Asymptotically exact mean field theory for the Anderson model including double occupancy

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The Anderson impurity model for finite values of the Coulomb repulsion $U$ is studied using a slave boson representation for the empty and doubly occupied $f$-level. In order to avoid well known problems with a naive mean field theory for the boson fields, we use the coherent state path integral representation to first integrate out the double occupancy slave bosons. The resulting effective action is linearized using two-time auxiliary fields. After integration over the fermionic degrees of freedom one obtains an effective action suitable for a $1/N_f$-expansion. Concerning the constraint the same problem remains as in the infinite $U$ case. For $T \to 0$ and $N_f \to \infty$ exact results for the ground state properties are recovered in the saddle point approximation. Numerical solutions of the saddle point equations show that even in the spin-degenerate case $N_f = 2$ the results are quite good.

I. INTRODUCTION

The Anderson impurity model (AIM)\cite{1} was proposed to gain insight into the physics of dilute magnetic alloys. Variations of this model describe e.g. thermodynamic, transport and spectroscopic properties of Ce mixed valence compounds surprisingly well\cite{2,3}. The strong on-site $f$-repulsion $U$ makes these compounds typical examples of strongly correlated electron systems.

Various reviews exist on the theoretical approaches to obtain exact or approximate solutions for the thermodynamics and correlation functions of the AIM\cite{3–5}. While exact solutions for thermodynamic properties are known for special cases using the Bethe-Ansatz\cite{5} the progress towards controlled approximations for spectral functions was mainly due to large $N_f$ expansions, where $N_f$ is the degeneracy of the $f$-level\cite{3}.

The two special cases for which the exact thermodynamics can be obtained via the Bethe-Ansatz are the infinite $U$ limit ($U = \infty, N_f$ arbitrary) and the spin-degenerate symmetric case ($2\varepsilon_f + U = 2\mu, N_f = 2$) where $\mu$ is the chemical potential which will be chosen as the zero of the one electron energies in the following and $\varepsilon_f$ is the bare $f$-level energy. The one-particle spectral functions which determine photoemission and inverse photoemission spectra are rather well understood in the infinite $U$ limit for arbitrary temperatures and degeneracies down to $N_f = 2$. For temperatures of the order of the Kondo temperature $T_K$ or smaller and $f$-occupancies close to one (spin-fluctuation limit) there is a sharp "Kondo-resonance" slightly above the Fermi energy and a broad resonance near $\varepsilon_f$. The knowledge about the position, the width and the weight of the Kondo resonance comes from three different approaches. It was first obtained for zero temperature using a variational ansatz for the ground state and a $1/N_f$ classification of intermediate states\cite{6,7}. The noncrossing approximation (NCA) which can be derived by different techniques works well for all temperatures except $T \ll T_K$\cite{8,9}.\
In the third approach a functional integral (FI) for the partition function is expressed in terms of an effective action for the slave boson, which is introduced to handle the constraint of at most single occupancy of the $f$-level. If the FI is evaluated in the saddle point approximation, corresponding to a simple mean field approximation for the slave boson, the exact ground state energy is recovered in the limit $N_f \to \infty$. Gaussian fluctuations around the saddle point yield $(1/N_f)^{-1}$-corrections in the very low temperature Fermi liquid regime. Due to the occupancy constraint the saddle point expansion is not a $(1/N_f)^{-1}$-expansion in the strict sense. This problem will be addressed later in this paper for finite values of $U$.

In the spindegenerate symmetric case the Kondo peak is at the Fermi level due to the particle-hole symmetry of the problem. For $N_f > 2$ this symmetry is no longer given even for symmetric parameters $2\varepsilon_f + U = 0$ and a symmetric band, and the position of the Kondo peak has not been reliably calculated except in the large $N_f$ limit. Also the position of the Kondo peak for nonsymmetric parameters and $N_f = 2$ is not yet well understood. For not too low Kondo temperatures the only reliable results are from quantum Monte Carlo calculations. The spectral function for the $N_f = 2$-AIM has recently gained renewed attention as its calculation is required as an intermediate step in the exact solution of the Hubbard model in infinite dimensions.

For the finite $U$ AIM and arbitrary degeneracy $N_f$ there exists a variational approach which go over to the corresponding $U = \infty$ theories in the large $U$ limit. A naive mean field theory for the slave bosons for the empty $f$-level as well as the doubly occupied $f$-level does not recover the exact ground state energy in the limit $N_f \to \infty$, as it completely misses to obtain the mathematical structure of an integral equation for finite $U$ in contrast to an transcendental equation for $U = \infty$. Similar deficiencies of mean field theories for double occupancy slave bosons occur for the Hubbard model.

It is the aim of this paper to present a generalized mean field theory for the finite $U$ Anderson model in the $f^0, f^1$ and $f^2$ subspace for arbitrary degeneracy $N_f$, which leads to the exact ground state energy in the limit $N_f \to \infty$. Starting from a coherent state path integral we integrate out the double occupancy bosons, which leads to four-fermion terms. Using a Stratonovich-Hubbard transformation which introduces two-time auxiliary fields an effective action appropriate for a large $N_f$ expansion is derived, apart from the problem with the occupancy constraint, similar to the infinite $U$ case. We study stationary solutions of the saddle point equations for which the additional auxiliary fields depend on the time difference only. This leads after Fourier expansion to a system of coupled nonlinear equations for the Fourier components. Analytic continuation from the Matsubara frequencies to the real axis leads to a system of integral equations, which for finite $N_f$ has to be solved numerically. In the limit $N_f \to \infty$
the equations simplify considerably and for $T \to 0$ we exactly recover the integral equation which determines the ground state energy.\[13\]

In section II we present the model and introduce the coherent state path integral formulation. An exact effective action for the empty $f$-level slave boson and the two-time auxiliary fields is derived. In section III the corresponding saddle point equations are derived. The simplified equations in the limit $N_f \to \infty$ are discussed. The numerical solutions for finite $N_f$ are presented in section IV. Some results of ref.\[13\] and details of various calculations are described in appendices.

II. THE MODEL

We consider the finite $U$ Anderson impurity Hamiltonian \[13\]

$$H_A = \sum_{\nu=1}^{N_f} \left[ \varepsilon \nu, \varepsilon \nu, d\varepsilon + \varepsilon_f f^+_\nu f^*_\nu + \int d\varepsilon \left[ V(\varepsilon) f^+_\nu \varepsilon \nu + h.c. \right] \right] + U \sum_{\nu, \mu} n_\nu n_\mu$$

\[1\]

where we have introduced a combined index, $\nu$, for the orbital and spin degeneracies. Spin-orbit and multiplet splittings are neglected. The first term describes the conduction states, with energy $\varepsilon$, and the second term the $f$-level with the (bare) energy $\varepsilon_f$. The third term leads to a hopping between these states where the $V(\varepsilon)$ can be chosen real and the last term describes the Coulomb interaction between the $f$-electrons. The Hamiltonian is studied in the subspace of at most double occupancy of the $f$-level i.e. in the $f^0, f^1$ and $f^2$ manifold. This restriction is incorporated using slave bosons.

In the infinite $U$ model Coleman\[9\] has introduced a single slave boson as a counting device for the number of $f$-electrons. For the finite $U$ model there are $N_f (N_f - 1) / 2$ different doubly occupied $f$-states. Therefore we introduce $N_f (N_f - 1) / 2$ additional "heavy bosons"\[14\]. If $|\{0\}\rangle$ denotes the ground state of the "light" and heavy bosons we make the correspondence

$$\mu > \nu : f^+_\mu f^*_\mu |\{n_\mu\}\rangle \rightarrow h^+_\mu |\{n_\mu\}\rangle \otimes |\{0\}\rangle$$

where $|\{n_\mu\}\rangle$ denotes an arbitrary band state and $h^+_\mu$ is the creation operator of a heavy boson. To remove the restriction $\mu > \nu$ it is useful to define boson operators for $\mu \leq \nu$ by $h^+_{\mu \nu} := -h^+_{\nu \mu}$ and $h_{\mu \mu} \equiv 0$.

We now construct a Hamiltonian acting on the product space of electrons and bosons which is equivalent to $H$ in the $\{f^0, f^1, f^2\}$ subspace

$$H = H_0 + \sum_{\mu > \nu} (2\varepsilon_f + U) h^+_{\mu \nu} h_{\mu \nu} + \int d\varepsilon \left[ \sum_{\nu=1}^{N_f} V(\varepsilon) f^+\nu \varepsilon \nu b + \sum_{\mu, \nu=1}^{N_f} V(\varepsilon) h^+_{\mu \nu} f^*\nu c_{\mu \nu} + h.c. \right]$$

\[3\]

Here $H_0$ is formally the same as in Eqn.\[14\]. The Hamiltonian $H$ commutes with the "charge operator" $\hat{Q}$ defined as
\[
\dot{Q} = b^+ b + \sum \nu f^+_{\nu} f_{\nu} + \sum_{\mu>\nu} h^+_{\mu\nu} h_{\mu\nu}
\] (4)

Therefore the subspaces \( F_Q \) with definite integer value \( Q \) can be treated separately. In the subspace \( F_1 \) the Hamiltonian \( H \) is equivalent to the Anderson Hamiltonian \( H_A \) in the subspace of \( f^0, f^1 \) and \( f^2 \) states. The partition function is therefore given by

\[
Z_A = Tr e^{-\beta H} = Z_1
\] (5)

where the trace is restricted to the subspace of states with \( Q = 1 \). This projection to the \( Q = 1 \) subspace can be expressed as a contour integral in a complex \( \lambda \)-plane \((Z \equiv Z_A)\)

\[
Z = \frac{\beta}{2\pi i} \int_C d\lambda e^{\beta \lambda} Tr \left( e^{-\beta H(\lambda)} \right)
\] (6)

where \( H(\lambda) \equiv H + \lambda \dot{Q} \) and the contour runs from \( \lambda_R - i\pi/\beta \) to \( \lambda_R + i\pi/\beta \), where the real \( \lambda_R \) is arbitrary. Since the trace has now to be performed over the full Hilbert space of fermions and bosons \( Z \) can be expressed as a coherent state functional integral

\[
Z = \int_C \frac{\beta d\lambda}{2\pi i} e^{\beta \lambda} \int Df D\bar{c} Dh D\bar{b} \exp \left\{ - \int_0^\beta (L_0(\tau) + L_1(\tau)) d\tau \right\}
\] (7)

where

\[
L_0(\tau) = \sum_{\nu=1}^{N_f} \left\{ \int d\varepsilon \bar{c}_{\nu}(\tau) \left[ \frac{\partial}{\partial \varepsilon} + \varepsilon \right] c_{\nu}(\tau) + f_{\nu}(\tau) \left[ \frac{\partial}{\partial \varepsilon} + \varepsilon_f + \lambda \right] f_{\nu}(\tau) \right\}
\]

\[+ b^*(\tau) \left[ \frac{\partial}{\partial \varepsilon} + \lambda \right] b(\tau) + \sum_{\mu>\nu} h^*_{\mu\nu}(\tau) \left[ \frac{\partial}{\partial \varepsilon} + 2\varepsilon_f + U + \lambda \right] h_{\mu\nu}(\tau) \] (8)

and

\[
L_1(\tau) = \sum_{\nu=1}^{N_f} \int d\varepsilon \left[ V(\varepsilon) \bar{f}_{\nu}(\tau) c_{\nu}(\tau) b(\tau) + V(\varepsilon) b^*(\tau) \bar{c}_{\nu}(\tau) f_{\nu}(\tau) \right]
\]

\[+ \sum_{\nu,\mu=1}^{N_f} \int d\varepsilon \left[ V(\varepsilon) h^*_{\mu\nu}(\tau) f_{\nu}(\tau) c_{\mu}(\tau) + V(\varepsilon) \bar{c}_{\mu}(\tau) \bar{f}_{\nu}(\tau) h_{\mu\nu}(\tau) \right] \] (9)

with \( \tau \)-dependent Grassmann fields \( c, \bar{c} \) and \( f, \bar{f} \) and complex fields \( b \) and \( h_{\mu\nu} \).

As the Grassmann fields enter the action \( S = \int_0^\beta d\tau L(\tau) \) with \( L(\tau) \equiv L_0(\tau) + L_1(\tau) \) quadratically it would be possible at this point to eliminate all fermionic variables by tracing over in the usual way. As we want to construct a mean field theory which becomes asymptotically exact in the large degeneracy and small temperature limit this procedure turns out **not** to be successful. The saddle point equations for the resulting effective action \( S_{eff}(b, h) \) do **not** produce the exact \( T = 0 \) results in the large degeneracy limit. This failure can be related to the fact that the term \( L_{11h}(\tau) \) in \( L_1(\tau) \) is not well suited for a large \( N_f \) saddle point expansion, because it consists of \( N_f^2 \) terms in which different orbital indices \( \mu, \nu \) are coupled.
we proceed differently, in a way which in the first step produces a seemingly more complicated effective action involving "four-fermion" terms. Factorizing these terms with a Stratonovich-Hubbard transformation leads to an interaction term in the effective action of the form needed for a large $N_f$ expansion.

In the first step the heavy bosons are integrated out. The Gaussian integrals are easily performed and yield using $h_{\nu\mu} = -\tilde{h}_{\nu\mu}$ in the interaction term $L_{1h}(\tau)$

\[
\int Dh \exp \left\{ - \int_0^\beta \left[ \sum_{\mu > \nu} h_{\nu\mu}^*(\tau) \frac{\partial}{\partial \tau} + 2\varepsilon_f + U + \lambda h_{\nu\mu}(\tau) + L_{1h}(\tau) \right] \right\} 
\]

\[
= Z_0^h(\lambda) \exp \left\{ - \sum_{\mu > \nu} \int d\varepsilon d\varepsilon' \int_0^\beta d\tau \int_0^\beta d\tau' V(\varepsilon) \left( \bar{c}_{\varepsilon\mu}(\tau) \bar{f}_{\varepsilon\mu}(\tau) - \bar{c}_{\varepsilon\mu}(\tau') \bar{f}_{\varepsilon\mu}(\tau') \right) \right\},
\]

where

\[
Z_0^h(\lambda) = \left( 1 - \exp[ -\beta(2\varepsilon_f + U + \lambda) ] \right)^{-N_f(N_f-1)/2}
\]

is the unperturbed partition function for the heavy bosons and

\[
G_0^h(\tau - \tau') \equiv -\langle \tau | (\partial_\tau + 2\varepsilon_f + U + \lambda)^{-1} | \tau' \rangle
\]

is the corresponding unperturbed propagator with the usual bosonic boundary conditions.

The exponent on the rhs of Eqn. (10) can be written in a form suitable for a Stratonovich-Hubbard transformation introducing

\[
Vc_{\mu}(\tau) \equiv \int d\varepsilon V(\varepsilon)c_{\mu\varepsilon}(\tau)
\]

with $V \equiv (\int |V(\varepsilon)|^2 d\varepsilon)^{1/2}$ and using

\[
\sum_{\mu > \nu}(\bar{c}_{\nu\mu}(\tau)\bar{f}_{\nu\mu}(\tau) - \bar{c}_{\nu\mu}(\tau')\bar{f}_{\nu\mu}(\tau'))(f_{\nu\mu}(\tau')c_{\nu\mu}(\tau') - f_{\nu\mu}(\tau)c_{\nu\mu}(\tau'))
\]

\[
= \left( \sum_{\mu} \bar{c}_{\mu}(\tau)c_{\mu}(\tau') \right) \left( \sum_{\nu} \bar{f}_{\nu}(\tau)f_{\nu}(\tau') \right) + \left( \sum_{\mu} \bar{f}_{\mu}(\tau)f_{\mu}(\tau') \right) \left( \sum_{\nu} \bar{c}_{\nu}(\tau)c_{\nu}(\tau') \right).
\]

As both terms on the rhs have a simple product form we can use the identity

\[
e^{CD} = A \int \frac{dRe \alpha \ dIm \alpha}{\pi} e^{-A|\alpha|^2 - \sqrt{A}(\alpha C + A*)} \]

valid for commuting variables $C$ and $D$ and $Re(A) > 0$. The auxiliary fields which have to be introduced to linearize the four-Grassmann terms depend on two time variables

\[
\exp \left\{ -V^2(\sum_{\mu} \bar{c}_{\mu}(\tau)c_{\mu}(\tau'))(\sum_{\nu} \bar{f}_{\nu}(\tau)f_{\nu}(\tau'))G_0^0(\tau - \tau') \right\}
\]

\[
= \frac{-1}{G_0^0(\tau - \tau')} \int d\mu(F(\tau, \tau')) \exp \left\{ \frac{|F(\tau, \tau')|^2}{G_0^0(\tau - \tau')} - F(\tau, \tau')V \sum_{\mu} \bar{c}_{\mu}(\tau)c_{\mu}(\tau') - F^*(\tau, \tau')V \sum_{\mu} \bar{f}_{\mu}(\tau)f_{\mu}(\tau') \right\}
\]

where $d\mu(F) = dRe F dIm F / \pi$. The second term in Eqn. (13) yields
\[
\exp \left\{ -V^2 \left( \sum_{\mu} \bar{c}_\mu(\tau) f_\mu(\tau') \right) \left( \sum_{\nu} \bar{f}_\nu(\tau)c_\nu(\tau') \right) G_h^0(\tau - \tau') \right\} 
\]
\[
= -\frac{1}{G_h^0(\tau - \tau')} \int d\mu(X(\tau, \tau')) \exp \left\{ \frac{|X(\tau, \tau')|^2}{G_h^0(\tau - \tau')} - V \sum_{\mu} (X(\tau, \tau') \bar{c}_\mu(\tau') + X^*(\tau, \tau') \bar{f}_\mu(\tau)c_\nu(\tau')) \right\}
\]

The linearization produces additional terms bilinear in the Grassmann variables. The first Grassmann term in the exponent on the rhs of Eqn. (15) corresponds to a separable perturbation \( \sim |c, \mu > < c, \mu | \), where

\[
|c, \mu > : = \frac{1}{V} \int d\varepsilon V(\varepsilon) |\varepsilon, \mu >
\]

are linear combinations of conduction states localized around the impurity. The other term in the exponent on the rhs of Eqn. (15) leads to a fluctuating f-level position \( \varepsilon_f + \lambda \rightarrow \varepsilon_f + \lambda + V F^*(\tau, \tau') \). The Grassmann terms in the exponent on the rhs of Eqn. (2.14) modify the hopping strength \( V b(\tau) \delta(\tau - \tau') \rightarrow V (b(\tau) \delta(\tau - \tau') + X^*(\tau, \tau')) \).

At the next step the Grassmann variables are formally integrated out

\[
Z = \int e^{\beta d \lambda} e^{\beta \lambda} Z^0(\lambda) \int Db DF DX e^{-S_{eff}}
\]

where the effective action \( S_{eff} \) is given by

\[
S_{eff} = \int_0^\beta b^*(\tau)(\partial_\tau + \lambda)b(\tau)d\tau - \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \frac{|X(\tau_1, \tau_2)|^2 + |F(\tau_1, \tau_2)|^2}{G_h^0(\tau_1 - \tau_2)} - N_f Tr \ln[\partial \otimes 1_e + 1_e \otimes h_0 + h_1]
\]

and the trace runs over the space of antiperiodic functions on the interval \([0, \beta]\) as well as the space of single electron states for a single channel. The operators \( h_0 \) and \( h_1 \) are given by

\[
h_0 = \int \varepsilon |\varepsilon > < \varepsilon | d\varepsilon +(\varepsilon_f + \lambda) | f > < f |
\]

\[
h_1 = V(F^* | f > < f | + F | c > < c | + (b^* + X) | c > < f | + (b + X^*) | f > < c |)
\]

The label of the electronic channel has been suppressed as each channel gives the same contribution leading to the factor \( N_f \) in front of the trace. Scaling all Bose fields by a factor \( \sqrt{N_f} \) i.e. \( b \rightarrow \sqrt{N_f} b \) etc. the effective action becomes proportional to \( N_f \) and a well defined large \( N_f \) expansion could be carried out, if not the same problem known from the infinite \( U \) case \( ^1 \) due to the constraint integral over \( \lambda \) would show up. The exponent \( \beta \lambda \) is not proportional to \( N_f \) which leads to a similar behaviour as discussed in detail for \( U = \infty \) \( ^2 \).

Nevertheless we treat the functional integral in Eqn. (10) by a saddle point approximation (without scaling of the Bose fields).
III. THE SADDLE POINT EQUATIONS

To derive the saddle point equations (SPE) the Bose fields and their complex conjugates \( F, F^* \) etc. are treated as independent variables and we replace \( F^* \to \bar{F} \) etc. to indicate that the saddle point values of \( F \) and \( \bar{F} \) etc. are in general not complex conjugate fields.

The functional derivatives of the effective action \( S_{\text{eff}} \) involve single electron propagators which we abbreviate as \( (i, j = f \text{ or } c) \)

\[
G_{ij}(\tau, \tau') \equiv -\langle i < \mid \partial \otimes \mathcal{1}_e + 1_{\tau} \otimes \mathcal{h}_0 + \mathcal{h}_1 \rangle^{-1} \mid j > \rangle \tag{20}
\]

which obey the usual fermionic boundary conditions. As the factor \( e^{\beta \lambda} Z_0^h(\lambda) \) is independent of the Bose fields the SPE from the derivatives with respect to the Bose fields read

\[
0 = \frac{\delta S_{\text{eff}}}{\delta b(\tau)} = (\partial_\tau + \lambda)b(\tau) + N_f V G_{fc}(\tau, \tau) \tag{21}
\]

\[
0 = \frac{\delta S_{\text{eff}}}{\delta \bar{b}(\tau)} = (\partial_\tau + \lambda)\bar{b}(\tau) + N_f V G_{cf}(\tau, \tau) \tag{22}
\]

\[
0 = \frac{\delta S_{\text{eff}}}{\delta X(\tau, \tau')} = -\frac{\bar{X}(\tau, \tau')}{G_h^0(\tau - \tau')} + N_f V G_{cf}(\tau', \tau) \tag{23}
\]

\[
0 = \frac{\delta S_{\text{eff}}}{\delta \bar{X}(\tau, \tau')} = -\frac{\bar{X}(\tau, \tau')}{G_h^0(\tau - \tau')} + N_f V G_{cf}(\tau', \tau) \tag{24}
\]

\[
0 = \frac{\delta S_{\text{eff}}}{\delta F(\tau, \tau')} = -\frac{\bar{F}(\tau, \tau')}{G_h^0(\tau - \tau')} + N_f V G_{cc}(\tau', \tau) \tag{25}
\]

\[
0 = \frac{\delta S_{\text{eff}}}{\delta \bar{F}(\tau, \tau')} = -\frac{F(\tau, \tau')}{G_h^0(\tau - \tau')} + N_f V G_{ff}(\tau') \tag{26}
\]

The generalization of the static approximation in the \( U = \infty \) case amounts to search for solutions with "time"-translational invariance, i.e. the two-time Bose fields depend on the "time"-difference only, while \( b \) and \( \bar{b} \) are constant. This yields the equations

\[
- \lambda b = N_f V G_{fc}(0) \tag{27}
\]

\[
- \bar{b} = N_f V G_{cf}(0) \tag{28}
\]

\[
\bar{X}(\tau - \tau') = N_f V G_h^0(\tau - \tau')G_{fc}(\tau' - \tau) \tag{29}
\]

\[
X(\tau - \tau') = N_f V G_h^0(\tau - \tau')G_{cf}(\tau' - \tau) \tag{30}
\]

\[
\bar{F}(\tau - \tau') = N_f V G_h^0(\tau - \tau')G_{cc}(\tau' - \tau) \tag{31}
\]

\[
F(\tau - \tau') = N_f V G_h^0(\tau - \tau')G_{ff}(\tau' - \tau) \tag{32}
\]

In the SPE from the constraint variable \( \lambda \) we have also to take into account the \( \lambda \)-dependence of the integrand in \( \{13\} \) not contained in \( S_{\text{eff}} \). As we are interested in the low temperature regime the partition function \( Z_h^0(\lambda) \) can be approximated by 1, but the factor \( e^{\beta \lambda} \) has to be kept. This yields

\[
0 = \frac{\delta (S_{\text{eff}} - \beta \lambda)}{\delta \lambda} \tag{33}
\]

\[
= - \int \bar{b}(\tau_1)b(\tau_1)d\tau - N_f \int G_{ff}(\tau, \tau + 0)d\tau - \beta
\]

\[
+ \int (X(\tau_1, \tau_2)\bar{X}(\tau_1, \tau_2) + (\bar{F}(\tau_1, \tau_2)\bar{F}(\tau_1, \tau_2))\frac{\partial}{\partial \lambda}(1/G_h^0(\tau_1 - \tau_2))d\tau_1 d\tau_2
\]
Using Eqn. (27-32) this SPE reads \((n_f)_{ps} = N_fG_{ff}(-0))\)

\[ |b|^2 + (n_f)_{ps} + A = 1 \quad (34) \]

where \(A\) is given by \((\bar{V}^2 \equiv N_fV^2)\)

\[ A = \bar{V}^2 \int d\tau [N_fG_{fe}(-\tau)G_{cf}(-\tau) + N_fG_{ff}(-\tau)G_{cc}(-\tau)] \frac{\partial}{\partial \lambda} G^0_{hf}(\tau) \quad (35) \]

As will be shown in appendix C, \(A\) presents the probability for the double occupancy of the \(f\)-level. To solve the SPE (27-32) and (34) we write the propagators as Fourier series

\[ G^0_{hf}(\tau - \tau') = \frac{1}{\beta} \sum_m e^{-\mu_m(\tau - \tau')} G^0_{hf}(i\mu_m) \quad (36) \]

\[ G_{ij}(\tau' - \tau) = \frac{1}{\beta} \sum_n e^{-i\omega_n(\tau' - \tau)} G_{ij}(i\omega_n) \quad (37) \]

where the Matsubara frequencies \(\nu_m = 2\pi m/\beta\hbar, m \in \mathbb{Z}\) are of the Bose type, while the \(\omega_n = 2\pi(n+1)/\beta\hbar, n \in \mathbb{Z}\) are fermionic frequencies. Then Eqns. (27-32) lead to equations for the Fourier coefficients, e.g.

\[ \tilde{X}(i\omega_n) = N_fV \frac{1}{\beta} \sum_m G^0_{hf}(i\nu_m) G_{fe}(i\nu_m - i\omega_n) \quad (38) \]

and corresponding equations for the other Bose fields. To calculate the \(G_{ij}(i\omega_n)\) one has to calculate the resolvent of the one electron operator \(h(i\omega_n) \equiv h_0 + h_1(i\omega_n)\)

\[ G_{ij}(i\omega_n) = \langle i | (i\omega_n - h(i\omega_n))^{-1} | j \rangle \quad (39) \]

The inversion is straightforward using a partitioning technique with the projector \(P = |f><f|\). With

\[ G^{00}_{cc}(z) \equiv \langle c | (z - h_0^M)^{-1} | c \rangle \quad (40) \]

and

\[ G^0_{cc}(i\omega_n) \equiv G^{00}_{cc}(i\omega_n)/(1 - VF(i\omega_n)G^{00}_{cc}(i\omega_n)) \quad (41) \]

the result for the \(f\)-propagator is given by \((\bar{\varepsilon}_f \equiv \varepsilon_f + \lambda)\)

\[ G_{ff}(i\omega_n) = [i\omega_n - \bar{\varepsilon}_f - V\bar{F}(i\omega_n) - V^2(b + \tilde{X}(i\omega_n))G^0_{cc}(i\omega_n)(\bar{b} + X(i\omega_n))]^{-1} \quad (42) \]

The other resolvent matrix elements are

\[ G_{cf}(i\omega_n) = G^{00}_{cc}(i\omega_n)V(\bar{b} + X(i\omega_n))G_{ff}(i\omega_n), \quad (43) \]

\[ G_{fc}(i\omega_n) = G^{00}_{ff}(i\omega_n)V(b + X(i\omega_n))G^0_{cc}(i\omega_n), \quad (44) \]

\[ G_{cc}(i\omega_n) = G^{00}_{cc}(i\omega_n) + G_{cf}(i\omega_n)V(b + \tilde{X}(i\omega_n)) \quad (45) \]

Alternatively \(G_{cc}\) can be written in the form

\[ G_{cc}(i\omega_n) = (i\omega_n - \bar{\varepsilon}_f - V\bar{F}(i\omega_n))G_{ff}(i\omega_n)G^0_{cc}(i\omega_n) \quad (46) \]

In the following we study the solution of the SPE with \(b, \bar{b}\) different from zero and define
\[ \bar{x}(i\omega_n) \equiv \bar{X}(i\omega_n)/b \]  
\[ x(i\omega_n) \equiv X(i\omega_n)/b \]  

Then the SPE (53, 55) take the form

\[ -\lambda = \tilde{V}^2 \frac{1}{\beta} \sum_n G_{ff}(i\omega_n) G_{00}(i\omega_n)(1 + \bar{x}(i\omega_n)) \]  
\[ \bar{x}(i\omega_n) = \tilde{V}^2 \frac{1}{\beta} \sum_m G_{00}(i\nu_m) G_{ff}(i\nu_m - i\omega_n) G_{00}(i\nu_m - i\omega_n) (1 + \bar{x}(i\nu_m - i\omega_n)) \]  
\[ V\bar{F}(i\omega_n) = \tilde{V}^2 \frac{1}{\beta} \sum_m G_{00}(i\nu_m) G_{00}(i\nu_m - i\omega_n) (i\nu_m - i\omega_n - \bar{\varepsilon}_f - V\bar{F}(i\nu_m - i\omega_n)) G_{ff}(i\nu_m - i\omega_n) \]  
\[ VF(i\omega_n) = \tilde{V}^2 \frac{1}{\beta} \sum_m G_{00}(i\nu_m) G_{ff}(i\nu_m - i\omega_n) \]  

The equations following from (28) and (30) involve \( x(i\omega_n) \). Comparing with Eqns. (49) and (50) leads to the identity \( \bar{x}(i\omega_n) = x(i\omega_n) \), i.e., we can drop the additional equations. Together with (50) the Eqns. (51-52) determine the Bose fields at the saddle point.

In order to obtain a first understanding of these equations we start with a discussion of the limit \( N_f \to \infty \). It is easy to see that it is consistent to assume that \( \bar{x}(i\omega_n), V\bar{F}(i\omega_n) \) and \( VF(i\omega_n) \) are of order unity in the limit \( N_f \to \infty \) with \( \tilde{V} \) constant. This implies

\[ G_{ff}(i\omega_n) \xrightarrow{N_f\to\infty} (i\omega_n - \bar{\varepsilon}_f - V\bar{F}(i\omega_n))^{-1} \equiv G_{ff}^0(i\omega_n) \]  

and \( G_{cc}(i\omega_n) \to G_{cc}^0(i\omega_n) \). This simplifies Eqns. (52) and (51) for \( F(i\omega_n) \) and \( F(i\omega_n) \)

\[ V\bar{F}(i\omega_n) = \tilde{V}^2 \frac{1}{\beta} \sum_m \frac{1}{[i\nu_m - (2\varepsilon_f + U + \lambda)]} \cdot \frac{1}{[i\nu_m - i\omega_n - \bar{\varepsilon}_f - V\bar{F}(i\nu_m - i\omega_n)]} \]  
\[ VF(i\omega_n) = \tilde{V}^2 \frac{1}{\beta} \sum_m \frac{1}{[i\nu_m - (2\varepsilon_f + U + \lambda)]} \cdot \frac{1}{[(G_{cc}^0(i\nu_m - i\omega_n))^{-1} - V\bar{F}(i\nu_m - i\omega_n)]} \]  

which now constitute a closed system of equations for a given value of \( \lambda \). At this point it is necessary to discuss the strategy to solve the SPE for the Fourier components. Guided by results of an expansion in powers of \( 1/U \) we will assume that an analytic continuation \( F(i\omega_n) \to F(z) \) etc. is possible, with \( F(z) \) etc. analytic functions except at (parts of) the real axis. As \( F \) and \( F \) are of order \( 1/U \) the leading order result for \( VF(i\omega_n) \) is obtained by neglecting \( V\bar{F}(i\nu_m - i\omega_n) \) in the denominator in Eqn. (54). Then the Matsubara sum can be performed in the usual way by contour integration and one obtains

\[ VF(i\omega_n) = \tilde{V}^2 \sum_n \frac{f(\varepsilon_f + \lambda)}{i\omega_n - \varepsilon_f - U} \]  

where \( f(\varepsilon) \) is the Bose function and \( n_-(\varepsilon) \) is the Fermi function. The leading order result for \( V\bar{F}(i\omega_n) \) is
\[ V F_0(i\omega_n) = \int \frac{|\tilde{V}(\varepsilon)|^2 (n_-(2\varepsilon_f + U + \lambda) + f(\varepsilon))}{i\omega_n + \varepsilon - (2\varepsilon_f + U + \lambda)} d\varepsilon \]  

(57)

To this order the analytical continuation is trivial and has the properties discussed above. In the low temperature limit the Bose functions at \( \tilde{\varepsilon}_U \equiv 2\varepsilon_f + U + \lambda \) can be neglected. At \( T = 0 \) the function \( V F_0(z) \) has a branch cut from \( \tilde{\varepsilon}_U \) to \( \tilde{\varepsilon}_U + B \). For the solution of Eqsns. (54, 55) for arbitrary \( U \) we now assume the spectral representations \( (i = c, f) \)

\[ G_{ii}^{(0)}(i\omega_n) = \int \frac{\rho_{ii}^{(0)}(\varepsilon)}{i\omega_n - \varepsilon} d\varepsilon \]  

(58)

Performing the Matsubara sums in Eqn. (54, 55) yields after analytic continuation

\[ V F(z) = \tilde{V}^2 \int \frac{\rho_{ff}^{(0)}(\varepsilon)(f(\varepsilon) + n_-(\tilde{\varepsilon}_U))}{z + \varepsilon - \tilde{\varepsilon}_U} d\varepsilon \]  

(59)

\[ V \tilde{F}(z) = \tilde{V}^2 \int \frac{\rho_{cc}^{(0)}(\varepsilon)(f(\varepsilon) + n_-(\tilde{\varepsilon}_U))}{z + \varepsilon - \tilde{\varepsilon}_U} d\varepsilon \]  

(60)

Together with Eqn. (53) and \( G_{ff}^{(0)}(z)^{-1} = G_{cc}^{(0)}(z)^{-1} - V F(z) \) this constitutes a system of integral equations for the spectral weight functions \( \rho_{ff}^{(0)} \) and \( \rho_{cc}^{(0)} \). As the finite temperature theory will be discussed later for arbitrary \( N_f \) we restrict ourselves here to the limit \( T \to 0 \). At the saddle point value of \( \lambda \) one expects \( \rho_{ff}^{(0)}(\varepsilon) \) to vanish for \( \varepsilon < \varepsilon_F \) as in the \( U = \infty \) case.\( ^3 \) In addition to the Kondo peak slightly above the Fermi energy \( \varepsilon_F = 0 \), \( \rho_{ff}^{(0)}(\varepsilon) \) has an \( f^2 \) contribution above \( \tilde{\varepsilon}_U \), as can be inferred form Eqn. (63). Therefore the integrand on the rhs of Eqn. (59) vanishes, i.e. \( V F(z) \equiv 0 \) at \( T = 0 \) in the limit \( N_f \to \infty \). This leads to \( G_{cc}^{(0)}(z) = G_{cc}^{(0)}(z) \) and

\[ G_{ff}^{(0)}(z) = (z - \tilde{\varepsilon}_f + \tilde{\Gamma}(2\varepsilon_f + U + \lambda - z))^{-1} \]  

(61)

with \( \tilde{\Gamma}(z) \) defined in (A.6).

For \( T \to 0 \) and \( N_f \to \infty \) Eqsns. (54) and (55) then simplify to

\[ -\lambda = \int_{-\tilde{B}}^{\tilde{B'}} |\tilde{V}(\varepsilon)|^2 1 \beta \sum_n \frac{1}{i\omega_n - \tilde{\varepsilon}_f + \tilde{\Gamma}(\tilde{\varepsilon}_U - i\omega_n)} \frac{1 + \tilde{x}(i\omega_n)}{(i\omega_n - \varepsilon)} d\varepsilon \]  

(62)

\[ \tilde{x}(i\omega_n) = \int_{-\tilde{B}}^{\tilde{B'}} |\tilde{V}(\varepsilon)|^2 1 \beta \sum_m \frac{1}{i\nu_m - \tilde{\varepsilon}_U} \frac{1}{[i\nu_m - i\omega_n - \tilde{\varepsilon}_f + \tilde{\Gamma}(\tilde{\varepsilon}_U - i\nu_m + i\omega_n)]} \frac{1 + \tilde{x}(i\nu_m - i\omega_n)}{(i\nu_m - i\omega_n - \varepsilon)} d\varepsilon \]  

(63)

In order to perform the Matsubara sums by contour integration it is necessary to analytically continue the Fourier coefficients \( \tilde{x}(i\omega_n) \). A useful guide is again to first calculate \( \tilde{x}(i\omega_n) \) to leading order in \( 1/U \), which amounts to iterate Eqn. (53). This calculation shows that \( \tilde{x}(i\omega_n) \) can be analytically continued and at \( T = 0 \) has a branch cut from \( \tilde{\varepsilon}_U \) to \( \tilde{\varepsilon}_U + B \). To evaluate the Matsubara sums in (62) we therefore assume that \( \tilde{x}(z) \) has a spectral representation with a branch cut starting at a positive
energy value. Then for $T \to 0$ only the last pole term on the rhs of (62, 63) contributes to the contour integral and one obtains after analytic continuation

$$-\lambda = \int_{-B}^{0} \frac{|V(\varepsilon)|^2 (1 + \bar{x}(\varepsilon))}{\varepsilon - \varepsilon_f - \lambda + \Gamma(2\varepsilon_f + U + \lambda - \varepsilon)} d\varepsilon$$

(64)

$$\bar{x}(z) = -\int_{-B}^{0} \frac{|V(\varepsilon)|^2 (1 + \bar{x}(\varepsilon))}{(2\varepsilon_f + U + \lambda - \varepsilon - z)[\varepsilon - \varepsilon_f - \lambda + \Gamma(2\varepsilon_f + U + \lambda - \varepsilon)]} d\varepsilon$$

(65)

If $z$ is chosen on the real axis $-B < Re z < 0$ the second equation is an integral equation for $\bar{x}(\varepsilon)$ with $\varepsilon \in [-B, 0]$ which together with (64) determines $\lambda$. With the identification $\bar{x}(\varepsilon) \leftrightarrow c(\varepsilon)$ and $\lambda \leftrightarrow -\Delta E$ these are exactly the equations which occur in the description of the ground state in the limit $N_f \to \infty$. This is discussed in appendix A. A direct proof for the relation $-\lambda = \Delta E$ valid at $T = 0$ in the limit $N_f \to \infty$ is presented in appendix B.

After this discussion of the limit $N_f \to \infty$ we return to the full SPE (40, 52) for finite values of $N_f$. We use the same strategy as for the solution of Equs. (54, 55) and assume that the Greens functions $\hat{G}_{ij}(i\omega_n)$ can be analytically continued, and as a function of the complex variable $z$ are analytic expect at (parts of) the real axis. This implies the spectral representation

$$\hat{G}_{ij}(z) = \int_{-\infty}^{\infty} \frac{\rho_{ij}(\varepsilon)}{z - \varepsilon} d\varepsilon$$

(66)

Using these spectral representations the Matsubara sums in Equs. (40, 52) can easily be performed. If we also introduce the functions $R_{ij}(z)$,

$$R_{ij}(z) = \int_{-\infty}^{\infty} \frac{\rho_{ij}(\varepsilon)f(\varepsilon)}{z - \varepsilon} d\varepsilon$$

(67)

we obtain

$$VF(z) = -\tilde{V}^2[n_-(\tilde{\varepsilon}_U)G_{ff}(\tilde{\varepsilon}_U - z) + R_{ff}(\tilde{\varepsilon}_U - z)]$$

(68)

$$\tilde{V} F(z) = -\tilde{V}^2[n_-(\tilde{\varepsilon}_U)G_{cc}(\tilde{\varepsilon}_U - z) + R_{cc}(\tilde{\varepsilon}_U - z)]$$

(69)

$$X(z) = -N_f V[n_-(\tilde{\varepsilon}_U)G_{cf}(\tilde{\varepsilon}_U - z) + R_{cf}(\tilde{\varepsilon}_U - z)]$$

(70)

Therefore $F$, $\tilde{F}$ and $X$ are also analytic except at the real axis and can also be expressed in terms spectral functions $\rho_F(x)$, $\rho_{\tilde{F}}(x)$ and $\rho_X(x)$. Together with the relations (42, 43) the equations (68-70) provide a set of nonlinear integral equations for these spectral functions for given values of $\lambda$ and $b$. In order to determine the saddle point values of $\lambda$ and $b$ we in addition have to use equation (49) and the constraint relations (54) which was irrelevant in the limit $N_f \to \infty$. Using the spectral representation (64) the probability for double occupancy $A$ (43) can be expressed in terms of the spectral functions. For temperatures $k_B T \ll \tilde{\varepsilon}_U$ one obtains

$$A = (N_f V)^2 \int d\varepsilon d\varepsilon' \frac{\rho_{ff}(\varepsilon)\rho_{cc}(\varepsilon') + \rho_{fc}(\varepsilon)\rho_{cf}(\varepsilon')}{(\tilde{\varepsilon}_U - \varepsilon - \varepsilon')^2} f(\varepsilon)f(\varepsilon')$$

(71)

The numerical solutions of the coupled system of equations is described in the next section.
IV. NUMERICAL SOLUTION OF THE SADDLE POINT EQUATIONS

In this section we present an outline of our numerical procedure to solve the SPE for a given band density of states, which determines the unperturbed band propagator $G_{cc}^{00}$. The equations (68-70) provide relations between the spectral functions $\rho_K(\varepsilon)$ with $K \in \{F, \bar{F}, X\}$ and the spectral functions $\rho_{ij}(\varepsilon)$ with $i, j \in \{f, c\}$. For $k_B T \ll \tilde{\varepsilon}_U$ they read

$$\rho_F(\varepsilon) = N_f V \rho_{ff}(\tilde{\varepsilon}_U - \varepsilon) f(\tilde{\varepsilon}_U - \varepsilon)$$  

$$\rho_{\bar{F}}(\varepsilon) = N_f V \rho_{cc}(\tilde{\varepsilon}_U - \varepsilon) f(\tilde{\varepsilon}_U - \varepsilon)$$  

$$\rho_X(\varepsilon) = -N_f V \rho_{fc}(\tilde{\varepsilon}_U - \varepsilon) f(\tilde{\varepsilon}_U - \varepsilon)$$

We solve the SPE iteratively using e.g. the results for $N_f \to \infty$ discussed in section III as the starting values for the $\rho_K$, $\lambda$, and $b$. From the $\rho_K$ we calculate the functions $\tilde{K}(\varepsilon + i0)$, which via equations (42-45) determine the propagators $G_{ij}(\varepsilon + i0)$ and their spectral functions $\rho_{ij}(\varepsilon)$. Using equations (72-74) we obtain new spectral functions $\rho_K(\varepsilon)$. The constraint relation (34) involves the pseudo $f$-occupancy $(n_f)_{ps}$

$$(n_f)_{ps} = N_f \int \rho_{ff}(\varepsilon) f(\varepsilon) d\varepsilon$$

and the probability for double occupancy $A$, which we evaluate using (71) and (72-74)

$$A = \int d\varepsilon d\varepsilon' \rho_F(\varepsilon) \rho_{\bar{F}}(\varepsilon') + \rho_X(\varepsilon) \rho_X(\varepsilon') f(\varepsilon) f(\varepsilon')$$

In order to obtain a numerically stable method to determine new values of $\lambda$ and $b$ we treat equations (34) and (27)

$$1 - (n_f)_{ps} - A - b^2 = 0$$

$$\lambda b + N_f V \int \rho_{fc}(\varepsilon) f(\varepsilon) d\varepsilon = 0$$

as a two dimensional system of equations and solve it by Newton’s method. We then go to the beginning of the loop and terminate the iterative procedure when the relative change of all propagators is less than $10^{-4}$ and $\lambda$ and $b$ solve (77) and (78) with an error less then $10^{-3}$. For the functions $\rho_K(\varepsilon)$ we usually used a 500 points logarithmic mesh, which was implemented by logarithmic submeshes to resolve characteristic features such as band edges.

In our calculations we used a semielliptical band density of states $2\sqrt{B^2 - \varepsilon^2}/\pi B^2$ with $B = 6$. The numerical results presented in this paper are restricted to the zero temperature limit. Compared to the $U = \infty$ limit the spectral functions $\rho_K$ corresponding to the two time auxiliary fields provide a new input for the calculation of the pseudo $f$-Greensfunction, which is given by $G_{ff}$. In figure 1 we show the spectral functions...
$\rho_f, \rho_F$, and $\rho_X$ for $N_f = 14$, $\varepsilon_f = -2.5$, $U = 8$ and $\Delta = 2V^2/B = 2.67$. The spectral functions are zero for energies less than $\tilde{\varepsilon}_U \equiv 2\varepsilon_f + \lambda + U \approx 6.25$ which is determined by $\lambda_{SP} \approx 3.25$. In the following the subscripts $SP$ will be dropped. These spectral functions together with $\lambda$ and $b$ determine the pseudo $f$-spectral function $(\rho_{ff})_{ps} \equiv \rho_{ff}$ defined in (60) which is shown in fig. 2. The main spectral feature is the “Kondo - peak” slightly above the chemical potential taken as the zero of energy. As can already be seen in the limit $N_f \to \infty$ (53) and discussed in detail in (54) the peak position is not given by $\varepsilon_f + \lambda$ as (for a flat band density of states) in the $U = \infty$ limit. There is additional spectral weight in the interval $[\tilde{\varepsilon}_U, \tilde{\varepsilon}_U + B]$ which is magnified in the inset of the figure. This is $f^2$ - weight is very small for the pseudo $f$ - spectral function, while it is large for the real $f$ - spectral function as discussed in references 13 and 11. The real $f$ - spectral function $(\rho_{ff})_{real}$ in the saddle point approximation consists of one contribution $|b|^2(\rho_{ff}(\varepsilon))_{ps}$, i.e. the Kondo peak position in $(\rho_{ff})_{real}$ is determined by the peak position in $(\rho_{ff})_{ps}$. There are additional terms in the expression for the real $f$ - Greens function (51) which are responsible for the large $f^2$ - weight in $(\rho_{ff})_{real}$.

The spectral functions $\rho_{cc}(\varepsilon)$ and $\rho_{fc}(\varepsilon)$ are shown in fig. 3. This dip in $\rho_{cc}(\varepsilon)$ at the position of the Kondo peak is readily understood from Eqn. (14). The occupancies $\langle P_n \rangle$ for the parameter values used in figs. 1-3 are $\langle P_0 \rangle = 0.144, \langle P_1 \rangle = 0.792, \langle P_2 \rangle = 0.063$. This corresponds to the real $f$ - occupancy $(n_f)_{real} = \langle P_1 \rangle = 2\langle P_2 \rangle = 0.92$.

The results shown so far correspond to $N_f = 14$, i.e. the large $f$ - degeneracy obtained by neglecting spin - orbit and crystal field splitting. As there are no exact results available for the model for arbitrary $N_f$ and $U$ the deviation of the the SPE results from the exact ones cannot be judged. A very stringent test of the quality of the saddle point results can be made for the most interesting value $N_f = 2$ of the degeneracy, i.e. the spindegenerate model, where exact results are available as discussed in the introduction. As the SPE provide the exact solution in the limit of infinite degeneracy one can hardly expect reliable results down to $N_f = 2$. The exact solution for $N_f = 2$ in the symmetric case $2\varepsilon_f + U = 0$ and a symmetric half-filled band has particle-hole symmetry, which leads to $\langle P_0 \rangle = \langle P_2 \rangle$ and a symmetric real $f$ - spectral function, i.e. the Kondo peak is located at the energy zero. In our approach the $f^0$ and the $f^2$ subspaces are treated in completely different ways and we there cannot expect the solution of the SPE for the symmetric $N_f = 2$ case to obey particle - hole symmetry. To test how well the behavior from the exact solution is reproduced by the solution of the SPE we show in fig. 4 we the probabilities $\langle P_n \rangle$ for $N_f = 2, \varepsilon_f = -2.5$ and $\Delta = 2.67$ as a function of $U$ for $U > 5$. In the exact solution the crossing between $\langle P_0 \rangle$ and $\langle P_2 \rangle$ curves occurs at $U = 5$, while the SPE crossing ist at $U = 5.4$. If one has symmetric parameters $2\varepsilon_f + U$ but $N_f > 2$ the exact Kondo peak lies at a small positive energy and its position for $N_f \to \infty$ is given by...
the solution of the SPE. While the peak position of the exact solution is only defined for integer values of $N_f$ we can study the peak position from the SPE as a continuous function of $N_f$. This is shown in fig. 6 for $\varepsilon_f = -2.5$, $U = 5$ and $\Delta = 1.33$. With the degeneracy approaching $N_f = 2$ the Kondo peak approaches zero, but does not quite reach it.

The results shown in figs. 5 and 6 indicate that the SPE are quite good even for rather small values of the degeneracy. A more detailed presentation of results for thermodynamic properties and the real $f$-spectral functions also at finite temperatures will be presented in a forthcoming publication.

V. SUMMARY

The generalized mean field theory for the Anderson impurity model including double occupancy presented in this paper has filled a well known gap in the approximate treatments of this model. In contrast to the mean field theory for the $U = \infty$ model our new approximation cannot alternatively be obtained from a simple factorization of higher correlations. The use of the coherent state functional integral and the introduction of two time auxiliary fields seems necessary to obtain the correct structure in the large degeneracy limit. In the saddle point approximation the theory yields the exact result for the ground state in the limit $N_f \to \infty$. For large but finite $N_f$ the solution of the SPE is expected to provide a good approximation for temperatures small compared to the Kondo temperature. The spindegenerate limit cannot be reproduced exactly, as the theory treats the $f^0$ - and $f^2$ - subspaces in completely different ways. The presented mean field theory can be generalized in a rather straightforward way from the impurity to the lattice model.

APPENDIX A:

In this appendix we present a short but selfcontained derivation of the integral equation which has to be solved to obtain the exact ground state in the infinite degeneracy limit $^3$. This equation also describes the exact ground state for finite $N_f$ if the valence band is completely filled.

Let $|0\rangle$ be the state with all conduction states below the Fermi energy, $\varepsilon_F = 0$, filled and the $f$-level empty. This state couples via $H_A$ to the states

$$|\varepsilon\rangle = \frac{1}{\sqrt{N_f}} \sum_{\nu} f_{\nu}^+ c_{\varepsilon\nu} |0\rangle,$$  \hspace{1cm} (A1)

in which one conduction electron below $\varepsilon_F$ has hopped into the $f$-level. These states couple to states in which the $f$-level is doubly occupied









as well as to states with the $f$-level empty and a particle hole-pair in the conduction band. The coupling to the latter states is smaller by a factor $1/\sqrt{N_f}$ and can therefore be neglected in the large $N_f$ limit. In this limit the ground state takes the form

$$ |\phi_0 \rangle = A \left[ |0\rangle + \int_{-B}^{0} d\varepsilon \, a(\varepsilon) |\varepsilon\rangle + \int_{B}^{0} d\varepsilon \int_{-B}^{\varepsilon} d\varepsilon' b(\varepsilon, \varepsilon') |\varepsilon, \varepsilon'\rangle \right] \quad (A3) $$

where $A$ is the normalization constant. Inserting into the Schrödinger equation $H_A |\phi_0 \rangle = E |\phi_0 \rangle > b(\varepsilon, \varepsilon')$ can be simply expressed in terms of $a(\varepsilon)$ and $a(\varepsilon')$ and one obtains the equations

$$ \Delta E = \int_{-B}^{0} \tilde{V}(\varepsilon) a(\varepsilon) d\varepsilon, \quad (A4) $$

$$ \left[ \varepsilon_f - \varepsilon - \Delta E - (1 - \frac{1}{N_f}) \tilde{\Gamma}(2\varepsilon_f + U - \varepsilon - \Delta E) \right] a(\varepsilon) + \tilde{V}(\varepsilon) \left[ 1 - (1 - \frac{1}{N_f}) \int_{-B}^{0} 2\varepsilon_f + U - \varepsilon - \Delta E - \varepsilon_1 d\varepsilon_1 \right] = 0 \quad (A5) $$

where $\Delta E \equiv E_0 - <0 | H | 0>$, $\tilde{V}(\varepsilon) = \sqrt{N_f}V(\varepsilon)$ and

$$ \tilde{\Gamma}(z) = \int_{-B}^{0} \frac{\tilde{V}(\varepsilon)^2}{z - \varepsilon} \quad (A6) $$

In the derivation the matrix elements $<\varepsilon | H | 0>$ are used. For the comparison with the saddle point equations we define the function $c(\varepsilon)$ for $-B < \varepsilon < 0$ by

$$ a(\varepsilon) \equiv \tilde{V}(\varepsilon) \frac{1 + c(\varepsilon)}{\Delta E - \varepsilon_f + \varepsilon + (1 - \frac{1}{N_f}) \tilde{\Gamma}(2\varepsilon_f + U - \varepsilon - \Delta E)} \quad (A8) $$

Then equations (A4) and (A3) read

$$ \Delta E = \int_{-B}^{0} \frac{|\tilde{V}(\varepsilon)|^2 \left(1 + c(\varepsilon)\right)}{\Delta E - \varepsilon_f + \varepsilon + (1 - \frac{1}{N_f}) \tilde{\Gamma}(2\varepsilon_f + U - \varepsilon - \Delta E)} \quad (A9) $$

$$ c(\varepsilon) + \int_{-B}^{0} \frac{1}{(2\varepsilon_f + U - \varepsilon - \Delta E - \varepsilon_1) \Delta E - \varepsilon_f + \varepsilon_1 + \tilde{\Gamma}(2\varepsilon_f + U - \varepsilon_1 - \Delta E)} d\varepsilon_1 = 0 \quad (A10) $$

In the limit $\varepsilon_f + U >> B$ the integral equation (A10) is of separable form. The function $c(\varepsilon)$ for $-B < \varepsilon < 0$ can be analytically continued using Eqn. (A10). Then $c(z)$ has a branch cut on the real axis from $2\varepsilon_f + U - \Delta E$ to $2\varepsilon_f + U - \Delta E + B$. The saddle point equations reduce at $T = 0$ in the large degeneracy limit to Eqn. (A9) and (A10) if one identifies $c(\varepsilon)$ with $\tilde{x}(\varepsilon)$ and $\Delta E$ with $-\lambda$. 

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APPENDIX B:

In this appendix we derive the expression for the grand canonical potential at the saddle point \( J_{SP} \) and discuss how it simplifies in the limit \( N_f \rightarrow \infty \).

We begin with the evaluation of the last term on the rhs of Eqn. \((17)\) for the effective action \( S_{eff} \). At the saddle point the fields \( F, F, X, \) \( \bar{X} \) depend on the time difference only and the "time-part" of the trace can be written as a sum over the fermionic Matsubara frequencies. If we denote the unperturbed propagators in accordance with Eq. \((10)\) as \( G^{00}(i\omega_n) \) we have to evaluate \( \text{tr} \ln [1 - G^{00}h_1] \) where the "small trace" runs over the one electron Hilbert space. We use \( \text{tr} \ln \hat{\alpha} = \ln \text{det} \hat{\alpha} \) as the determinant is easily calculated using the special form of \( h_1 \) \((13)\)

\[
\det(1 - G^{00}(i\omega_n)h_1(i\omega_n)) = (1 - f | G^{00} | f > V F)(1 - c | G^{00} | c > V F) - V^2(b + X) < c | G^{00} | c > (b + \bar{X}) < f | G^{00} | f >
\]

\[
= 1 - V F(i\omega_n)G^{cc}_{00}(i\omega_n) - V F(i\omega_n)G^{cc}_{00}(i\omega_n) = 1 - V F(i\omega_n)G^{cc}_{00}(i\omega_n)
\]

(B1)

In the second equality we have used \((11)\) and \((12)\). The Matsubara sum is now performed as a contour integral using the assumptions about the analytic continuation of the auxiliary fields discussed in section II. This yields

\[
-I = N_f Tr \ln[\partial \otimes 1_c + 1_c \otimes h_0 + h_1] |_{SP} = J_M^0 + J_f^0 + (\Delta J)_1
\]

(B2)

with

\[
(\Delta J)_1 = N_f \int \frac{d\varepsilon}{2\pi i} f(\varepsilon) \left\{ \ln \left[ \frac{1 - V F(\varepsilon + i0)G^{cc}_{00}(\varepsilon + i0)}{1 - V F(\varepsilon - i0)G^{cc}_{00}(\varepsilon - i0)} \right] + \ln \left[ \frac{(\varepsilon - \varepsilon_f + i0)G_{ff}(\varepsilon - i0)}{\varepsilon - \varepsilon_f + i0} \right] \right\}
\]

(B3)

and \( J_M^0 + J_f^0 \) the grand canonical potential for a system noninteracting electrons described by \( h_0 \).

If we denote the double integral on the rhs of \((17)\) by \( \beta I \) we obtain using the SPE

\[
I = N_f V \int \frac{d\varepsilon}{2\pi i} f(\varepsilon) | (FG_{cc} + XG_{fc})_{\varepsilon - i0} - (FG_{cc} + XG_{fc})_{\varepsilon + i0} | \]

(B4)

Using \((14)\) with \( Z_h^h(\lambda) \approx 1 \) for the interesting temperature regime we finally obtain

\[
J_{SPA} = J_M^0 + J_f^0 + (\Delta J)_1 - I + \lambda | b |^2 - \lambda
\]

(B5)

For \( T \rightarrow 0 \) this expression simplifies considerably in the large \( N_f \) limit. Then \( VF \) and \( G_{ff} - G_{ff}^0 \) are of order \( 1/N_f \) and the logarithms in \((B3)\) can be expanded. To the same order in \( 1/N_f \) the Greens functions in \((B4)\) can be replaced by the unperturbed functions \( G^{cc}_{cc} \) and \( G^{cc}_{fc} \). Then in order \( 1/N_f^0 \) all terms in the expression for \( J_{SPA} \) cancel except the first and the last one. With \( E_0^{(0)} \equiv < 0 | H | 0 > \) this yields

\[
(E_0)^{SPA} = E_0^{(0)} - \lambda
\]

(B6)

as mentioned following Eqn. \((54-55)\).
APPENDIX C:

In this appendix we discuss how the "real $f$-occupancy" in the saddle point approximation $\langle n_f \rangle_{\text{real}}^{\text{SPA}}$ can be expressed in terms of the "pseudo-$f$-occupancy" $\langle n_f \rangle_{\text{ps}}^{\text{SPA}} = N_f G_{ff}^{\text{SPA}}(\tau = 0)$. The calculation shows that the constant $A$ defined following Eq. (34) presents the probability for the double occupancy of the $f$-level.

The real $f$-occupancy can be calculated from the grand canonical potential $J = -\ln Z/\beta$ with $Z$ defined in (6) by differentiation with respect to the $f$-level energy $\varepsilon_f$

$$\langle n_f \rangle_{\text{real}} = \frac{\partial J}{\partial \varepsilon_f}$$

(C1)

In the SPA the grand canonical potential is given in (B5). With $h \equiv h_0 + h_1$ given in (18-19) we obtain

$$J_{\text{SPA}} = -\left(\frac{N_f}{\beta}\right) \text{Tr} \ln(\partial + h) + I + \lambda(| b |^2 - 1) \equiv J_h - I + \lambda(| b |^2 - 1)$$

(C2)

In the following the label SPA at all fields and Greens functions will be suppressed. The contribution to $\langle n_f \rangle_{\text{real}}$ from the first term on the rhs of (C.2) is

$$\frac{\partial J_h}{\partial \varepsilon_f} = \left(\frac{N_f}{\beta}\right) \text{Tr}(G \frac{\partial h}{\partial \varepsilon_f})$$

(C3)

and with $h = 1_\tau \otimes h_0 + h_1$ given in (B4) we obtain

$$\frac{\partial J_h}{\partial \varepsilon_f} = \left(1 + \frac{\partial \lambda}{\partial \varepsilon_f}\right) \langle n_f \rangle_{\text{ps}} + \frac{1}{\beta} \left[ N_f V \text{tr}_\tau(G_{ff} \frac{\partial \bar{F}}{\partial \varepsilon_f}) + N_f V \text{tr}_\tau(G_{cf} \frac{\partial F}{\partial \varepsilon_f}) \right]$$

(C4)

where $\text{tr}_\tau$ denotes the "time"-integration part of the trace. Differentiating the double integral (B4) yields

$$\frac{\partial I}{\partial \varepsilon_f} = \frac{1}{\beta} \int d\tau d\tau' \left[ \frac{1}{G_0^{\text{SR}}(\tau - \tau')} \left\{ \frac{\partial \bar{X}(\tau - \tau')}{\partial \varepsilon_f} X(\tau - \tau') + \bar{X}(\tau - \tau') \frac{\partial X(\tau - \tau')}{\partial \varepsilon_f} \right\} + \frac{\partial \bar{F}(\tau - \tau')}{\partial \varepsilon_f} F(\tau - \tau') + \bar{F}(\tau - \tau') \frac{\partial F(\tau - \tau')}{\partial \varepsilon_f} \right] - (2 + \frac{\partial \lambda}{\partial \varepsilon_f}) A$$

(C5)

and from the last term on the rhs of (C.2) we obtain

$$\frac{\partial}{\partial \varepsilon_f}\lambda(| b |^2 - 1) = \frac{\partial \lambda}{\partial \varepsilon_f}(| b |^2 - 1) + \lambda(\frac{\partial \bar{b}}{\partial \varepsilon_f} + \bar{b} \frac{\partial b}{\partial \varepsilon_f})$$

(C6)

If we add up all contributions and use the SPE (27-32) and (34) we obtain the simple result

$$\langle n_f \rangle_{\text{real}} = \langle n_f \rangle_{\text{ps}} + 2A$$

(C7)

This suggests that $A$ is the probability for the double occupancy of the $f$-level. This is readily verified by calculating $\langle P_2 \rangle$, where $P_n$ is projection operator for
the $f$-level occupied by $n$ electrons. A calculation very similar to the one presented above yields in SPA

$$< P_2 > = \frac{\partial J}{\partial U} = A \quad \text{(C8)}$$

In the limit $N_f \to \infty$ and $T \to 0$ this identity can be explicitly checked using the results of appendix A and the expression for $< P_2 >$ presented in ref. 13. From (C.7) and (C.8) and $\sum_{n=0}^{\infty} < P_n > = 1$ we also obtain $< P_1 > = (n_f)_p$, and $< P_0 > = |b|^2$, which elucidates the meaning of the SPE (24).

The generalization of (C.8) beyond the SPA is given by using (16) to evaluate $\partial J/\partial U$. This yields

$$< P_2 > = \frac{1}{Z} \int_C \frac{\beta d\lambda}{2\pi i} e^{\beta \lambda} \int D\beta D\gamma DX \left( \int d\tau d\tau' |X(\tau, \tau')|^2 + |F(\tau, \tau')|^2 \frac{\partial}{\partial \lambda} G_h^0(\tau - \tau') \right) e^{-\beta S_{eff}} \quad \text{(C9)}$$

where we have taken $Z_h^0(\lambda) \approx 1$ as usual. If we take the $FI$ on the rhs of (C.9) as the generalized expression for $A$, equation (C.7) also holds generally.

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FIG. 1. The spectral functions $\rho_F$, $\rho_F$ and $\rho_X$ for $N_f = 14$, $\varepsilon_f = -2.5$, $U = 8$ and $\tilde{\Delta} = 2.67$.

FIG. 2. The pseudo $f$-spectral function $(\rho_{ff})_{ps}$. The inset shows the additional spectral weight in the interval $[\tilde{\varepsilon}_U, \tilde{\varepsilon}_U + B]$. The parameters are the same as in fig. 1.

FIG. 3. $\rho_{cc}(\varepsilon)$ and $\rho_{fc}(\varepsilon)$ are shown. The parameters are the same as in fig. 1.

The spectral functions

FIG. 4. The occupation probabilities $\langle P_n \rangle$ for $N_f = 2$, $\varepsilon_f = -2.5$ and $\tilde{\Delta} = 2.67$ as a function of $U$.

FIG. 5. The position of the Kondo peak as a function of $N_f$ for $\varepsilon_f = -2.5$, $U = 5$ and $\tilde{\Delta} = 1.33$. 

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Figure 1

\begin{center}
\includegraphics[width=\textwidth]{figure1.png}
\end{center}

Legend:
- $\rho_F$
- $\rho_F^r$
- $-\rho_X$
Figure 3

Graph showing two curves, one labeled $\rho_{cc}$ and the other $\rho_{cf}$, as functions of $\varepsilon$. The $\rho_{cc}$ curve is a smooth arch, while the $\rho_{cf}$ curve has a sharp peak at $\varepsilon = 0$ and decreases as $\varepsilon$ moves away from zero.
Figure 4
Figure 2
