the impurity spin is never lifted. Hence in the absence of a spin ordering transition which lifts the degeneracy, or a superconducting transition, each cloud contributes a “spin disorder scattering” which leads to a violation of Bloch’s theorem [7,9]. Such a result is reminiscent of magnetic rare earth intermetallics such as Gd [10], but such resistivities are well understood through lowest order golden rule estimates of the scattering from the bare local moments, rather than a complex many body spin cloud.

The application of a spin or channel symmetry breaking field for a single two-channel impurity drives the physics to that of a Fermi liquid [8]. For the case of a field $H_{sp}$ which couples linearly to the impurity spin, it is well established that the Fermi level one-particle phase shift tends to $\pm \pi/4$ for spin $\pm \bar{a}$ [8]. The crossover temperature for this behavior is $T_{sp} = H_{sp}^2/T_K$ (the moment is included in $H_{sp}$). Hence, for $T > T_{sp}$ the system looks like a two-channel lattice with $\rho(T)$ headed towards the unitarity limit at low $T$. For $T < T_{sp}$, $\rho(T)$ must drop towards zero with a $T^2$ Fermi liquid behavior. For an applied channel field $H_{ch}$ coupling linearly to the channel spin, one channel will pop to zero phase shift at $T = 0$, the other to $\pi/2$, making for a “half insulator/half metal”: the zero phase shift channel will short circuit the resonant channel, leading to zero resistance at $T = 0$, but no conduction will be possible in the resonant channel. The crossover temperature in this case is $T_{ch} = H_{ch}^2/k_B T_K$. In either case, the resistivity should be described by a universal scaling function below the crossover scale (based on the results of Ref. [5]), of the form $\rho(H_{ch}, T) \sim F(H_{ch}^2/T)$ where $\alpha = sp, ch$. The schematic resistivity behavior expected for the two-channel model is illustrated in the Figure.

These resistivity results are obtained within an enforced normal, paramagnetic phase. The onset of a magnetic, superconducting, or channel field instability would clearly alter the structure of the schematic resistivity curves.

I now turn to a discussion of the heavy fermion materials and the possible relevance of these considerations there. For UBe$_3$, it has been proposed that a two-channel quadrupolar Kondo lattice model may provide an appropriate description [12]. This metal has, reproducibly, $\rho(T_\alpha) \approx 100 \mu\text{Ω cm}$. The extrapolated value for $\rho(0)$ is nearly as large and (i) vanishes in applied pressure, (ii) goes to zero in applied field with a scaling function form $\rho(H, T) \sim F(H^2/(T - T_0))$ where values of $\beta = 1.0, T_0 = 0$ [13] and $\beta = 1.67, T_0 = 0.75 K$ [14] have been observed. Since there is no evidence of magnetic or quadrupolar order at any temperature above the superconducting transition, I speculate that the unusual residual resistivity of this material may provide an example of the incoherent metal scenario describe above, with the differing values of $\beta, T_0$ from the infinite dimension Lorentzian DOS description deriving from finite dimensionality effects. In this case the magnetic field should initially behave as a channel field, since the effective impurity spin is quadrupolar and the channel index is magnetic, while for sufficiently large fields the magnetic field induced quadratic splitting of the non-magnetic ground state will render it an effective spin field.

For UPt$_3$, a quadrupolar Kondo lattice Hamiltonian may also prove a suitable starting point for theoretical modeling [8], although the low temperature behavior in this system is clearly that of a Fermi liquid and weak in-plane magnetic order is observed in this material [1]. The in-plane order serves as a channel symmetry breaking field. Since the crossover effects in the two-channel model scale with the square of the applied field, I speculate that it is sufficient to have a molecular field induced value to $H_{ch}^2$ which is certain to be non-vanishing for a lattice model. Thus the Fermi liquid scale would be set by the crossover temperature proportional to the
molecular field induced value of $H_{sp,ch}^2/T_K$. To study this idea further dilution on the uranium sublattice is desirable; unfortunately no suitable reference compound exists. URu$_2$Si$_2$ offers a more promising possibility, particularly in view of evidence for the two channel Kondo effect in Th$_{1-x}$U$_x$Ru$_2$Si$_2$[10].

In summary, a study has been made of the low temperature resistivity of the one and two-channel Kondo lattice models in infinite dimension assuming an underlying Lorentzian DOS for the conduction electrons in an enforced paramagnetic state. At particle hole symmetry, the two channel lattice is an incoherent metal, with finite residual resistivity due to spin-disorder scattering off of the degenerate two-channel screening clouds. This may be altered to ordinary metallic behavior by application of spin or channel symmetry breaking fields. This novel result may explain the unusual resistivity of UBe$_{13}$. Though the Lorentzian DOS gives reasonable results for the one channel model (e.g., an insulator at half filling), it will be important to study a non-Lorentzian DOS in the future to ensure that the results obtained are not pathological.

It is a pleasure to acknowledge useful conversations with M. Aronson, M. Jarrell, A. Ludwig, H. Pang, Th. Pruschke, A. Ruckenstein, and J.W. Wilkins. This research was supported by a grant from the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Research.

[1] N. Grewe and F. Steglich, in Handbook on the Physics and Chemistry of Rare-Earths, vol 14, edited by Gschneidner and Eyring (North-Holland, Amsterdam, 1991).
[2] K. Ueda, H. Tsunetsugu, and M. Sigrist, Phys. Rev. Lett. 68, 1030 (1992); C.C. Yu and S.R. White, Phys. Rev. Lett. 71, 3866 (1993).
[3] M. Jarrell, H. Akhlaghpour, and Th. Pruschke, Phys. Rev. Lett. 70 (1993) 1670; M. Jarrell, private communication, 1994.
[4] P. Nozières and A. Blandin, J. Phys. (Paris) 41, 193 (1980).
[5] A.W.W. Ludwig and I. Affleck, Phys. Rev. Lett. 57, 3160 (1991); Nuc. Phys. B, (1994).
[6] I. Affleck, et al., Phys. Rev. B46, 7918 (1992).
[7] V. Emery and S. Kivelson, Phys. Rev. B46, 10812 (1992).
[8] D.L. Cox, Physica B 186-188, 312 (1993).
[9] C.L. Seaman, et al., Phys. Rev. Lett. 67, 2882 (1991).
[10] H. Amitsuka et al., Physica B 186-188, 337 (1993).
[11] B. Andraka, Phys. Rev. B49, 3589 (1994).
[12] D.L. Cox, Phys. Rev. Lett. 59, 1240 (1987).
[13] B. Batlogg et al., J. Magn. Mag. Mat. 63& 64, 441 (1987).
[14] B. Andraka and G.R. Stewart, Phys. Rev. B (Rap. Comm.), to be published (May 1994).
[15] M.C. Aronson et al., Phys. Rev. Lett. 63 2311 (1989).
[16] This is inferred from Eq. (5.84) in The Kondo Problem to Heavy Fermions by A. Hewson, (Cambridge Press, Cambridge, 1993), p. 121.
[17] D.L. Cox and A.E. Ruckenstein, Phys. Rev. Lett. 71, 1613 (1993).
[18] See, for example, D. Vollhardt, to appear in Correlated Electron Systems, ed. V.J. Emery (World Scientific, Singapore, 1993).
[19] Q. Si and G. Kotliar, Phys. Rev. Lett. 70, 3143 (1993).
[20] E. Müller-Hartmann, Z. Phys. B74, 507 (1989).
[21] See, for example, Eq. (7.1.3) in Many Particle Physics by G.D. Mahan (Plenum, New York, 1990), p. 604.
[22] D.L. Cox and N. Grewe, Zeitschrift für Physik B-Condensed Matter 71, 321 (1988).
[23] C. Sanchez-Castro, K.S. Bedell, and B.R. Cooper, Phys. Rev. B 47, 6879 (1993).
[24] J. Gan, N. Andrei and P. Coleman, Phys. Rev. Lett. 70, 686 (1993).
[25] K.N.R. Taylor and M.I. Darby, Physics of Rare Earth Solids (Chapman and Hall, London, 1972) p. 206.

Figure. Schematic form of the resistivity of the two-channel Kondo lattice in infinite dimensions for a bare Lorentzian conduction density of states. The solid line is for no symmetry breaking, the dashed line in the case of applied spin or channel field $H_{sp,ch}$, with $T_{sp,ch} = H_{sp,ch}^2/T_K$. 