

Magnetoresistance in the Two-Channel Anderson Lattice

F. B. Anders,¹ Mark Jarrell,² and D. L. Cox¹

¹*Department of Physics, The Ohio State University, Columbus, Ohio 43210*

²*Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221*

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The paramagnetic phase of the two-channel Anderson lattice model in the Kondo limit is investigated in infinite spatial dimensions using the noncrossing approximation. The resistivity exhibits a Kondo upturn with decreasing T , followed by a slow decrease to a finite value at $T = 0$. The decrease reflects lattice coherence effects in concert with particle-hole symmetry breaking. The magnetoresistance obeys an approximate scaling relation, decreasing towards coherent Fermi liquid behavior with increasing field. The magnetic field induces a Drude peak in the optical conductivity. [S0031-9007(97)02707-5]

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Heavy fermion (HF) materials [1] have been under investigation for two decades. Characteristic of these materials is a 100–1000 fold enhanced electronic specific heat coefficient $\gamma(T) = C(T)/T$ and very large and strongly temperature dependent resistivity $\rho(T)$ (of the order of 100 $\mu\Omega$ cm). In most of these intermetallic compounds magnetic and/or superconducting ground states are found. The physics of these interesting anomalous metals is related to strongly correlated electrons in $4f/5f$ orbitals. Some of these systems are well described as Landau Fermi liquids of massive quasiparticles.

Recently, a number of non-Fermi liquid (NFL) HF alloys have been found which display, e.g., logarithmically divergent $\gamma(T)$ [2]. The superconducting HF compound UBe_{13} also has NFL behavior in γ , possesses a very large residual resistivity ($\approx 100 \mu\Omega$ cm) at the superconducting transition even in high quality samples (as determined by a large T_c and sharp resistive transition). Such NFL behavior is consistent with a two-channel Kondo model description of the physics, such as has been proposed for UBe_{13} on symmetry grounds [3]. In this picture, *electrical quadrupole moments* of the twofold nonmagnetic Γ_3 ground state of the U ion are screened by orbital motion of the conduction electrons. Because the magnetic moment of the electrons is a spectator to this process, there are two screening channels. Reversal of spin and orbital indices allows for a two-channel magnetic Kondo effect for a Ce^{3+} ion in a cubic environment [4]. The two-channel Kondo impurity model for these cases [3,5] has been investigated essentially exactly with different techniques [6]. However, little is known about the corresponding lattice model [7,8].

In this paper we present a solution of one-particle properties of the two-channel Anderson lattice (TCA) model in infinite spatial dimensions. To obtain the solution of the effective two-channel single impurity problem, the noncrossing approximation (NCA) [9] is used. Although this method fails to solve the infinite dimension single channel Anderson lattice at temperatures less than the lattice Kondo temperature T^* [10], it works

well in the low temperature region of the two-channel impurity model [3,4,11]. The calculated resistivity $\rho(T)$ agrees well with recent quantum Monte Carlo (QMC) results [8]. For lower temperatures than accessible by QMC, however, we find a decrease in $\rho(T)$ for decreasing T . A strong negative magnetoresistivity at temperatures below the resistivity maximum in an applied magnetic field indicates a recovery of Fermi-liquid behavior. At the same time, an onset of a Drude peak in the optical conductivity is found which is absent in the zero field solution. We briefly discuss the possible relevance of these results to experiment at the end.

Theory.—The two-channel Anderson lattice Hamiltonian under investigation reads

$$\hat{H} = \sum_{\alpha(i,j)} \frac{t^*}{\sqrt{d}} c_{i\alpha\sigma}^\dagger c_{j\alpha\sigma} + \sum_{i\sigma} E_\sigma X_{\sigma,\sigma}^{(i)} + \sum_{i\sigma\alpha} V \{c_{i\alpha\sigma}^\dagger X_{\alpha,\sigma}^{(i)} + \text{H.c.}\}. \quad (1)$$

X are the usual Hubbard operators, d being the spatial dimension, i the lattice site, t^* the reduced hopping matrix element of the conduction electron between nearest neighbors which carry a spin σ , and a channel index $\alpha = (1, 2)$. The conduction electrons couple via hybridization matrix element V to the ionic many-body states on each lattice site. The symmetry breaking magnetic field enters by a Zeeman term in $E_\sigma = \varepsilon_f + g|\mu_b|\sigma H$. The Zeeman splitting of the conduction electrons only results in a shift of the band centers and turns out to be a small correction. When $|E_\alpha - E_\sigma|$ is much larger than the hybridization width $\Gamma_0 = \pi\rho V^2$, the model can be mapped onto a two-channel Kondo model [3] via the Schrieffer-Wolff transformation.

The local approximation for the Anderson lattice [10] is exact in the limit $d \rightarrow \infty$ [12] and can capture the important physical effects of real ($d = 3$) materials. The method proceeds with an appropriate rescaling of the effective hopping. We choose one f site as an *effective impurity* site which is self-consistently embedded in an effective medium that includes the contributions from

the rest of the lattice. In a single impurity problem only the bare medium one-particle self-energy enters, given by $\Delta_{\alpha\sigma}^0(z) = N_s^{-1} \sum_{\underline{k}} d_{\alpha\sigma}(\underline{k}, z) = N_s^{-1} \sum_{\underline{k}} V^2(z - \varepsilon_{\underline{k}\alpha\sigma})^{-1}$. In the $d = \infty$ lattice the local f -Green's function (GF) has to be equal to the \underline{k} -summed lattice GF

$$\frac{1}{N_s} \sum_{\underline{k}} \frac{1}{1 - \tilde{F}_{\alpha\sigma}(z)[d_{\alpha\sigma}(\underline{k}, z) - \tilde{\Delta}_{\alpha\sigma}(z)]} = 1, \quad (2)$$

where $\tilde{\Delta}_{\alpha\sigma}(z)$ is the self-consistent one body self-energy of the local "impurity" propagator $\tilde{F}_{\alpha\sigma}(z) = \langle\langle \hat{X}_{\alpha,\sigma}^{(i)} | \hat{X}_{\sigma,\alpha}^{(i)} \rangle\rangle(z)$. The effective hybridization width $\tilde{\Gamma}_{\alpha\sigma}(\omega) = \frac{\text{Im}}{\pi} \tilde{\Delta}_{\alpha\sigma}(\omega - i\delta)$ then enters the local two-channel effective impurity problem. The self-energy of the conduction electrons is given by

$$\Sigma_{\alpha\sigma}(z) = \frac{V^2 \tilde{F}_{\alpha\sigma}(z)}{1 + \tilde{F}_{\alpha\sigma}(z) \tilde{\Delta}_{\alpha\sigma}(z)}. \quad (3)$$

In the single channel case, the fact that the T matrix $\tilde{T}(z) = V^2 \tilde{F}(z)$ is at the unitarity limit (for $z, T \rightarrow 0$) leads to Fermi-liquid behavior of the conduction band self-energy, viz. $-\text{Im} \Sigma_{\alpha\sigma}(\omega + i0^+) \propto aT^2 + b\omega^2$. Since the value of the T matrix at the chemical potential and $T \rightarrow 0$ is smaller than the unitarity limit in the two-channel case Eq. (3) tells us immediately that the corresponding conduction band self-energy for the exact solution in the paramagnetic phase of the lattice has to be finite. This has been recently called an *incoherent metal* [7,8]. The physical origin is the following: the local spin is overcompensated by two conduction electron spins. On each lattice site a residual free thermodynamically fluctuating degree of freedom (DOF) acts as a scatterer for conduction electrons. A residual entropy of $1/2 \log(2)$ per site is associated with this DOF which has been interpreted as a free Majorana fermion [13]. The finite self-energy yields a finite value for $\rho(T \rightarrow 0, H = 0)$. Since in a translationally invariant system a vanishing dc resistivity is expected for $T \rightarrow 0$, this indicates that the paramagnetic state is *not* the ground state of the two-channel Anderson lattice.

In the absence of a magnetic field the NCA equations of the effective impurity are equivalent to a resonant level system with an effective Anderson width $\tilde{\Gamma}_0 = 2\Gamma_0$. The so-called NCA "pathology" in the local GF becomes the physical Abrikosov-Suhl resonance (ASR) in the two-channel case [3–5]. In limit of infinite spin N and channel M degeneracy with a fixed ratio N/M the NCA becomes exact [11], and gives exact leading susceptibility and next leading resistivity exponents for all N, M , including $N = M = 2$ for which amplitudes are also in good agreement [4,11]. The effective local GF is given by the convolution

$$\tilde{F}_{\alpha\sigma}(i\omega_n) = \frac{1}{\tilde{Z}_f} \oint_C \frac{dz}{2\pi i} e^{-\beta z} \tilde{P}_{\alpha}(z) \tilde{P}_{\sigma}(z + i\omega_n), \quad (4)$$

where \tilde{Z}_f is the effective local partition function. Even though higher order vertex corrections [14] will modify the spectral distribution, the leading physical effect and

the correct thermodynamics are captured correctly within the NCA. Since the saturation value of the effective site T matrix is half the unitary limit, no pseudogap develops in the quasiparticle spectrum as in the one-channel lattice [15].

In infinite spatial dimensions the vertex corrections in the two-particle propagators vanish [12] and the conductivity itself is a $1/d$ correction which can be calculated by evaluating the lowest order bubble diagram [16], given by

$$\begin{aligned} \sigma^{(\alpha)}(\omega) &= A \int_{-\infty}^{\infty} d\omega' \frac{[f(\omega') - f(\omega + \omega')]}{\omega} \\ &\times \int_{-\infty}^{\infty} d\varepsilon \rho_0(\varepsilon) \sum_{\sigma} \text{Im} G_{\alpha\sigma}^{(c)}(\omega' - i\delta, \varepsilon) \\ &\times \text{Im} G_{\alpha\sigma}^{(c)}(\omega' + \omega - i\delta, \varepsilon), \end{aligned} \quad (5)$$

where $A = \pi e^2 a^2 t^{*2} N (hdVol)^{-1} = t^* \omega_p^2 / 4\pi$, $\rho_0(\varepsilon)$ is the bare Gaussian density of states, $G_{\alpha\sigma}^{(c)}(z)$ the conduction electron GF, and a the lattice constant of the d -dimensional hypercube. The f electrons do not contribute to the conductivity since the hybridization is assumed \underline{k} independent. The dc conductivity is obtained by the limit $\sigma_{\text{dc}}(T) = \lim_{\omega \rightarrow 0} \sigma(\omega, T)$.

Results.—We numerically obtained a self-consistent solution of the lattice problem. The error in the norm of $\tilde{P}(z)$ reaches 0.01%, the sum rule for the self-energy is obeyed within 0.02%, and the maximum iterative difference of effective hybridization widths is bounded by $\max\{|\tilde{\Gamma}_n(\varepsilon) - \tilde{\Gamma}_{n-1}(\varepsilon)|\} < 10^{-8}$. All energies, if not otherwise stated, are measured in the original Anderson width Γ_0 . We chose $\varepsilon_f = E_{\sigma} - E_{\alpha} = -3\Gamma_0$ in the absence of H and $t^* = 10\Gamma_0$ with a band center at $\omega = 0$. $T_K = 0.016\Gamma_0$. In Fig. 1 $\rho(T, H)$ normalized to the estimated $T \rightarrow 0$ value of the QMC data [8] is shown for different values of the applied magnetic field measured in units of $H_K = k_B T_K / g\mu_B$. We have fixed the lattice scale $T_0 = 1.3T_K$ by matching to the QMC resistiv-

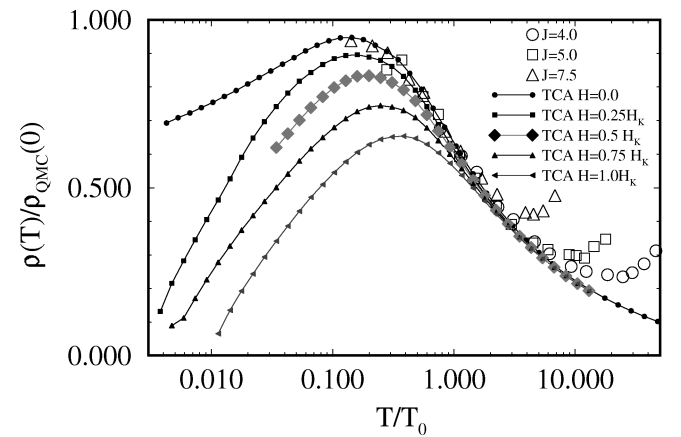


FIG. 1. Resistivity for the TCA vs temperature for different magnetic fields. We have normalized to the estimated $\rho(T = 0)$ values of the QMC data, temperature for the same parameters. The open symbols are the QMC results for different J in the two-channel Kondo lattice model.

ity data. The agreement with the higher temperature data for the Kondo lattice—the open symbols—is excellent. Nevertheless, the resistivity has a maximum and slowly decreases with decreasing temperature, as expected from a lattice calculation. While for $H = 0$ a positive intercept occurs at $T = 0$ consistent with an infinitely degenerate ground state, a crossover to Fermi-liquid behavior is expected in an applied field. A simple explanation of this is that the field lifts the degeneracy of the ground doublet, making the problem formally equivalent to the spin 1/2 Anderson lattice model in the extreme mixed valent regime (empty orbital lower than occupied orbital). This will have a Fermi-liquid normal state. Note that the $\rho(T, H)$ linearly extrapolates to a negative value. This results from being in the crossover regime above an expected T^2 behavior. Although the NCA cannot access to the Fermi-liquid regime for $H > 0$ and $T \rightarrow 0$ [10], we can access the crossover regime. Evaluation of the constants for A in Eq. (5), assuming a lattice constant of 5 \AA and two electrons per unit cell in a three dimensional lattice, gives a resistivity prefactor of $\approx 12.6 \mu\Omega \text{ cm}/\Gamma_0^2$ which leads to a resistivity maximum of $\approx 250 \mu\Omega \text{ cm}$ using our absolute maximum of $20\Gamma_0^2$. This is very close to the experimentally found value of $\approx 190 \mu\Omega \text{ cm}$ for UBe_{13} [17].

Motivated by the experimental data for $\rho(T, H)$ for UBe_{13} [18], we have attempted to scale our $\rho(T, H)$ data with the ansatz $\Delta\rho/\rho = [\rho(T, H) - \rho(T, 0)]/\rho(T, 0) \propto f[H/(T + T^*)^\beta]$. While for the impurity model, we expect $T^* = 0$, $\beta = 1/2$, we find approximate scaling for $T^* = 0.006T_K$, $\beta = 0.39$, as plotted in Fig. 2. The inset of the figure shows the imaginary part of the conduction electron self-energy $\Sigma_c(\omega)$ (3) for $H = 0$ shown for two different temperatures. It shows a shift of the maxima away from the chemical potential in this metallic regime. Very close to $\omega = 0$ a very small onset of coherence is observed for $T \rightarrow 0$, but the relaxation rate remains of the order of $2\Gamma_0$.

We have calculated the complex frequency dependent optical conductivity $\sigma(\omega, T) = \sigma_1(\omega, T) + i\sigma_2(\omega, T)$, with $\sigma_1(\omega, T)$ displayed in Fig. 3. When $H = 0$ and $T \lesssim T_K$, the qualitative features are similar to those reported earlier [8], with a low frequency pseudogap and a large charge fluctuation peak (here at $\approx 0.9\Gamma_0$). With decreasing temperatures the optical conductivity develops a pseudogap, and as a result spectral weight is transferred to high frequencies to satisfy the f -sum rule [19]. This spectral weight shift to higher frequencies is seen clearly in the figure by comparing the $T = 10T_K$ and $T = T_K$ curves (note that the logarithmic plot overemphasizes the area of the pseudogap). At low temperatures a small increase in $\sigma(\omega)$ can be observed when $\omega \rightarrow 0$. Nevertheless, no clear Drude peak is seen even for $T = 0.01T_K$, one decade lower than the observed maximum in $1/\sigma(0, T)$. However, in a magnetic field of $H = H_K$ a low frequency ‘‘Drude’’ peak develops again, consistent with the return to Fermi-liquid behavior suggested in $\rho(T, H)$. Note that in the single channel Anderson lattice

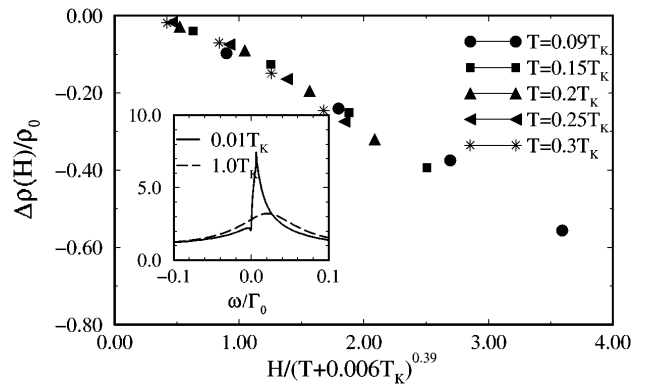


FIG. 2. Magnetoresistance $[\rho(T, H) - \rho(T, 0)]/\rho(T, 0)$ vs scaling variable $x = H/(T + 0.006T_K)^{0.39}$. Inset: Imaginary part of the conduction band self-energy vs frequency in the vicinity of the chemical potential $\mu = 0$ for two different temperatures.

a clear Drude peak develops already a little below the maximum in $1/\sigma(0, T)$.

With the phenomenological ansatz $\sigma_{\text{opt}}(\omega) = \omega_p^2/(4\pi) \{\Gamma_{\text{opt}}(\omega) - i\omega[1 + \lambda(\omega)]\}^{-1}$ the dynamical optical relaxation rate $\Gamma_{\text{opt}}(\omega)$ and the dimensionless mass enhancement factor $\lambda(\omega)$ have been determined. In Fig. 4(a) $\Gamma_{\text{opt}}(\omega)$ is plotted for the same parameters as in Fig. 3. While for temperatures $T > 0.1T_K$ $\Gamma_{\text{opt}}(\omega)$ is nearly frequency independent for low frequencies, at the lowest temperature $\Gamma_{\text{opt}}(0)$ has decreased reflecting the decrease of the dc resistivity. The low frequency behavior has an exponent slightly lower than for $n = 1$. We emphasize the *difference* between $\text{Im}\Sigma_c(\omega)$ and $\Gamma_{\text{opt}}(\omega)$: the first is a true *one-particle* relaxation rate; the second, however, reflects the two-particle nature of the energy absorption process associated with electrical charge transport. Generally, only for a Fermi liquid at very low temperatures and frequencies should

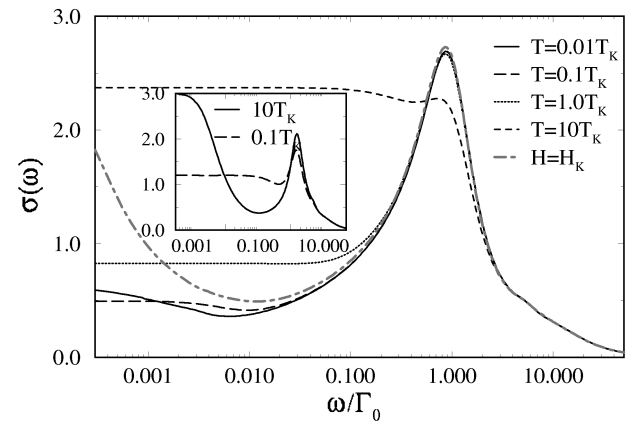


FIG. 3. Optical conductivity per channel in units of $\omega_p^2/4\pi$ vs frequency for covering three decades in temperature. The dash-dotted line is calculated with $T = 0.01T_K$, $H = H_K$. In the inset the corresponding curves for the single channel PAM for the two highest temperatures are shown in the same units.

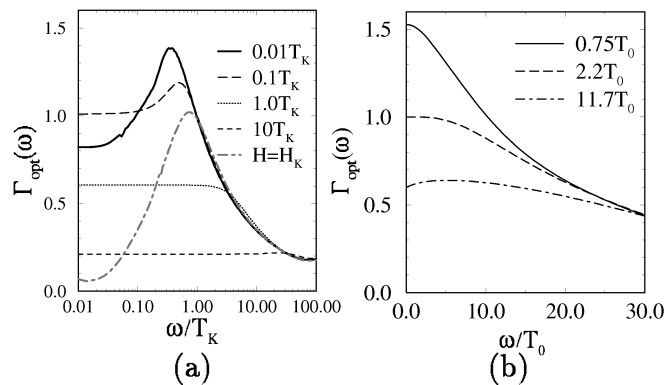


FIG. 4. Relaxation rate $\Gamma_{\text{opt}}(\omega)$ in units of Γ_0 (a) per channel for the two-channel Anderson lattice measured versus ω/T_K and (b) QMC data for the two-channel Kondo lattice (parameter: $J = 4\Gamma_0$, $T_0 = 0.281\Gamma_0$).

$\Gamma_{\text{opt}} = 2\text{Im}\Sigma_c(\omega)$. In an applied magnetic field $H = H_K$ and low temperatures $T = 0.01T_K$ the optical relaxation rate $\Gamma_{\text{opt}}(0)$ shows the expected trend to Fermi-liquid behavior. Figure 4(b) shows the QMC calculation of $\Gamma_{\text{opt}}(\omega)$ for the two-channel Kondo lattice at particle-hole symmetry. A strict quantitative comparison with NCA results is not possible because: (i) T_0 and the Kondo interaction J overlap to within an order of magnitude in the QMC calculations (T_0 is well separated from high energy scales here), and (ii) because the particle-hole symmetry removes the nonmonotonicity experienced in the NCA calculations. Modulo these concerns, the separate calculations agree qualitatively in the overlapping temperature and frequency regions.

Comparison to experiment.—As mentioned earlier, $\rho(T, H = 0)$ is reminiscent in form and magnitude of UBe_{13} [17]. The magnetoresistance also resembles that of UBe_{13} , though our scaling form is different in detail [18]. However, a strict comparison is not possible, since assuming a quadrupolar Kondo model applies to UBe_{13} , we should rather split $|\alpha i\rangle$ states (order H) and quadratically split $|\sigma i\rangle$ states (Van Vleck processes). Other recent data suggest a possible $\text{U}^{3+}\text{-U}^{4+}$ configuration degeneracy which is lifted by Th substitution [20]. We defer the necessary intermediate valence calculation to a future work. In this case, a crossover from NFL to Fermi-liquid physics is still expected. Our $\sigma(T, \omega)$, $\Gamma_{\text{opt}}(\omega)$ calculations are very compatible with data for the alloys $\text{Y}_{0.8}\text{U}_{0.2}\text{Pd}_3$ and $\text{Th}_{1-x}\text{U}_x\text{Pd}_2\text{Al}_3$ [21], as well as the compound UBe_{13} [22]. Because of the incoherent normal metal phase, we expect little qualitative difference between these more dilute alloys and the lattice. For UBe_{13} , the existing optical data only go to $50\text{ cm}^{-1} \approx (5-6)k_B T_K$ in frequency [22,23], and it is clearly desirable to extend these measurements to lower frequencies. We remark that for $\text{Th}_{1-x}\text{U}_x\text{Pd}_2\text{Al}_3$, if a hexagonal quadrupolar Kondo

picture applies, a c -axis magnetic field will split the $|\sigma i\rangle$ levels [5], permitting comparison to our calculations.

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