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CONSERVING SLAVE BOSON APPROACH TO STRONGLY CORRELATED FERMI SYSTEMS: SINGLE-IMPURITY ANDERSON MODEL

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We propose a general and systematic method for the study of correlated Fermi systems, based on an auxiliary slave boson representation and a self-consistent partial resummation of Feynman diagrams. The time-independent local constraint is treated in the saddle point approximation, rendering the theory tractable both in the impurity and lattice cases. Our approach avoids slave boson condensation and preserves local gauge invariance. We apply the method to the one-impurity, infinite-U Anderson model as a test case, and discuss how unphysical singularities present in earlier theories may be eliminated.

THEORETICAL EFFORTS to explain high T_c superconductivity [1], heavy fermion systems [2] and other recently discovered materials have focused on models of strongly correlated Fermi systems. Generally, one attempts to model the correlated electrons in these compounds by strong repulsive on-site interactions U for d- or f-electrons. As $U \to \infty$, the interaction effectively limits electrons to the part of the Hilbert space with no doubly occupied sites. It is this projection of the dynamics into a subspace of Hilbert space which is difficult to describe with conventional many-body techniques [3]. In order to circumvent the technical difficulties caused by projection operators, Barnes [4] proposed sometime ago that the projection may be accomplished by introducing auxiliary or "slave" Bose fields describing the empty lattice site, and a local constraint ensuring that each site is either empty or singly occupied (i.e. the sum of the occupation numbers of bosons and fermions adds up to one). This approach has been pioneered by Coleman [5] and by Read and Newns [6] in conjunction with a $1/N$ expansion for the N-orbital single impurity Anderson model. Later versions of the technique have been applied to the Anderson lattice model, the Hubbard model and its derivatives and other models of correlated fermions.

The conventional $1/N$ slave boson method has enjoyed a good deal of success and apparently gives much of the correct qualitative physics already in mean field theory [6]. However, it is flawed by the occurence of a spurious Bose condensation transition at finite temperature, which makes it impossible to describe the crossover from low temperature to high temperature regime correctly. We believe [7] that Bose condensation should be inhibited by the local constraint, even though the number of bosons n_b is, in general, finite in the limit $T \to 0$. This may happen if the Bose spectral function $A_b(\omega)$ acquires spectral weight at negative ω (where it attains negative values), such that in the limit $T \to 0$,

$$n_b = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} A_b(\omega) b(\omega) \to - \int_{-\infty}^{0} \frac{d\omega}{\pi} A_b(\omega) > 0,$$

where $b(\omega) = (e^{\omega/T} - 1)^{-1}$. It appears that the corresponding change in the spectral function from its form in mean field theory requires the summation of contributions in all orders of $1/N$, or even nonanalytic contributions [5] in $1/N$. This has been attempted for the Anderson impurity model in the so-called "non-crossing approximation" (NCA) [8, 9], in which all Keiter–Kimball diagrams [3] with non-crossing electron propagator lines are summed. For larger degeneracy $N \geqslant 4$ and in the Kondo regime the NCA results are in excellent agreement with exact Bethe-ansatz results, except for the low temperature regime $T < T_{\mathrm{NCA}} \ll T_{\mathrm{Kondo}}$, where spurious singularities appear and the exact Fermi liquid behaviour of this model is badly violated [9]. Application of the NCA scheme to lattice models requires additional assumptions [10]. To some extent these problems have been addressed by Jin and Kuroda [11], who showed that the bose condensation problem could be overcome in an unconventional $1/N$ slave boson scheme for the Anderson model to order $1/N^2$. While their results

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reproduce the known low temperature behaviour and provide a smooth crossover to the high temperature regime, some singularities have to be removed in an *ad hoc* way. Any of the above theories has difficulties for the canonical case of spin 1/2 ($N = 2$).

We propose here a slave boson approach to models of strongly correlated Fermi systems of the impurity or lattice type which allows one, for any degeneracy N, to separate the constraint problem from the problem of treating the intrinsic dynamics in a controlled way. As opposed to some of the above-mentioned approaches, our theory is based on time-ordered Green's functions. One may construct approximations respecting all exact symmetries of such models. As a test case we consider the infinite-U single impurity Anderson model of a magnetic impurity in a host metal because it allows for comparison with available exact results. In addition, dynamical quantities such as the d-electron spectral function cannot be obtained exactly and would be interesting to calculate in a controlled approximation. In terms of slave boson and pseudofermion operators b and f_σ for the d-electrons with $d_\sigma^\dagger = f_\sigma^\dagger b$ and conduction electron operators $c_{\mathbf{k},\sigma}^\dagger$, the effective Hamiltonian is given by

$$H = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} + E_d \sum_\sigma f_\sigma^\dagger f_\sigma + V \sum_{\mathbf{k},\sigma} (c_{\mathbf{k},\sigma}^\dagger f_\sigma b^\dagger + \text{h.c.}), \tag{1}$$

restricted to the subspace of eigenstates of the charge operator $Q = \Sigma_\sigma (f_\sigma^\dagger f_\sigma + b^\dagger b - 1)$ with eigenvalue zero. This spin label σ runs from 1 to N. The charge Q is conserved, i.e. $[Q, H] = 0$, and as a consequence the Hamiltonian is invariant under local gauge transformations $f_\sigma \to f_\sigma e^{i\Theta}$, $b \to b e^{i\Theta}$.

The constraint is conveniently taken into account in the path integral formulation, e.g. of the partition function Z [6],

$$Z = \int_0^{2\pi T} \frac{d\lambda}{2\pi T} e^{-S_{\text{eff}}(\lambda)}, \tag{2}$$

where TS_{eff} is the grand potential of the system with fixed λ, given by

$$Z(\lambda) = e^{-S_{\text{eff}}} = \int D[f, \bar{f}] D[b, \bar{b}] D[c, \bar{c}]\, e^{-S} \tag{3}$$

with

$$S = \int_0^{1/T} d\tau \left[\sum_\sigma \left(\sum_{\mathbf{k}} \bar{c}_{\mathbf{k},\sigma} \partial_\tau c_{\mathbf{k},\sigma} + \bar{f}_\sigma (\partial_\tau + i\lambda) f_\sigma \right) + \bar{b}(\partial_\tau + i\lambda) b + H(\tau) - i\lambda \right]. \tag{4}$$

In writing equation (2), it is assumed that $S_{\text{eff}}(\lambda)$ is an analytic function of λ in the interval $[0, 2\pi T]$. Otherwise, the integration contour has to be shifted along the imaginary axis to avoid any singularities. In particular, shifting the contour to $-i\infty$ is equivalent to taking the limit $i\lambda \to \infty$ of $Z(\lambda)$. The single-particle Green's function may be expressed likewise as

$$G_d(\omega_n) = \frac{1}{Z} \int_0^{2\pi T} \frac{d\lambda}{2\pi T} e^{-S_{\text{eff}}(\lambda)} G_d(\omega_n, \lambda), \tag{5}$$

where $G_d(\omega_n, \lambda)$ is the d-electron Green's function for a fixed λ. It may be shown that the above representation gives the correct result in the limit hybridization $V \to 0$ (atomic limit).

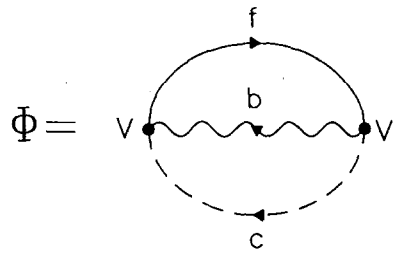

Fig. 1. Diagram for the generating functional Φ in lowest order in V.

We now proceed to discuss approximations for $G_d(\omega_n, \lambda)$. Since in deriving equation (5) we made use of the local gauge invariance of $G_d(\omega_n, \lambda)$, any approximation used in equation (5) must be gauge invariant, too, *guaranteeing the conservation of Q in time*. Such approximations may be conveniently derived from a generating functional Φ [12]. In the limit of small hybridization V, the lowest order diagram for Φ is second order in V and contains one Green's function of each kind, G_f, G_b, G_c (Fig. 1). As discussed below, this approximation is sufficient to give the correct qualitative behaviour both above and below the Kondo temperature, except for very low temperatures. For the moment, our intent is principally to show that conserving approximations can be constructed. It is one of the virtues of this formulation that any extension to higher order processes is straightforward.

Functional differentiation with respect to G_i yields the self-energies Σ_i, i.e.

$$\begin{aligned} \Sigma_{f_\sigma}(w_n) &= -V^2 T \sum_{\omega_n'} G_b(\omega_n') G_{c\sigma}(\omega_n - \omega_n'), \\ \Sigma_b(w_n) &= V^2 T \sum_\sigma \sum_{\omega_n'} G_{f\sigma}(\omega_n + \omega_n') G_{c\sigma}(\omega_n'), \\ \Sigma_{c\sigma}(w_n) &= -V^2 T \sum_{\omega_n'} G_{f\sigma}(\omega_n + \omega_n') G_b(\omega_n'), \end{aligned} \tag{6}$$

which, together with the slave particle Green's functions $G_b(\omega_n) = (i\omega_n - i\lambda - \Sigma_b)^{-1}$ and $G_{f\sigma}(\omega_n) = (i\omega_n - i\lambda - E_d - \Sigma_{f\sigma})^{-1}$ as well as the local c-electron Green's function $G_c(\omega_n) = [(G_c^0) - \Sigma_c]^{-1}$, form

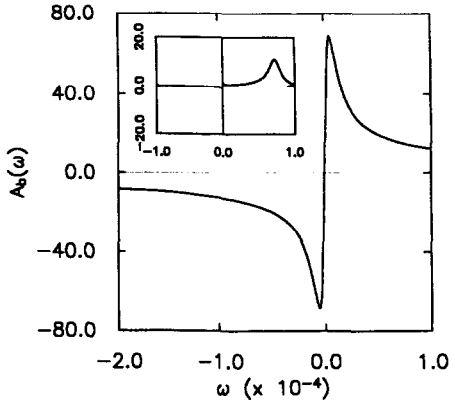

Fig. 2. Boson spectral function $A_b(\omega)$ vs ω near $\omega = 0$ in saddle point approximation for $N = 2$, $E_d = -0.67$, $\Gamma = 0.15$, $T_K \simeq 5 \times 10^{-4}$ at $T = 5 \times 10^{-6}$, using conduction electron density of states $N(\varepsilon) = \pi^{-1/2} \exp(-\varepsilon^2)$ and chemical potential $\mu = 0$. The inset shows the broadened peak at $\omega \simeq \lambda_0 \simeq |E_d|$.

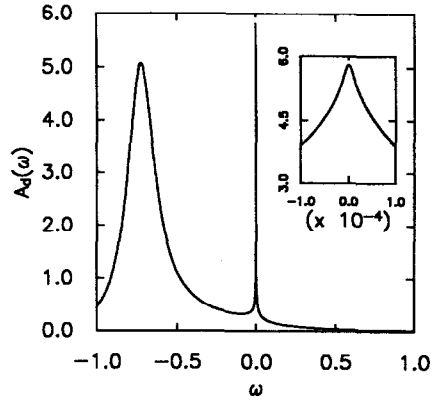

Fig. 3. The d-electron spectral function $A_d(\omega)$ vs frequency, in saddle point approximation (parameters as in Fig. 2). The inset shows the Kondo resonance peak near $\omega = 0$. The exact $T = 0$ value of $A_d(0)$ following from the Friedel–Langreth sum rule is 6.2.

a complete set of self-consistent equations. Here $G_c^0(\omega_n) = \int d\varepsilon\, N(\varepsilon)/(i\omega_n - \varepsilon)$, where $N(\varepsilon)$ is the c-electron density of states. Note that $i\lambda$ plays the role of a chemical potential with the unusual property of being complex-valued. The d-electron Green's function is given exactly in terms of Σ_c as

$$G_d(\omega_n, \lambda) = \frac{1}{V^2} \frac{\Sigma_c(\omega_n)}{1 - \Sigma_c(\omega_n) G_c^0(\omega_n)}. \tag{7}$$

It can be shown that expression (7) for $G_d(\omega_n, \lambda)$, with Σ_c given by equation (6), is gauge-invariant.

We evaluate the λ integral over $G_d(\omega_n, \lambda)$ in equation (5) approximately by determining the saddle point of $\exp\{-S_{\text{eff}}(\lambda)\}$. The saddle point condition $dS_{\text{eff}}/d\lambda = 0$ translates into $\langle Q \rangle = 0$ using the thermodynamic relation $\langle Q \rangle = -iT\, dS_{\text{eff}}/d\lambda$. We have solved the self-consistent equations (6) and (7) numerically at the saddle point. The saddle point value λ_0 is found to be purely imaginary, corresponding to a real valued chemical potential $i\lambda_0$ for the pseudofermions and the slave boson. The pseudofermion spectral function is characterized by a single peak around $\omega = 0$, while the slave boson spectral function has a broad peak at $\omega \simeq |E_d|$ and a sharp structure near zero frequency (Fig. 2), extending to negative ω, as anticipated. The corresponding d-electron spectral function shows the expected features: a broad peak at $\omega \simeq |E_d|$ and a Kondo resonance near the Fermi energy at $\omega = 0$ (Fig. 3). The width of the resonance is correctly given by the Kondo scale $T_K = D \exp\{-\pi |E_d| N\Gamma\}$, where $\Gamma = \pi N(0) V^2$ is the bare hybridization width and D is the conduction bandwidth. However, at temperatures $T \ll T_K$ the slave boson and the pseudofermion spectral functions $A_b(\omega)$ and $A_{f\sigma}(\omega)$ appear to develop singularities at $\omega = 0$ at least down to the lowest temperatures of about 10^{-2} T_K of our numerical evaluation. Also the fluctuations in Q appear to tend to zero with T as $\Delta Q^2 \sim T$, implying that the projection onto the $Q = 0$ sector may become exact at $T = 0$ even in the saddle point approximation. The singularities are not unexpected, since both the pseudofermions and the slave boson Green's functions involve intermediate states in sectors of Hilbert space different from $Q = 0$ which are orthogonal to the $Q = 0$ states and hence lead to an orthogonality catastrophe [13]. Another way to view the singularities is to notice that in order to have a non-integer value $n_f < 1$ for the fermion occupation number at $T = 0$, as enforced by the constraint, the real part of $G_{f\sigma}(\omega - i0)$ needs to change sign at $\omega = 0$ [14]. This requires $G_{f\sigma}(\omega - i0)$ to diverge at $\omega = 0$, since $\text{Im}\ \Sigma_{f\sigma}(\omega - i0) \to 0$ as well [see equation (6)]. The d-electron spectral function is finite, but develops a cusp at $\omega = 0$ in the limit $T \to 0$, which conflicts with the exact Fermi-liquid behaviour known to exist for this model [15].

In fact, the results of the saddle point approximation to equations (4)–(6) are very similar to those obtained within the NCA. The NCA equations are obtained from equation (6) by taking the limit $i\lambda \to \infty$, which effects the exact projection onto the subspace $Q = 0$. Therefore it does not appear to be essential to improve on the saddle point approximation by calculating the effect of fluctuations. Nevertheless we would like to point out a difficulty in the fluctuation calculation. Since $S_{\text{eff}}(\lambda)$ as well as $G_d(\omega_n, \lambda)$ have branch cuts in the complex λ-plane along $\text{Re}\{\lambda\} = 0$ and $\text{Re}\{\lambda\} = \pi T$ (and periodically continued at intervals of $2\pi T$), the initial integration

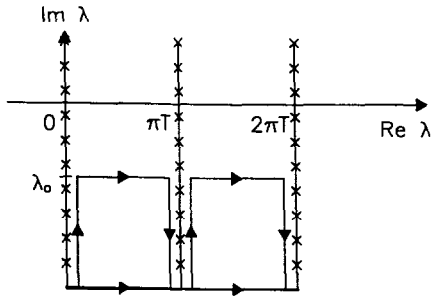

Fig. 4. Contours in the complex $i\lambda$-plane for the integrations in equations (4) and (5). The branch cuts of $S_{\text{eff}}(\lambda)$ and $G_{d\sigma}(\omega_n, \lambda)$ are indicated by crosses.

contour from $\lambda = -i\lambda_1$ to $\lambda = -i\lambda_1 + 2\pi T$, $\lambda_1 \to \infty$, may not just be shifted parallel to the real axis until it traverses the saddle point at $\lambda = \lambda_0$ (i.e. choosing $-\lambda_1 = \lambda_0$). Instead, the contour wraps around the branch cuts in the way shown in Fig. 4. Thus there is an extra contribution of the fluctuations around the saddle point from the part of the integration contour along the branch cuts.

In the chosen approximation for the generating functional (Fig. 1), the formation of the Kondo singlet ground state is not accounted for in an explicit way. In the NCA, this deficiency is reflected in the appearance of spectral anomalies at very low temperatures, destroying the expected Fermi liquid behaviour [8, 9, 15] To recover the correct low-energy behaviour in this formulation, it appears necessary to include higher order diagrams. For example, multiple scattering of pseudofermions and conduction electrons shown in Fig. 5 should lead to the formation of the bound state [16]. We have analyzed the corresponding scattering amplitude in the exactly projected case, where the integral equation represented by Fig. 5 simplifies considerably, and found numerically that a pole indeed exists on the real axis in the spin singlet channel. The pole contribution to the self-energies $\Sigma_{f,b}$ causes the infrared singularities to be cut off on the scale T_K, thus restoring analytical behaviour of the d-electron Green's function. It remains to be seen whether this behaviour persists in the saddle point approximation. A full numerical evaluation is in progress.

We note that in the model of spinless fermions ($N = 1$), there is no possibility of a pole in the f–c correlation function and hence the infrared singularities remain. In renormalization group language, the $N > 1$ system scales, initially with decreasing temperature, towards the X-ray threshold fixed point (FP), but at low temperature flow towards the Fermi liquid FP characteristic of the noninteracting system.

An advantage of the approach presented here, as compared to generalizations of the NCA, is that it may be extended to the lattice case in a straightforward way. Although the evaluation of the saddle point equations will be more difficult on the lattice, we expect the fluctuation expansion to be well-defined, since the singularities peculiar to single-impurity problems will be integrated over. We are in the process of applying the approach to lattice models such as the periodic Anderson model, and the t–J and Hubbard models.

In summary, we have presented a systematic and general approach to strongly interacting many-body systems by combining slave particle representations with conserving self-consistent approximations and a controlled implementation of the local constraint inherent to such theories. As a first test, we have applied the method to the single impurity Anderson model, which has been notoriously difficult to describe in a standard field theoretical treatment. Our formulation is free of spurious slave boson condensation and provides a systematic method for handling infrared singularities present in earlier similar theories.

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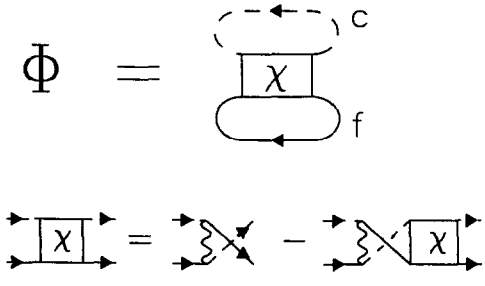

Fig. 5. Correction to generating functional from f–c ladders.

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