Two-Scale Analysis of the SU(N) Kondo Model

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We show how to resolve coherent low-energy features embedded in a broad high-energy background by use of a fully self-consistent calculation for composite particle operators. The method generalizes the formulation of Roth, which linearizes the dynamics of composite operators at any energy scale. Self-consistent equations are derived and analyzed in the case of the single-impurity SU(N) Kondo model.

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The development of effective methods for describing correlated electron systems has been the subject of intensive activity over the last decade, spurred by the experimental discoveries of the heavy fermion systems, the high-temperature superconductivity, and, generally, a revival of interest in transition metal-oxide physics [1].

The Roth method for the correlation problem [2] in the context of the Hubbard model [3] is based on an ansatz which reduces the dynamics of field operators to a linearized one. The essential idea is to select a basis of fermionic operators ψ_i, write their equations of motion which involve operators J_i, and then close these equations by projecting J_i onto the basis by using the Roth projector $\mathcal{P}$ defined by

$$\mathcal{P}(J_l) = \sum_{rs} \langle\{J_l, \psi_r^\dagger\}\rangle I_{rs}^{-1} \psi_s \,, \qquad (1)$$

where $I_{rs} = \langle\{\psi_r, \psi_s^\dagger\}\rangle$, with $\{\_,\_\}$ denoting the anticommutator. In this approach the determination of the Green's functions is then reduced to the evaluation of certain static thermal averages: $\langle\{\psi_r, \psi_s^\dagger\}\rangle$ and $\langle\{J_l, \psi_r^\dagger\}\rangle$. When these parameters are connected to matrix elements of the Green's functions associated with the basis, one has a self-consistent scheme for their calculation. However, this is often not the case, and further approximations are introduced to establish the connections and get the self-consistency. The application of this method, as well as similar methods [4], has recently been reviewed by Mancini and collaborators [5]. Through careful comparison with existing numerical data, they concluded that good results for many physical quantities are obtained by requiring that the Green's functions fulfill exact equal-time identities accompanying the fermionic character of the operators.

In spite of its intuitive appeal, there are several serious difficulties with Roth's method. Recent advances in the study of correlated electron systems converge upon a picture of the one-particle Green's function made up of incoherent broad spectral features in addition to more dispersive quasiparticle bands which exist at lower energies [6,7]. The Roth approach describes the Green's functions in terms of a finite number of sharp poles which are a poor description of the incoherent structure of the high-energy spectra. Also, the presence of low-energy features embedded in a broad high-energy background precludes the straightforward extension to low-energy scales of this approach. Indeed, low-energy features cannot be resolved increasing the size of the basis. Increasing the size of the basis only amounts to calculating self-consistently a larger number of spectral moments [8] which are dominated by high-energy contributions. A clear example of this dramatic failure is provided by the Kondo impurity model, where it has been proved impossible to derive the existence of a Kondo resonance in the spectra within a projection scheme.

In this Letter, we present a generalization of Roth's projection technique which overcomes the limitations discussed above and, as an illustration of the technique, we investigate the single-impurity SU(N) Kondo model [9]. Our goal is to introduce a general technique in a simple context which is well understood, but so far has not been successfully treated by techniques based on the equations of motion. We will demonstrate that our method reproduces all the well-known spectral features of the impurity model.

The method carries out the following steps. (i) In the first step, we write the equations of motion for the operators of physical interest in terms of higher order ones (or *composite operators*). Similarly, we express the Green's functions of interest in terms of the Green's functions of the composite operators. The composite operators should not have components on the physical fields at high energies. (ii) Then, we evaluate the Green's functions of the composite operators by a technique which is valid at high energies, such as the mode-coupling approximation [10]. Use of the mode-coupling approximation is motivated by the fact that it more clearly reflects that the high-energy part of the spectra is quite incoherent. At this stage, we divide the composite operators into (a) a high-energy part, described by the mode-coupling approximation, and (b) a low-energy part, to be determined by a nonperturbative closure of the equations of motion. The necessity for this step is checked by writing the expressions for the moments and noting that the mode-coupling approximation fails to give the spectral weights, as expected from an independent evaluation of the moments. (iii) The

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low-energy closure of the equations of motion is dictated by the physics of the problem and is inspired by the successes of the slave boson techniques [11]. It is a simple quasiparticle theory which involves unknown parameters such as the low-energy spectral weights. The self-consistent determination of the low-energy parameters completes the full determination of the physical Green's functions.

The SU(N) Kondo model is described by the following Hamiltonian:

$$H = \sum_{\mathbf{k},\mathbf{k}'} c^\dagger(\mathbf{k}) \cdot \left[\delta_{\mathbf{k}\mathbf{k}'}\varepsilon_c(\mathbf{k}) + 2J_\mathrm{K} \frac{1}{NN_s} \vec{\tau}_N \vec{n}^d \right] c(\mathbf{k}'), \tag{2}$$

where $c(\mathbf{k})$ denotes the conduction electron operator, and $\vec{n}^d$ represents the spin operator at the impurity site [$\vec{n}^d \cdot \vec{n}^d = N(N+1)/2$]. $\varepsilon_c(\mathbf{k})$ and J_K are the conduction electron energy and the Kondo coupling, respectively. N_s is the number of atomic sites of the host metal responsible for the orbitals which form the conduction band. τ_N^a are the $N^2 - 1$ traceless generators of SU(N) [$\vec{\tau}_N \cdot \vec{\tau}_N = 2(N^2-1)/N$]. From (2), we have

$$i \frac{\partial}{\partial t} c(\mathbf{k}) = \varepsilon_c(\mathbf{k}) c(\mathbf{k}) + 2J_\mathrm{K} \frac{1}{NN_s} \sum_{\mathbf{q}} \vec{\tau}_N \cdot \vec{n}^d c(\mathbf{q}). \tag{3}$$

Next, we introduce the composite Heisenberg field operator,

$$\psi^\dagger = (\psi_1^\dagger, \psi_2^\dagger) = \left(c_0^\dagger, 2\frac{1}{N} c_0^\dagger \vec{\tau}_N \cdot \vec{n}^d \right), \tag{4}$$

where $c_0 = (1/\sqrt{N_s}) \sum_{\mathbf{q}} c(\mathbf{q})$ is the electron at the impurity site. The field ψ_2 in (4) abides by the criterion required by the method in (i). In fact, when $\langle\{\psi_2, \psi_1^\dagger\}\rangle$ is regarded as the scalar product of the field ψ_2 with the field c_0, there is no component of ψ_2 on c_0 at any energy scale since $\langle\{\psi_2, \psi_1^\dagger\}\rangle = 0$. Then, using Eq. (3) we can express the Green's functions of the first field in terms of the Green's function for the composite operator ψ_2. We have

$$G_{11}(\omega) = \Gamma_0(\omega) + J_\mathrm{K}^2 \Gamma_0(\omega) G_{22}(\omega) \Gamma_0(\omega), \tag{5}$$

$$G_{12}(\omega) = J_\mathrm{K} \Gamma_0(\omega) G_{22}(\omega), \tag{6}$$

where $G_{\alpha\beta}(\omega)$ is the thermal Green's function associated with the basis in (4) and $\Gamma_0(\omega) = \frac{1}{N_s}\sum_{\mathbf{q}} \frac{1}{\omega - \varepsilon_c(\mathbf{q})}$ is the free propagator of the field c_0. The total spectral weight attached to the second composite field ψ_2 is

$$I_{22} = 4\frac{N+1}{N^2} + 4K_D, \tag{7}$$

where the Kondo amplitude $K_D = \langle \psi_1 \psi_2^\dagger \rangle = -2\frac{1}{N^2}\langle \psi_1^\dagger \cdot \vec{\tau}_N \psi_1 \vec{n}^d \rangle$ describes the binding between the localized spin and the spin excitations of the field c_0. In order to resolve low-energy features embedded in a high-energy background, we write

$$G_{22}(\omega) = G_{22}^H(\omega) + G_{22}^L(\omega), \tag{8}$$

where $G_{22}^H(\omega)$ keeps the information about the band structure and is not sensitive to features which are small with respect to the bandwidth $2D$. In contrast, $G_{22}^L(\omega)$ mostly takes coherent contribution from low energies and depends only weakly on the high-energy part of the spectrum. Such a decomposition corresponds to decomposition of the composite field ψ_2 as $\psi_2 = \psi_2^H + \psi_2^L$, with ψ_2^H giving rise to incoherent broad features, whereas ψ_2^L emerges as an observable quasiparticle at low energies.

In the high-energy regime, time-dependent correlation functions can be treated within the mode-coupling approximation in terms of electron-hole and charge-spin fluctuations. By the use of mode coupling in the paramagnetic case, we have for the time ordered Green's function $S_{22}^H(\omega)$,

$$S_{22}^H(\omega) = 8\frac{N^2-1}{N^3} \frac{i}{2\pi} \int d\Omega\, S_{11r}(\omega - \Omega) S_{11}(\Omega), \tag{9}$$

where

$$S_{11r}(t_i, t_j) = \langle \mathcal{T}[n_r^d(t_i) n_r^d(t_j)] \rangle \qquad r = 1, \ldots, N^2 - 1. \tag{10}$$

The spectral weight absorbed by the propagator $G_{22}(\omega)$ in the mode-coupling form (9) is $4(N+1)/N^2$. As we are here computing the high-energy component of G_{22}, we can safely take the atomic limit for the Bose propagator, so that $G_{22}^H(\omega) = 4\frac{N+1}{N^2} G_{11}(\omega)$. In the high-energy regime, any other treatment for the Bose propagator would not substantially affect our results for the fermionic spectral function (i.e., by taking the atomic limit we already get an accuracy of the same order of the energy scale we are computing).

From the Hamiltonian (2) it is direct to derive

$$i\frac{\partial}{\partial t}\psi_2 = 2\frac{1}{N}\vec{\tau}_N \cdot \vec{n}^d c_\varepsilon + 2J_\mathrm{K}\frac{1}{N}\vec{\tau}_N \cdot \vec{n}^d \psi_2 + 8if_{abc}^N J_\mathrm{K} \frac{1}{N^2} \tau_N^a [c_0^\dagger \cdot \tau_N^b c_0] n_c^d c_0, \tag{11}$$

where f_{abc}^N are the structure constants of the SU(N) Lie algebra ($[\tau_N^a, \tau_N^b] = 2if_{abc}^N \tau_N^c$) and $c_\varepsilon = (1/\sqrt{N_s})\sum_{\mathbf{q}} \varepsilon_c(\mathbf{q}) c(\mathbf{q})$. It is worth noting that the source (11) has a direct component on the field c_0 [$2J_\mathrm{K}/N \vec{\tau}_N \cdot \vec{n}^d \psi_2 = 4J_\mathrm{K}(N+1)/N^2 c_0 + \ldots$] which disappears for $N \to \infty$ being the coefficient $4J_\mathrm{K}(N+1)/N^2$ (for $N = 2$, $2J_\mathrm{K}/N \vec{\tau}_N \cdot \vec{n}^d \psi_2 \to 3J_\mathrm{K} c_0 - 2J_\mathrm{K}\psi_2$).

In the low-energy regime, we assume the following dynamics for the field ψ_2:

$$i\frac{\partial}{\partial t}\psi_2^L = \aleph \psi_1. \tag{12}$$

This corresponds to the physical assumption that at low energies (i.e., at energies much smaller than J_K and D)

we have a quasiparticle theory. Indeed, the ansatz in (12) can be described as an application of Roth's projection idea to a field ψ_2^L which has most of its spectral weight at low energies. Thus, the high-energy spectral weight is already accounted for by the mode-coupling approximation. This is the second main departure from the original Roth approach, where an equation of motion for the field ψ_2 would have been projected onto ψ_1 and ψ_2 itself. This field would have spectral weight at all frequencies [e.g., $4(N+1)/N^2$] and from it a Kondo scale cannot be estimated. Once again, noteworthy is the fact that the basis defined in (4) alone is inadequate to capture both low- and high-energy physics of the Kondo model once a Roth truncation is realized. At this level of approximation, in the scattering matrix [i.e., $J_K^2 G_{22}(\omega)$] there is only one energy scale that cannot mimic a crossover between the two regimes. This is set by I_{22} where the high-energy spectral weight [i.e., $4(N+1)/N^2$] prevents the low-energy scale from emerging.

By combining (3) and (12) it is direct to show that

$$G_{22}^L(\omega) = \frac{I_{22}^L}{\omega - J_K^2 I_{22}^L \Gamma_0(\omega)}, \qquad (13)$$

being $\aleph = J_K I_{22}^L$, after projecting (12) on the field ψ_1. We have defined I_{22}^L as the spectral weight of $G_{22}(\omega)$ in the low-energy region. Also, it is implicitly assumed that $\langle\{\psi_2^L, \psi_2^{H\dagger}\}\rangle = 0$ because they span different energy sectors of the Hilbert space. In conclusion, we have

$$G_{11}(\omega) = \frac{\Gamma_0(\omega)}{1 - 4\frac{N+1}{N^2} J_K^2 \Gamma_0^2(\omega)} + \frac{J_K^2 \Gamma_0^2(\omega)}{1 - 4\frac{N+1}{N^2} J_K^2 \Gamma_0^2(\omega)} \frac{I_{22}^L}{\omega - J_K^2 I_{22}^L \Gamma_0(\omega)}, \qquad (14)$$

$$G_{12}(\omega) = \frac{4\frac{N+1}{N^2} J_K \Gamma_0^2(\omega)}{1 - 4\frac{N+1}{N^2} J_K^2 \Gamma_0^2(\omega)} + \frac{J_K \Gamma_0(\omega)}{1 - 4\frac{N+1}{N^2} J_K^2 \Gamma_0^2(\omega)} \frac{I_{22}^L}{\omega - J_K^2 I_{22}^L \Gamma_0(\omega)}, \qquad (15)$$

$$G_{22}(\omega) = \frac{4\frac{N+1}{N^2} \Gamma_0(\omega)}{1 - 4\frac{N+1}{N^2} J_K^2 \Gamma_0^2(\omega)} + \frac{1}{1 - 4\frac{N+1}{N^2} J_K^2 \Gamma_0^2(\omega)} \frac{I_{22}^L}{\omega - J_K^2 I_{22}^L \Gamma_0(\omega)}. \qquad (16)$$

At this stage of the method, once I_{22}^L is evaluated, the problem is solved, as in point (iii) referred to above. From Eq. (7) it is clear that I_{22}^L is connected to K_D. However, it is crucial to note that it represents the low-energy spectral weight and is a distinct object in respect to the K_D parameter which also contains contributions from energies of the order J_K. For the determination of this low-energy scale, we need to call upon some self-consistent condition. Evaluating the Kondo amplitude K_D using $G_{12}(\omega)$,

$$K_D = -T \sum_n G_{12}(i\omega_n), \qquad \omega_n = (2n+1)\pi T, \qquad (17)$$

and inserting this into Eq. (7), we give a relation between I_{22} and I_{22}^L of the form $I_{22} = F[I_{22}^L]$. To get the self-consistent equation, we estimate $I_{22}^H = F[I_{22}^L = 0, T = J_K]$ which results in an equation for the low-energy spectral weight of the form $I_{22}^L = I_{22} - I_{22}^H$. In other words, we choose J_K as the energy above which the one-particle Green's function is made up of incoherent high-energy contributions with no relevant temperature dependence. While the equations resemble the slave boson equations, they differ in a significant way from them. These equations do not introduce additional redundant phases and Lagrange multipliers, and avoid all the difficulties associated with the treatment of the gauge fields. The slave boson method has been very successful in obtaining low-energy information. High-energy information can also be obtained by performing fluctuations around the mean-field solutions, but this gets increasingly difficult, particularly in lattice models [12].

We now present some results. For the numerical solution of the equations we used a constant density of states $\rho = \frac{1}{2D}\theta(D - |\omega|)$ for the field c_0 so that $\Gamma_0^R(\omega) = \frac{1}{2D}\ln|\frac{D+\omega}{D-\omega}| - i\pi\frac{1}{2D}\theta(D - |\omega|)$. In Figs. 1 and 2, the Kondo amplitude K_D and I_{22}^L are shown as functions of the temperature for $J_K = 0.08$ and $N = 2$. D has been set equal to 1. In Fig. 2 we also show the solution for $N = \infty$ and the one after replacing $I_{22}^H = F[I_{22}^L = 0, T = J_K]$ with $I_{22}^H = F[I_{22}^L = 0]$. Both these solutions give a spurious transition at a characteristic temperature which is the signature of the Kondo crossover in the exact solution. As in the slave boson approximation, this is due to the absence of a small inhomogeneous term which is present in our method and mimics mixing effects between high- and low-energy contributions. The quantities in Fig. 2 coincide only in the limit of large spin

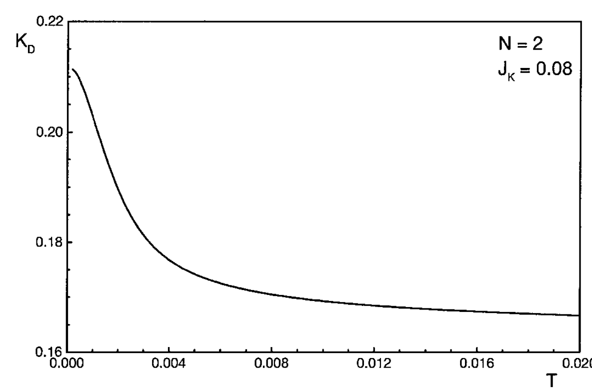

FIG. 1. The Kondo amplitude K_D is plotted as a function of the temperature for $J_K = 0.08$ and $N = 2$.

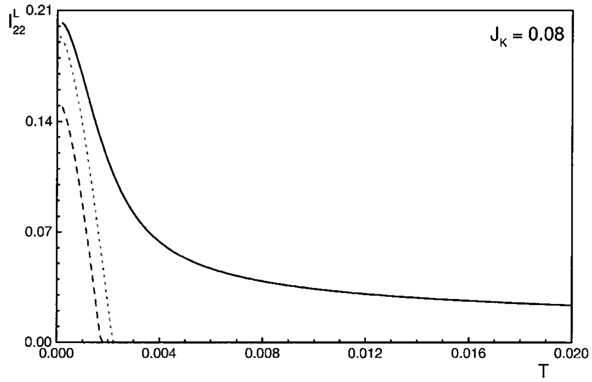

FIG. 2. The low-energy spectral weight I^L_{22} is given as a function of the temperature for $J_K = 0.08$ and $N = 2$ (solid line). As a point of reference, we give the solution after $I^H_{22} = F[I^L_{22} = 0]$ (dashed line) and for $N = \infty$ (dotted line).

degeneracy (i.e., $N \to \infty$) where the method recovers the exact results [9]. Our numerical estimate for the Kondo temperature T_K agrees well with the exact solution [9,13]. At this temperature ($T_K \simeq 0.002$), I^L_{22} has a change in the concavity of its slope when plotted as a function of the temperature. In Fig. 3, we present the spectral density $\sigma_{22}(\omega) = (-\frac{1}{\pi})\mathrm{Im}[G^R_{22}(\omega)]$ for two different temperatures. Again, it is clear that at high temperatures (i.e., $T \geq J_K$) only a high-energy incoherent background is left. A well-defined singlet excitation mode no longer exists, even if some residual spin-spin interaction persists in being energetically favored by a finite bandwidth (i.e., K_D is nonzero at any temperature as in Fig. 1).

In conclusion, we have shown how to resolve coherent low-energy features embedded in a broad high-energy background by the use of a fully self-consistent calculation for composite particle operators. In a problem with more than one energy scale, which is typical of strongly correlated systems, we succeeded in capturing low-energy features. Our scheme extends and improves upon Roth's method by combining the advantages of the methods based on the equations of motion and the slave boson techniques. Lastly, we note that when there is an expansion parameter such as the size of the group, or the size of the representation, our approach can be formulated so as to reduce to the correct solution in the exactly soluble limit. We have illustrated this here with the Kondo model in the limit of the large spin symmetry group which has often been shown to retain many crucial aspects of low-energy physics [6].

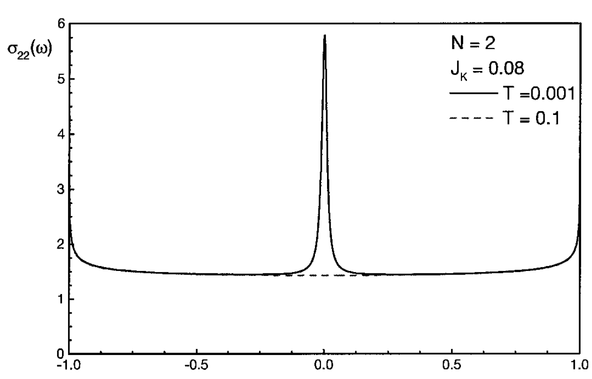

FIG. 3. The spectral density $\sigma_{22}(\omega)$ is reported for $T = 0.001$ (solid line) and $T = 0.1$ (dashed line). $J_K = 0.08$ and $N = 2$.

Finally, our approach is directly applicable to lattice models and work in this direction is currently in progress.

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