Magneto-Resistance in the Two-Channel Anderson Lattice

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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 non-crossing 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 magneto-resistance 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.

Introduction. Heavy fermion (HF) materials have been under investigation for two decades. Characteristic for 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 $100 \mu \Omega \text{cm}$). In most of these intermetallic compounds magnetic or/and 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 quasi-particles.

Recently, a number of non-Fermi liquid (NFL) HF alloys have been found which display, e.g., logarithmically divergent $\gamma(T)$ \cite{1}. The superconducting HF compound UBe\textsubscript{13} also has NFL behavior in $\gamma$, and moreover possesses a very large residual resistivity ($\approx 100 \mu \Omega \text{cm}$) at the superconducting transition even in high quality samples (as determined by a large $T_c$ and sharp resistive transition). Such NFL behavior may be possible from a two-channel Kondo model description of the physics, such as has been proposed for UBe\textsubscript{13} \cite{1} on symmetry grounds. In this picture, \textit{electrical quadrupole moments} of the two-fold non-magnetic $\Gamma_3$ 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 \cite{2}. The two channel Kondo impurity model for these cases \cite{3,4} has been investigated essentially exactly with different techniques \cite{5}. However, little is known about the corresponding lattice model \cite{6}.

In this paper we present a solution of one particle properties of the two channel Anderson lattice model in infinite spatial dimensions. To obtain the solution of the effective two channel single impurity problem, the Non-Crossing-Approximation (NCA) \cite{6,7,8} is used. Although this method fails to solve the infinite dimension single channel Anderson lattice at temperatures less than the lattice Kondo-temperature $T^*$ \cite{9}, it works well in the low temperature region of the two-channel model \cite{6,7,8}. The calculated resistivity $\rho(T)$ agrees well with recent Quantum-Monte-Carlo (QMC) results \cite{8}. For lower temperatures than accessible by QMC, however, we find a decrease in $\rho(T)$ for decreasing $T$. A strong negative magneto-resistivity at temperatures below the resistivity maximum in an applied magnetic field indicates a recovery of Fermi-liquid behaviour. 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

$$\hat{H} = \sum_{\alpha<\alpha',\sigma> \sigma',\alpha\neq\alpha'} \frac{t^{*}}{d} d_{\alpha\sigma}^{\dagger} j_{\alpha\sigma} + \sum_{\alpha\sigma} E_{\alpha} X_{\alpha\sigma}^{(i)} + \sum_{i\alpha\sigma} V \left\{ \epsilon_{\alpha\sigma} X_{\alpha\sigma}^{(i)} + \hbar c \right\} . \quad (1)$$

$X$ 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 neighbours which carry a spin $\sigma$ 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 $E_{\alpha} = \xi_f + g \mu_B \sigma H$. The Zeeman splitting of the conduction electrons only result in a shift of the band centers and turn 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 an two channel Kondo model \cite{8} via the Schrieffer-Wolff transformation \cite{9}.

In the local approximation for the Anderson Lattice \cite{10}, which is equivalent to the limit $d \rightarrow \infty$ \cite{11} with an appropriate rescaling of the effective hopping \cite{10}, we choose one $f$-site as an effective ”impurity” site which is self-consistently embedded in an effective medium reflection the rest of lattice. While in a single impurity problem only the bare medium $\Delta_{\alpha\sigma}^0(z) = N_s^{-1} \sum_{\alpha} d_{\alpha\sigma} (\hat{k}, z) = N_s^{-1} \sum_{\alpha} V^2(z - \varepsilon_{\alpha\sigma})^{-1}$ enters, in
the lattice the condition that the local $f$-Green’s function (GF) has to be equal to the $\bar{k}$-summed lattice GF

$$\frac{1}{N_s} \sum_{\bar{k}} \frac{1}{1 - \hat{F}_{\alpha\sigma}(\bar{k}, z) - \Delta_{\alpha\sigma}(z)} = 1. \quad (2)$$

where $\Delta_{\alpha\sigma}(z)$ is the self-consistent one body self energy of the local "impurity" propagator $\hat{F}_{\alpha\sigma}(z) = \langle \langle \bar{X}^{(\alpha)}_{\sigma} | \bar{X}^{(\alpha)}_{\sigma} \rangle \rangle (z)$. The effective hybridization width $\tilde{\Gamma}_{\alpha\sigma}(\omega) = \frac{3m}{T} \Delta_{\alpha\sigma}(\omega - i\delta)$ enters then the local two channel impurity problem. The self-energy of the conduction electrons is given by

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

In the single channel case, the unitarity limit of the $T$-matrix $\bar{T}(z) = V^2 \hat{F}(z)$ leads to the Fermi-liquid behaviour of the conduction band self-energy $\Sigma_{\alpha}(z) \sim aT^2 + bv^2$. Since the value of the $T$-matrix at the chemical potential and $T \to 0$ is smaller than the unitarity limit in the two(multi)-channel case Eqn.(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 [8]. The physical origin is the following: the local spin is over-compensated 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. An residual entropy of $1/2 \log(2)$ per site is associated with this DOF freedom which has been interpreted as a free Majorana fermion [17]. The finite self-energy yields a finite value for $\rho(T \to 0, H = 0)$. Since in translational invariant system a vanishing dc resistivity is expected 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

$$\Sigma_{\alpha}(z) = \frac{1}{\pi} \sum_{\sigma} \int_{-\infty}^{\infty} \tilde{\Gamma}_{\alpha\sigma}(\varepsilon) f(\varepsilon) \hat{P}_{\sigma}(z + \varepsilon) \quad (4)$$

$$\Sigma_{\sigma}(z) = \frac{1}{\pi} \sum_{\alpha} \int_{-\infty}^{\infty} \tilde{\Gamma}_{\alpha\sigma}(\varepsilon) f(-\varepsilon) \hat{P}_{\alpha}(z - \varepsilon) \quad (5)$$

are equivalent to a resonant level system with an effective Anderson width $\tilde{\Gamma}_0 = 2\tilde{\Gamma}_0$. The NCA pathology in the local GF becomes the physical Abrikosov-Suhl-resonance (ASR) in the two channel case [3-4]. The NCA threshold exponents of the effective ionic propagators $\hat{P}$ [15] have the exact value of $1/2$ calculated within a conformal field theory approach [19]. In limit of infinite spin $N$ and channel $M$ degeneracy with a fix ratio $N/M$ the NCA becomes exact [13]. The effective local GF is given by the convolution

$$\hat{F}_{\alpha\sigma}(i\omega_n) = \frac{1}{Z_f} \int d\varepsilon \frac{dz}{2\pi i} e^{-\beta z} \hat{P}_{\varepsilon}(z) \hat{P}_{\sigma}(z + i\omega_n), \quad (6)$$

where $Z_f$ is the effective local partition function. Even though higher order vertex corrections [20] will modify the spectral distribution, the leading physical effect and the correct thermodynamics is captured correctly within the Eqns.(4) and (5). Since the saturation value of the effective site $T$-matrix is half the unitary limit no pseudo-gap develops in the quasi-particle spectrum as in the one-channel lattice [21].

In infinite spatial dimensions the vertex corrections in the two-particle propagators vanish [22] and the conductivity itself is a $1/d$ correction which can be calculated by evaluating the lowest order bubble diagram [23], given by

$$\sigma_{\alpha}(\omega) = A \int d\omega' \frac{[f(\omega') - f(\omega + \omega')]}{\omega} \int d\varepsilon \rho_0(\varepsilon) \sum_{\sigma} 3m G_{\alpha\sigma}(\omega' - i\delta, \varepsilon) 3m G_{\alpha\sigma}(\omega' + \omega - i\delta, \varepsilon) , \quad (7)$$

which can be written as an integral over four complex error function; $A = \pi e^2 a^2 t^2 N/(h\nu dV)$. The Gaussian density of states $\rho_0(\varepsilon) [16]$, $G_{\alpha\sigma}(\varepsilon)$ 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 $k$ independent. The dc-conductivity is obtained by the limit $\sigma_{dc}(T) = \lim_{\omega \to 0} \sigma(\omega, T)$.

**Results.** To obtain a self-consistent solution of the lattice problem, (i) the effective hybridization with $\tilde{\Gamma}(\varepsilon)$ has been treated with the same accuracy as the threshold singularity of the ionic propagators in Eqns.(4) and (5), and (ii) only 10% of the calculated change of $\tilde{\Gamma}(\varepsilon)$ is added in each lattice iteration step, i.e. the lattice is switched on adiabatically. The error in norm of the $\tilde{P}(z)$ reaches 0.01%, the sum rule for the self-energy is obeyed within 0.02% and the maximum norm $max\{|\tilde{\Gamma}_n(\varepsilon) - \tilde{\Gamma}_{n-1}(\varepsilon)|\} < 10^{-6}$. All energies, if not otherwise stated, are measured in the original Anderson-width $\Gamma_0$. We chose $\varepsilon_f = E_\sigma - E_{\bar{\sigma}} = -3\Gamma_0$ in the absence of $H$ and $t^* = 10\Gamma_0$ with a band center at $\omega = 0$. $T_K = 0.016\Gamma_0$ [24].

In Fig. 3 $\rho(T, H)$ normalized to the estimated $T \to 0$ value of the QMC data [3] is shown for different values of the the applied magnetic field measured in units of $H_K = k_B T_K/(g\mu_B)$. We have fix the lattice scale $T_0 = 1.3T_K$ [24] by matching the QMC resistivity 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. The calculations are done slightly below half-filling and with fixed chemical potential. At half-filling in the Kondo-regime an the analytical solution
obtained with an artificial Lorentzian density of states predicts a resistivity of $\rho(T) = \rho(0)(1 - a\sqrt{T})$ at low temperature. While for $H = 0$ still a positive intercept at $T = 0$ is expected consistent with an infinitely degenerated ground state, clearly a crossover to Fermi-liquid is found within an applied field. The NCA patholog
ing of the optical conductivity has been calculated. With the $T$ below the maximum in $1/\sigma$, a clear Drude peak develops already a little higher than $T = 0$, and this is very close to the experimentally found value of $\approx 190 \mu \Omega \cdot cm$ for UBe$_{13}$.

Motivated by the experimental data for $\rho(T, H)$ for UBe$_{13}$, we have attempted to scale our $\rho(T, H)$ data with the Ansatz $\Delta \rho/\rho = |\rho(T, H) - \rho(T, 0)|/\rho(T, 0) \propto f(H/(T + T^*)^3)$. While for the impurity model, we expect $T^* = 0$, $\beta = 1/2$, we find approximate scaling for $T^* = 0.006 T_K$, $\beta = 0.39$, as plotted in Fig. 3. The inset of the figure shows the imaginary part of the conduction electron self-energy $\Sigma_c(\omega - i\delta)$ for $H = 0$ is plotted for four different temperatures in Fig. 2. 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 $T \to 0$, but the relaxation rate remains of the order of $2\Gamma_0$.

Now we focus on the optical conductivity, displayed in figure 3. The large peak at $\approx 0.9 \Gamma_0$ results from high energy charge excitations. With decreasing temperatures the optical conductivity develops a pseudo-gap. The $f$-sum rule relates the integrated optical conductivity

$$\int_0^{\infty} \sigma_\alpha(\omega) d\omega = \frac{\pi^2 e^2 q^2 t^2}{h} \frac{1}{V \Omega_l} \sum_\sigma \ll T_x \gg \propto \frac{1}{d}$$

(8)

to the average kinetic energy in the direction of the current flow, which is checked numerically. It indicates a shift of small amount of spectral weight to higher frequencies. This can be seen clearly in the figure by comparing the $T = 10 T_K$ and the $T = T_K$ curve (note that the logarithmic plot overemphasizes the area of the gap). At low temperatures a small increase in $\sigma(\omega)$ can be observed when $\omega \to 0$. Nevertheless, no clear Drude peak is seen even for $T = 0.01 T_K$, 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 behaviour suggested in $\rho(T, H)$. Note that in the single channel Anderson lattice a clear Drude peak develops already a little below the maximum in $1/\sigma(0, T)$.

Using the Kramers-Kronig relation the imaginary part of the optical conductivity has been calculated. With the phenomenological Ansatz

$$\sigma_{opt}(\omega) = \sigma(\omega) + i\sigma''(\omega) = \frac{\omega^2}{4\pi \Gamma_{opt}(\omega) - i\omega(1 + \lambda(\omega))}$$

(9)

the dynamical optical relaxation rate $\Gamma_{opt}(\omega)$ and the dimensionless mass enhancement factor $\lambda(\omega)$ have been determined. In Fig. 3 a) $\Gamma_{opt}(\omega)$ is plotted for the same parameters as in Fig. 3. While for temperatures $T > 0.1 T_K$ $\Gamma_{opt}(\omega)$ is nearly frequency independent for low frequencies, at the lowest temperature $\Gamma_{opt}(0)$ has decreased reflecting the decrease of the dc-resistivity. The low frequency behaviour has an exponent slightly lower then $n = 1$. We emphasize the difference between $3m \Sigma(\omega)$ and $\Gamma_{opt}(\omega)$: 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 $\Gamma_{opt} = -23 m \Sigma(\omega)$. In an applied magnetic field $H = H_K$ and low temperatures $T = 0.01 T_K$ the optical relaxation rate $\Gamma_{opt}(0)$ shows the expected trend to Fermi-liquid behaviour.

Fig. 3(b) shows the quantum Monte Carlo (QMC) calculation of $\Gamma_{opt}(\omega)$ for the two-channel Kondo lattice at particle hole symmetry. A strict quantitative calculation is not possible because: (i) of the overlap of $T_0$ and the Kondo interaction $J$ to within an order of magnitude in the QMC calculations (in the Anderson model calculations of this paper $T_0$ is well separated from high energy scales), and (ii) because the particle-hole symmetry removes the non-monotonicity 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 to UBe$_{13}$. The magneto-resistance also resembles that of UBe$_{13}$, though our scaling form in detail is different. However, a strict comparison is not possible, since assuming a quadrupolar Kondo model applies to UBe$_{13}$, we should rather split $\lvert \alpha i \rvert >$ states (order H) and quadratically split $\lvert \alpha i \rvert >$ states (van Vleck processes). Additionally, recent experiments suggest a possible $U^{3+}$-$U^{4+}$ configuration degeneracy with is lifted with Th substitution. We refer the necessary intermediate valance calculation to a future work. In this case, a crossover from NFL to Fermi-liquid physics is still expected. Our $\sigma(T, \omega), \Gamma_{opt}(\omega)$ calculations are very compatible with data for the alloys Y$_{0.8}$U$_{0.2}$Pd$_3$ and Th$_{1-x}$U$_x$Pd$_{2}$Al$_3$, as well as the compound UBe$_{13}$. Because of the incoherent normal metal phase, we expect little qualitative differences between these more dilute alloys and the lattice. For UBe$_{13}$, the existing optical data only go to 50 cm$^{-1}$, $\approx 2 - 3k_B T_K$ in frequency, and it is clearly desirable to extend these measurements to lower frequencies. We remark that for Th$_{1-x}$U$_x$Pd$_2$Al$_3$, if a hexago-
nal quadrupolar Kondo picture applies, a c-axis magnetic field will split the \(|\sigma_i >|\) levels \(|5\rangle\) permitting comparison to our calculations. In addition, it should be interesting to test whether a magnetic two-channel lattice picture applies to CeCu$_2$Si$_2$ \(|4\rangle\) and thus have detailed optical conductivity measurements carried out in applied field for this system.

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FIG. 1. Resistivity for the two channel Anderson lattice model (TCA) vs. temperature for different magnetic fields. We have normalized to the estimated ρ(T = 0) values of the Quantum-Monte-Carlo (QMC) data, temperature for the same parameters. The open symbols are the QMC results for different J in the two-channel Kondo lattice model. The inset shows the scaling of the position of the dc maxima vs H. Parameters: εf = −3Γ0, t∗ = 10Γ0, T0 = 0.02Γ0.
$\Delta \rho(H)/\rho_0$ 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 four different temperatures. Parameters: $\varepsilon_f = -3\Gamma_0$, $t^* = 10\Gamma_0$. 

FIG. 2. Magneto-resistance $(\rho(T, H) - \rho(T, 0))/\rho(T, 0)$ 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 four different temperatures. Parameters: $\varepsilon_f = -3\Gamma_0$, $t^* = 10\Gamma_0$. 

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FIG. 3. Optical conductivity per channel in units of $\omega^2_p/(4\pi)$ vs. frequency for covering three decades in temperature. In the inset the corresponding curves for the single channel PAM for the two highest temperatures are show in the same units. The dash-dotted line is calculated with $H = H_K$. Parameters: $\varepsilon_f = -3\Gamma_0$, $t^* = 10\Gamma_0$. 
FIG. 4. Relaxation rate $\Gamma_{\text{opt}}(\omega)$ in units of $\Gamma_0$ (a) per channel for the two channel Anderson lattice measured versus $\omega/T_K$ (Parameters: $\varepsilon_f = -3\Gamma_0$, $t^* = 10\Gamma_0$) and (b) QMC data for the two channel Kondo lattice (Parameter: $J = 4\Gamma_0$, $T_0 = 0.281\Gamma_0$).