Self-consistent Treatment of Crystal-Electric-Field-Levels in the Anderson Lattice

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We consider an Anderson lattice model with a spin 1/2 degenerated conduction electron band and localized ionic CEF-levels, classified according to the irreducible representation of the point group of the lattice. We present the self-consistency equations for local approximations ("d → ∞" approximation) for the periodic Anderson model. It leads to a matrix formulation of the effective local density of states and the lattice f-Green’s function. We derive the quasi-particle life-time which enters the Boltzmann transport equations. The impact of a k-dependent hybridization is discussed. We prove that vertex corrections will vanish, as long as all states of an irreducible representation couple to the conduction electron band with a hybridization matrix element of the same parity.

Keywords: Crystal Electric Field Effects, Heavy-Fermions, Anderson Lattice

I. INTRODUCTION

In Heavy Fermion (HF) materials [1], especially in Uranium based compounds, a simple Anderson-lattice model with single N-fold degenerate ionic ground-state, cannot explain the rich variety of transport measurements in the whole accessible temperature range. The additional maxima found experimentally in the specific heat, the resistivity and the thermo-power are related to higher Crystal-Electric-Field (CEF) levels and have been used to propose CEF level schemes for many different HF compounds using high temperature impurity approaches. Many theoretical attempts have been put forward to include CEF effects in a many body description of HF materials [2]. For magnetic impurities the high temperature spin-disorder resistance calculations [2] have been extended to describe anisotropy of transport of CePt2Si2 [3] in third order perturbation theory neglecting lattice coherence effects, for the low temperature phase it can included within some limits in a non-crossing approximation (NCA) calculation [3-5].

Nevertheless a theoretical approach for the lattice problem is missing. Additionally, the low temperature scale \( T^* \) will reflect higher excited multiplets due to the remaining virtual fluctuations in the ground state. Since in Uranium based compounds the bare spectroscopic CEF structure is still unsettled and a CEF singlet cannot be ruled out as ground state a model for competition between CEF and Kondo singlet was put forward only recently [7]. But for the Anderson lattice, approaches for including CEF effects exist only within the slave boson mean field theory [3]. The aim of this paper is to present a formalism to incorporate CEF-levels in a dynamical mean field (local) approximation [3] which is independent of the method used to effect the site problem. Even though we will restrict ourselves to one unoccupied state, and singly occupied CEF-multiplets transforming according to different irreducible representations \( \Gamma_i \) of the point group of the lattice, we can extend our method to address the question how to generate a multi-channel Kondo lattice model from first principles.

II. THEORY

It is assumed that a spin degenerate conduction electron band couples to localized ionic states via hybridization matrix elements. The matrix elements can be derived by expanding the conduction band locally in the irreducible representations of the point group [3]. First we introduce the Hamiltonian and the notation used throughout the paper.

\[
H = \sum_{k\sigma} \epsilon_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\nu\Gamma} E_{\Gamma\alpha} X_{\nu,\Gamma\alpha} c_{\nu,\Gamma\alpha}^\dagger c_{\nu,\Gamma\alpha} + \sum_{\nu,\Gamma\alpha, k\sigma} V_{\Gamma\alpha}(k\sigma) e^{i k \cdot R} c_{k\sigma}^\dagger X_{\nu,\Gamma\alpha} + h.c.
\]

The ionic states are labeled by their corresponding irreducible representation of the point group and an index \( \alpha \) which is a shorthand notation for all other quantum numbers, like occupation number \( n \), spin, or orbit quantum number, and \( X_{\nu,\Gamma\alpha} \equiv |\Gamma'\alpha' > < \Gamma\alpha| \) at the site \( \nu \). It is the most general formulation of the periodic Anderson model which takes into account only local hybridization. In this paper we concentrate on local fluctuations between singly and empty states only (\( U \to \infty \)).

While propagating through the lattice, the conduction electrons are scattered by the CEF states via the local T-matrix \( V_{\Gamma\alpha}(k\sigma)F_{\Gamma\alpha,\Gamma\alpha'}(z) \), where \( F_{\Gamma\alpha,\Gamma\alpha'}(z) \equiv \tau_0 X_{\tau_0,\Gamma\alpha}^\dagger X_{\tau_0,\Gamma\alpha'} \) is the local Green’s function. In the summation of all scattering processes of the conduction electrons, terms of the structure

\[
\sum_{\Gamma\alpha} \sum_{\sigma} \sum_{\Gamma'\alpha'} V_{\Gamma\alpha,\Gamma'\alpha'}(k\sigma) \frac{1}{z - E_{\Gamma\alpha}(k\sigma)F_{\Gamma\alpha,\Gamma'\alpha'}(z)V_{\Gamma'\alpha'}(k\sigma)}
\]

occur which can be identified as a component of a matrix product \( (d(k, z) \cdot F(z))_{\Gamma_1,\Gamma_2} \) where we have defined
the conduction electron matrix
\[
d(k,z) = \sum_{\sigma} d(k,\sigma,z) = \sum_{\sigma} V(k\sigma) \frac{1}{z - \varepsilon_{k\sigma}} V^T(k\sigma)
\]
and
\[
V^T(k\sigma) = \left\{ V_{1,\alpha_1}(k\sigma), V_{1,\alpha_2}(k\sigma), \ldots, V_{1,\alpha_n}(k\sigma) \right\}.
\]
The F-Green's function \( F(z) \) is a \( N \times N \) matrix, where \( N \) is the number of singly occupied states included in \( \varepsilon_{k\sigma} \).

The local ("d → ∞") approximation:
The local approximation \( \frac{1}{d} \), which is equivalent to the limit \( d \to \infty \) with an appropriate rescaling of the effective hopping \( \frac{1}{d} \), choose one f-site as an effective site which is embedded in an effective medium Green's function generated self-consistently by the rest of lattice. While in a single impurity problem the bare medium GF \( \Delta_n(z) = \frac{1}{N_s} \sum_k d(k,z) \) enters, the condition that the local f-Green's function has to be equal to the \( k \)-summed lattice Green's function
\[
\frac{1}{N_s} \sum_k \frac{1}{1 - \tilde{F}(z) [d(k,z) - \Delta(z)]} = 1 .
\]
determined self-consistently the renormalized media \( \Delta(z) \). The effective Anderson width \( \sum_k(z) = \frac{1}{N_s} \Delta(z) \) and the Green's function of the effective site \( \tilde{F}(z) \) are block-diagonal in the irreducible representations of the point group, since they are local quantities.

The lattice Green’s-functions
The f-Green’s-function (GF) matrix \( \tilde{F}(k,z) \) is obtained by summing over all possible intermediate scattering events taking an electron from site \( i \) to \( j \) and Fourier transforming the result in the reciprocal lattice space is
\[
\tilde{F}(k,z) = \frac{1}{\tilde{F}^{-1}(z) \left( d(k,z) - \Delta(z) \right)} .
\]

While the self-consistency condition (SCC) of the so-called lattice-NCA, another well-established local approximation for the Anderson lattice, is derived from a different philosophy \( \frac{1}{N_s} \), the structure of the lattice Green’s function can be obtained from \( \frac{1}{N_s} \) by replacing \( \Delta(z) \) by the bare \( \Delta_n(z) \). Even though \( \tilde{F}(z) \) and \( \Delta_n(z) \) transform according to the irreducible representations of the point group, the term \( d(k,z) \) mixes different representations for an arbitrary \( k \)-point destroying the point-group symmetry in \( k \)-space.

Via the exact equation of motion
\[
G_{k\sigma}(z) = G_{k\sigma}^{(0)}(z) + G_{k\sigma}^{(0)}(z) T_{k\sigma}(z) G_{k\sigma}^{(0)}(z) = \frac{1}{G_{k\sigma}^{(0)}(z) - \Sigma_{k\sigma}(z)}
\]
and
\[
T_{k\sigma}(z) = \sum_{\Gamma,\Gamma',\alpha'} V_{\Gamma \Gamma',\alpha'}(k) F_{\Gamma',\alpha'}(k,z) V_{\Gamma,\alpha'}(k) \]
\[
= V^T(k\sigma) \tilde{F}(k,z) V(k\sigma)
\]
a compact equation for the \( k \)-dependent self-energy
\[
\Sigma_{k\sigma}(z) = \frac{V^T(k\sigma) F(k\sigma) V(k\sigma)}{1 + G_{k\sigma}^{(0)}(z) V^T(k\sigma) F(k\sigma) V(k\sigma)} = \frac{V^T(k\sigma) \tilde{F}^{-1}(z) + \Delta(z) - d(k,-\sigma,z) V(k\sigma)}{1}
\]
is obtained from with the \( k \)-dependent inverse relaxation time \( \tau^{-1}(k\sigma,\omega) = 2 \Im \Sigma_{k\sigma}(\omega - i\delta) \) is calculate entering Boltzmann transport theory. Even though a local approximation has been used in deriving Eqn. \( \frac{1}{N_s} \) the self-energy is anisotropic due the \( k \)-dependence of the hybridization.

Example: Two Kramers Doubles:
The \( 4 \times 4 \) problem separates in two identical \( 2 \times 2 \) matrices for each pseudo-spin. Using the Faddeeva-function \( w(z) \), the diagonal elements \( F_1(z) \) and \( F_2(z) \) of the Green’s function matrix \( \tilde{F}(z) \) and angular averaged hybridized, we obtain two SCC
\[
\frac{1}{1 + \tilde{F}_\alpha(z) \Delta_\alpha(z)} \left[ 1 - i \, w \left( \sqrt{2} \, \rho_0(z - \Sigma_\alpha(z) - \varepsilon_0) \right) \right]
\]
\[
= \frac{\pi V^2 \rho_0 \tilde{F}_\alpha(z)}{1 + \tilde{F}_\alpha(z) \Delta_\alpha(z)} = 1 \quad \alpha = 1, 2
\]
which are only coupled via the self-energy of the conduction electrons
\[
\Sigma_\sigma(z) = \sum_\alpha \frac{V^2 \tilde{F}_\alpha(z)}{1 + \tilde{F}_\alpha(z) \Delta_\alpha(z)} .
\]
found from Eqn. \( \frac{1}{N_s} \). The averaging of anisotropy effects is justified in the SCC, since only the effective density of states enters the local approximation. For the transport calculation, however, the full angular dependence of the hybridization gives rise to the anisotropy of the transport properties even though a local approximation has been used. From Eqn. \( \frac{1}{N_s} \) it is clearly seen that the different position of the Abricosov-Suhl resonances in the two \( \tilde{F}_\alpha(z) \) will produced two maxima in the resistivity, as demonstrated in \( \frac{1}{N_s} \).

Vertex corrections in the Transport Theory:
Normally a vertex function enters the calculation of transport properties:
\[
\Gamma_{k}(z,\nu) = \left[ \frac{\partial \varepsilon_k}{\partial \varepsilon_k} + \sum_{k'} \frac{\partial \varepsilon_{k'}}{\partial \varepsilon_k} G_{k'}(z) \right] G_{k}\nu(z,\nu) W_{k\nu}(z,\nu,\nu)
\]
\( W_{k\nu}(z,\nu,\nu) \) being the irreducible two particle propagator. If we restrict ourself to the same Hund’s rule multiplet, the hybridization matrix element coupling both conduction electron Green’s function \( G_{k\sigma}(z) \) to a local \( f \) site will have the same parity. The total parity of the \( k \)-momentum loop is
given by $\partial_k \varepsilon_k$. Therefore the vertex correction will be exactly zero in a lattice with inversion symmetry and $\Gamma_k(z, z + \nu) = \partial_k \varepsilon_k$. Nevertheless, the total current has contributions from conduction and $f$-electrons when a $k$-dependent hybridization is present \[13\].

### III. CONCLUSION

We have developed a formalism to include local CEF-levels in a local approximation. The lattice coherence effects, which have been neglected in previous approaches have been taken into account. Eqn. (3) and Eqn. (6) show how the point group symmetry, which is present in all local quantities is destroyed for a general $k$-point. Vertex corrections to transport properties vanish identically on symmetry grounds if we restrict ourselves to the lowest lying Hund’s rule multiplet. Anisotropy effects enter via angular dependent hybridization matrix elements in the conduction electron self-energy, Eqn. (3). In the case of two doublets we can interpret the derived conduction electron self-energy as a superposition of contributions of individual symmetry channels which recovers the proposed semi-phenomenological extension of the LNCA [13]. Additional maxima in the resistivity arise naturally from contributions of the different Abricosov-Suhl resonances from additional CEF levels.

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