Unified Description of Fermi and Non-Fermi Liquid Behavior in a Conserving Slave Boson Approximation for Strongly Correlated Impurity Models

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We show that the presence of Fermi or non-Fermi liquid behavior in the SU(N) × SU(M) Anderson impurity models may be read off the infrared threshold exponents governing the spinon and holon dynamics in a slave boson representation of these models. We construct a conserving T-matrix approximation which recovers the exact exponents with good numerical accuracy. Our approximation includes both coherent spin flip scattering and charge fluctuation processes. For the single-channel case the tendency to form bound states drastically modifies the low energy behavior. For the multichannel case in the Kondo limit the bound state contributions are unimportant.   [S0031-9007(97)03563-1]

Impurity models with internal degrees of freedom and strong local correlations coupled to a fermionic bath have been of considerable interest recently [1–5]. The prototype is the Anderson impurity model, involving a localized electron level (called d level in the following) hybridizing with one or several conduction bands [6]. The strong Coulomb repulsion U ($U \to \infty$) between electrons in the localized state effectively restricts the d-level occupancy to $n_d \leq 1$. The ensuing projection of Hilbert space onto the physical subspace without multiple occupancy is a problem of fundamental importance in the theory of strongly correlated Fermi systems in general. As a consequence, the Anderson model displays many of the salient features of strongly correlated systems, including the formation of local magnetic moments and a competition between non-Fermi liquid behavior caused by an incipient orthogonality catastrophe, to which the system scales initially, and a Fermi liquid (FL) fixed point, which is realized at energies below a characteristic scale, the Kondo temperature T_K, if the local moment can be completely screened by the conduction electron spin system. This model can, therefore, serve as a test case for the regime of strong correlations and at the same time for developing new methods which may later be applied to lattice problems as well.

In terms of pseudofermion and slave boson operators f_σ, b_m ($\sigma = 1, \dots, N$, $m = 1, \dots, M$) [7–9] the M-channel Anderson model is defined by the Hamiltonian

$$H = H_0 + E_d \sum_\sigma f_\sigma^\dagger f_\sigma + V \sum_{\vec{k}, \sigma, m} (c_{\vec{k}, \sigma, m}^\dagger b_m^\dagger f_\sigma + \text{H.c.}),$$

(1)

where $H_0 = \sum_{\vec{k}, \sigma, m} (\varepsilon_{\vec{k}} - \mu) c_{\vec{k}\sigma m}^\dagger c_{\vec{k}\sigma m}$. $\varepsilon_{\vec{k}}$ is the conduction band energy, $c_{\vec{k}\sigma m}^\dagger$ creates a conduction electron in band m with spin projection σ and momentum $\vec{k}$, and E_d denotes the energy of the N-fold degenerate local d level at position $\vec{R} = 0$. V is the hybridization matrix element and μ the chemical potential. A physical electron in the local level is created by the electron operator $d_\sigma^\dagger = \sum_m f_\sigma^\dagger b_m$, where the condition of no double occupancy is effected by the local operator constraint $Q = \sum_\sigma f_\sigma^\dagger f_\sigma + \sum_m b_m^\dagger b_m = 1$. The effective coupling constant in the constrained Hilbert space is given by $\Gamma = \pi V^2 N(0)$, with $N(0)$ the conduction electron density of states at the Fermi level. In the Kondo limit ($n_d \to \lambda$) the Anderson model [Eq. (1)] can be mapped onto the SU(N) × SU(M) Coqblin-Schrieffer model. The latter has been studied extensively by the Bethe ansatz method [10], conformal field theory (CFT) [2], and self-consistent slave boson theory [5].

In this Letter we focus on the auxiliary particle Green's functions $G_{f\sigma}(\tau_1 - \tau_2) = -\langle T\{f_\sigma(\tau_1) f_\sigma^\dagger(\tau_2)\}\rangle$, $G_{bm}(\tau_1 - \tau_2) = -\langle T\{b_m(\tau_1) b_m^\dagger(\tau_2)\}\rangle$. The angular brackets denote the statistical average in the grand canonical ensemble, $\langle (\dots) \rangle = \text{tr}\{(\dots)\exp[-\beta(H - \lambda Q)]\}/\text{tr}\{\exp[-\beta(H - \lambda Q)]\}$. The exact projection onto the subspace $Q = 1$ is achieved by differentiating with respect to the fugacity $\exp(-\beta\lambda)$ and taking the limit $\lambda \to \infty$ [7,8,11]. This procedure ensures that the projected propagators obey Wick's theorem, and self-energies $\Sigma_{f,b,c}(i\omega_n)$ may be defined by $G_{f,b,c}(i\omega_n) = \{[G_{f,b,c}^o(i\omega_n)]^{-1} - \Sigma_{f,b,c}(i\omega_n)\}^{-1}$, where $G_{f\sigma}^o(i\omega_n) = (i\omega_n - E_d - \lambda)^{-1}$, $G_{bm}^o(i\omega_n) = (i\omega_n - \lambda)^{-1}$, and $G_{cm\sigma}^o(i\omega_n) = \sum_{\vec{k}}(i\omega_n - \varepsilon_{\vec{k}})^{-1}$. The d electron Green's function may be expressed in terms of Σ_c as discussed in Ref. [11]. The projected spectral functions $A_x(\omega) = \text{Im} G_x(\omega - i0)$ exhibit divergent threshold behavior at $\omega = 0$ with a proper choice of the zero of the auxiliary particle energy [11]: $A_x(\omega) \propto \omega^{-\alpha_x}$, $x = f, b$.

For the single-channel model with spin degeneracy N, which is known to have a FL ground state, the exact exponents $\alpha_{f,b}$ have been determined [12] by Wilson's numerical renormalization group (NRG) approach for the cases $N = 1, 2$, $M = 1$. They may also be deduced for arbitrary N by the following argument [13]: (i) In the spin screened FL state ($\omega, T < T_K$) the impurity is seen by the conduction electrons as a pure potential scattering center. (ii) The infrared (IR) threshold behavior of $G_{f,b}$ is then entirely due to the orthogonality catastrophe of the overlap of the Fermi sea without the impurity level and the fully interacting conduction electron sea affected by the potential

scattering phase shifts δ_σ. The corresponding exponent is given by $\alpha = 1 - \sum_\sigma (\delta_\sigma/\pi)^2$. (iii) The phase shifts follow from the Friedel sum rule $\Delta n_\sigma = \delta_\sigma/\pi$, where Δn_σ is the change in the number of conduction electrons at the impurity caused by the interaction with the impurity. (iv) For the boson spectral function the initial state is the empty impurity, which for each spin species fills up with $\Delta n_\sigma = n_d/N$ conduction electrons in the final state, until the correct impurity level occupation n_d is reached. It follows that

$$\alpha_b = 1 - n_d^2/N. \tag{2}$$

For the spectral function of fermions with spin σ the initial state is defined by a full impurity level with spin σ with the remaining $N - 1$ impurity levels empty. The corresponding change of conduction electron number in the final state with occupation n_d is $\Delta n_\sigma = n_d/N - 1$ and $\Delta n_{\sigma'} = n_d/N$, $\sigma' \neq \sigma$, and hence

$$\alpha_f = (2n_d - n_d^2)/N. \tag{3}$$

We emphasize that the expressions Eqs. (2) and (3) for the exponents have been confirmed using the Bethe ansatz solution and boundary CFT [14]. In the Kondo limit ($n_d = 1$), $\alpha_f = 1/N$, in disagreement with a result derived from a self-consistent parquet analysis [15]. Note that complete spin screening is crucial for this derivation of the exponents in terms of scattering phase shifts to be applicable: For the multichannel model ($M > 1$), which exhibits a non-FL ground state, the exponents in the Kondo limit are known from CFT [2] to be $\alpha_f = M/(N + M)$, $\alpha_b = N/(N + M)$, while the above argument would yield the wrong result $\alpha_f = 1 - M + (2n_d - n_d^2/M)/N$, $\alpha_b = 1 - n_d^2/(NM)$. Therefore, *the IR threshold exponents of the auxiliary particles are indicators, i.e., a necessary and sufficient condition, for FL or non-FL behavior, respectively.* There is evidence [16] that α_f has also observable relevance in that it governs the physical electron spectral function at intermediate frequencies $\omega \gtrsim T_K$.

We now turn to an approximation scheme [17] which is capable of recovering the above (exact) IR dynamics. As a minimal requirement, the constraint $Q = 1$ has to be fulfilled in any approximate theory. The constraint is closely related to the invariance of the system under a simultaneous local (in time) gauge transformation $f_\sigma(\tau) \rightarrow \exp[i\Theta(\tau)]f_\sigma(\tau)$, $b_m(\tau) \rightarrow \exp[i\Theta(\tau)]b_m(\tau)$. The Lagrange multiplier λ assumes the role of a local gauge field and transforms as $\lambda \rightarrow \lambda - i\partial\Theta/\partial\tau$. Any approximation scheme respecting the gauge symmetry will preserve the charge Q in time. We shall call approximations of this type conserving. Symmetry conserving approximations of the self-energies $\Sigma_{b,f,c}$ and the irreducible vertices Γ_{xy} may be generated by functional

differentiation from a functional Φ of closed skeleton diagrams as $\Sigma_x(\tau_1 - \tau_2) = \delta\Phi/\delta G_x(\tau_1 - \tau_2)$, $\Gamma_{xy} = \delta^2\Phi/\delta G_x\delta G_y$, and $x, y = f, b, c$.

We will be interested in the limit of weak hybridization, such that the dimensionless parameter $VN(0) \ll 1$. Thus, let us first discuss the lowest order approximation, which is of second order in V. The conserving approximation scheme requires the self-energies to be determined self-consistently, which amounts to an infinite resummation of perturbation theory even if only the second order skeleton diagram for Φ is kept. The resulting scheme is known as the "noncrossing approximation" (NCA) [18–20]. It should be a qualitatively correct approximation, provided the perturbation series for Φ converges, i.e., *if* there are no additional collective effects causing singularities. The NCA leads to very good results in the absence (i.e., in the multichannel case) or sufficiently far away from a FL fixed point: A comparison of NCA results for the auxiliary particle and d-electron spectral functions A_f, A_b, A_d, and exact results obtained for the single-channel case using the NRG method shows [11] that (i) the NCA auxiliary particle spectral functions are even quantitatively correct at energies ω above the Kondo scale $T_K = D(M\Gamma/\pi D)^{(M/N)}\exp[-\pi|E_d|/(N\Gamma)]$, where D is the high energy cutoff, but (ii) their low energy behavior ($\omega < T_K$) is incorrect. The latter appears to be due to a lack of vertex corrections. Within NCA the exponents of the above-mentioned threshold power laws may be determined analytically as $\alpha_f^{\text{NCA}} = M/(N + M)$, $\alpha_b^{\text{NCA}} = N/(N + M)$ [5,20]. For the case $M = 1$, these values disagree strongly with the exact results discussed above. In the multichannel case ($M > 1$), on the other hand, the NCA exponents agree with the exponents found for the fundamental fields and their correlation functions in CFT [2] in the Kondo limit. This suggests that the NCA describes the low energy properties correctly in the non-FL regime of the SU(N) × SU(M) Anderson model for $n_d = 1$ and that the generic behavior of the model is that of a non-FL.

It may be shown by power counting arguments that there are no corrections to the NCA exponents in any finite order of perturbation theory [5]. However, additional collective effects, e.g., the formation of the Kondo singlet state, lead to FL behavior. Thus, it is natural to search for singularities in the pseudofermion-conduction electron scattering channel. In particular, we consider the class of diagrams which, at any given order of V^2, represents processes with the maximum number of spin flips. The summation of the corresponding ladder diagrams can be performed by solving the integral equation for the c-f T matrix [Fig. 1(a)],

$$T_{s\sigma,s'\sigma'}^{(cf)}(i\omega_n, i\omega_n', i\Omega) = -V^2 G_b(i\omega_n + i\omega_n' - i\Omega)\delta_{s\sigma'}\delta_{s'\sigma} + V^2 T \sum_{\omega_n''} G_b(i\omega_n + i\omega_n'' - i\Omega)G_{f\sigma}(i\omega_n'')$$
$$\times G_{cs}(-i\omega_n'' + i\Omega)T_{\sigma s,s'\sigma'}^{(cf)}(i\omega_n'', i\omega_n', i\Omega). \tag{4}$$

Inserting NCA Green's functions for the intermediate state propagators of Eq. (4), we find numerically at low temperatures a pole of $T^{(cf)}$ in the singlet channel as a function of the center-of-mass (COM) frequency Ω in the Kondo regime
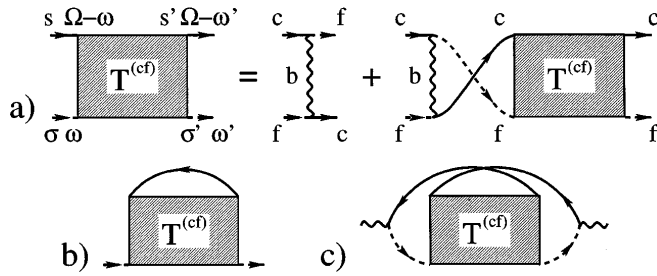
FIG. 1. (a) Diagrammatic representation of the conduction electron-pseudofermion T matrix $T^{(cf)}$. (b) Pseudofermion and (c) slave boson self-energies $\Sigma_{f\sigma}$, Σ_b. The terms corresponding to $T^{(cb)}$ are obtained by interchanging $f \leftrightarrow b^\dagger$.

$(n_d \gtrsim 0.7)$ [17,21]. This signals the tendency to form a singlet bound state at $\Omega = \Omega_{cf} \simeq -T_K$. In the empty orbital regime $(n_d \to 0)$ the behavior of the system is governed by charge fluctuations. The dominating contributions in this low density region may be expected to result from conduction electron-boson scattering. The corresponding scattering amplitude $T^{(cb)}$ is obtained from Eq. (4) by interchanging pseudofermions and antibosons, again leading to a pole, at $\Omega_{cb} < 0$. In the mixed valence regime $(n_d \simeq 0.5)$, the poles in both $T^{(cf)}$ and $T^{(cb)}$ are of equal importance.

In order to guarantee gauge invariance, self-consistency has to be imposed. The self-energies Σ_f, Σ_b calculated from $T^{(cf)}$ and $T^{(cb)}$ then follow from a generating functional Φ [17] and are depicted in Figs. 1(b) and 1(c). They are given as nonlinear and nonlocal (in time) functionals of the Green's functions. The Green's functions in turn are expressed in terms of the self-energies, closing the set of self-consistent equations [conserving T-matrix approximation (CTMA)]. Note that the contribution to Φ containing one boson rung corresponds to NCA. The diagram with two rungs is excluded since it is not a skeleton. The sum of the Φ diagrams with up to four rungs constitutes a large N expansion correct up to $O(1/N^2)$ and is identical to the diagram class used in Ref. [22]. We emphasize that the CTMA, i.e., the *self-consistent* summation of the *infinite* series of all diagrams shown in Fig. 1 is justified on physical as well as formal grounds: At any loop order of Φ it includes (1) the maximum number of spin flip as well as charge fluctuation processes; (2) all leading and subleading IR singular contributions, because all terms not included cancel pairwise in the IR regime [23]. The threshold property of the auxiliary spectral functions implies that the exact T matrices $T^{(cf)}$ and $T^{(cb)}$ have no spectral weight at negative COM frequencies Ω, in contrast to the poles appearing in the "perturbative" evaluation, i.e., inserting NCA propagators as discussed after Eq. (4). Consequently, these poles are shifted to $\Omega = 0$ by self-consistency, where they merge with the continuous spectral weight present for $\Omega > 0$, thus renormalizing the threshold exponents of the auxiliary spectral functions, as seen below. This is an expression of the fact that the

Kondo singlet is not a two-particle bound state but rather a collective many-particle state.

After analytical continuation to the real frequency axis we have solved the CTMA numerically by iteration. In the Kondo regime $(n_d \gtrsim 0.7)$ of the $N = 2$, $M = 1$ model, we have obtained reliable results down to temperatures of the order of $10^{-2}T_K$ (note that $T_K \to 0$ in the Kondo limit). In the mixed valence and empty impurity regimes, significantly lower temperatures may be reached, compared to the low temperature scale of the model. As is shown in Fig. 2(a), the spectral functions obtained are in good agreement with the results of NRG (zero temperature results), given the uncertainties in the NRG at higher frequencies. Typical behavior in the Kondo regime [Fig. 2(a)] is recovered: a broadened peak in A_b at $\omega \simeq |E_d|$, representing the hybridizing d level and a structure in A_f at $\omega \simeq T_K$. Both functions display power law behavior at frequencies below T_K, which at finite T is cut off at the scale $\omega \simeq T$. The exponents extracted from the frequency range $T < \omega < T_K$ of our finite T results compare well with the exact result also shown (see insets of Fig. 2). A similar analysis has been performed for a number of parameter sets spanning the complete range of d-level occupation numbers n_d. The extracted power law exponents are shown in Fig. 3,
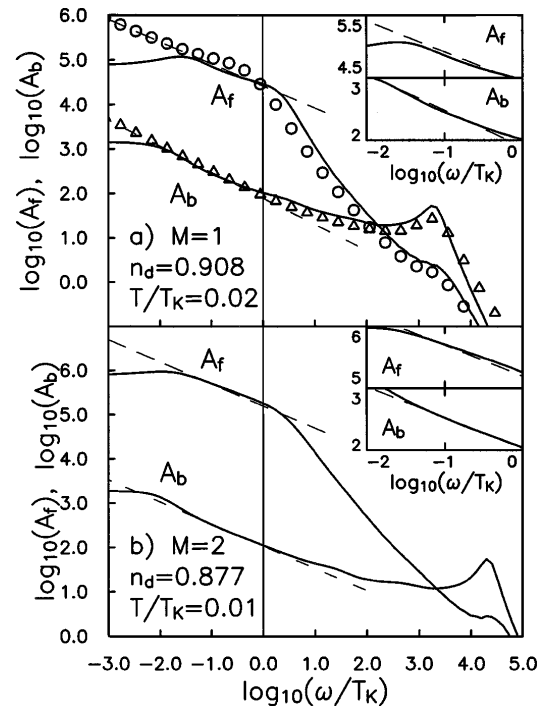

FIG. 2. Pseudofermion and slave boson spectral functions A_f and A_b in the Kondo regime ($N = 2$; $E_d = -0.05$, $\Gamma = 0.01$ in units of the half-bandwidth), for (a) the single-channel ($M = 1$) and (b) the multichannel ($M = 2$) case. In (a) the symbols represent the results of NRG for the same parameter set, $T = 0$. The slopes of the dashed lines indicate the exact threshold exponents as given by Eqs. (2) and (3) for $M = 1$ and by CFT for $M = 2$. Deviations from the power laws at low frequencies ω shift towards $\omega = 0$ as $T \to 0$, i.e., are finite T effects. Insets show magnified power law regions.
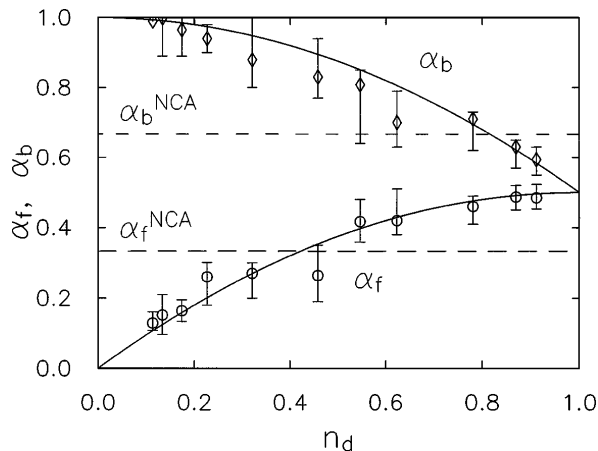
FIG. 3. CTMA results (symbols with error bars) for the threshold exponents α_f and α_b of A_f and A_b, $N = 2$, $M = 1$. Solid lines: exact [Eqs. (2) and (3)], dashed lines: NCA results.

together with error bars estimated from the finite frequency ranges over which the fit was made. The comparatively large error bars in the mixed valence regime arise because here spin flip and charge fluctuation processes are of equal importance, inhibiting the convergence of the numerical procedure. In this light, the agreement with the exact results is very good. This is evidence that *the CTMA recovers the signature of FL behavior present in the exact auxiliary particle dynamics of the single-channel Anderson model.* As a consequence of the conserving scheme, the FL behavior should be reproduced in physical properties as well, when derived from the same generating functional Φ. These evaluations are in progress.

In the multichannel case with $M > 1$, $N = M$, it follows from the symmetry of the model under the transformation $f_\sigma \rightarrow b_\sigma^\dagger$, $b_m \rightarrow f_m^\dagger$, $E_d \rightarrow -E_d$ that $\alpha_{f,b}(n_d) = \alpha_{b,f}(1 - n_d)$. For $n_d = 1$, $\alpha_{f,b}$ are known from CFT (see above). It follows that NCA yields the exact exponents both in the Kondo and in the empty impurity limits of the multichannel model. At present, it is not known whether this is the case for arbitrary n_d. Using NCA Green's functions as discussed above, we find again a pole in the spin singlet channel of the T matrix of pseudo-fermions (f_s, $s = \uparrow, \downarrow$) and conduction electrons of flavor m ($c_{\sigma m}$) for $n_d < 1$. However, the weight of the pole vanishes for $n_d \rightarrow 1$, and a numerical solution of the self-consistent CTMA equations for $M = N = 2$, $n_d = 0.877$ indeed yields exponents $\alpha_f \simeq 0.44$, $\alpha_b \simeq 0.49$, very close to the exact value of $1/2$ for $n_d = 1$ [Fig. 2(b)]. This is consistent with the fact that there should not be a bound state contribution in the overscreened case.

In this Letter we have considered the dynamics of the auxiliary particles for the (N, M) generalized Anderson impurity model with particular emphasis on the realization of FL behavior. We have shown that the occurrence of FL behavior can be deduced from the IR threshold exponents of the auxiliary particle spectral functions. A conserving self-consistent approximation incorporating an infinite number of coherent spin flip and charge transfer

processes (CTMA) leads to singular contributions which renormalize the threshold exponents by self-consistency. There cannot be a renormalization of the exponents in any finite order self-consistent summation. A numerical evaluation of the CTMA yields good agreement with the known exact values in the single-channel case, indicating that CTMA recovers the FL behavior. By contrast, in the multichannel case the singular contributions are ineffective in the limit $n_d \rightarrow 1$ of the two-channel Anderson model, i.e., the non-FL state persists and the exponents known from CFT are recovered.

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