An Enhanced Perturbational Study on Spectral Properties of the Anderson Model

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Abstract

The infinite-$U$ single impurity Anderson model for rare earth alloys is examined with a new set of self-consistent coupled integral equations, which can be embedded in the large $N$ expansion scheme ($N$ is the local spin degeneracy). The finite temperature impurity density of states (DOS) and the spin-fluctuation spectra are calculated exactly up to the order $O(1/N^2)$. The presented conserving approximation goes well beyond the $1/N$-approximation ($NCA$) and maintains local Fermi-liquid properties down to very low temperatures. The position of the low lying Abrikosov-Suhl resonance (ASR) in the impurity DOS is in accordance with Friedel’s sum rule. For $N = 2$ its shift toward the chemical potential, compared to the $NCA$, can be traced back to the influence of the vertex corrections. The width and height of the ASR is governed by the universal low temperature energy scale $T_K$. Temperature and degeneracy $N$-dependence of the static magnetic susceptibility is found in excellent agreement with the Bethe-Ansatz results. Threshold exponents of the local propagators are discussed. Resonant level regime ($N = 1$) and intermediate valence regime ($|\epsilon_f| < \Delta$) of the model are thoroughly investigated as a critical test of the quality of the approximation. Some applications
to the Anderson lattice model are pointed out.

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I. INTRODUCTION

Recently a major improvement has been reported on the perturbational approach to the single impurity Anderson-model (SIAM) with $N$-fold degenerate local state in the limit of infinitely large Coulomb repulsion $U$. The aim of this paper is to present in detail the results obtained so far with this so-called Post-NCA theory ($PNCA_\infty$). This approximation contains a resumation of infinite numbers of skeleton diagrams and is exact up to order $O(1/N^2)$. The skeleton diagrams included physically describe complicated multi-excitation processes.

The paper is organized as follows: in section 2, the large-$N$ expansion is used to derive the self-consistent coupled integral equation for the self-energies and the vertex-function. The physical processes included will be explained. In section 3 numerically obtained solutions for the local propagators will be presented and their threshold exponents related to results furnished by other methods. A detailed analysis of the one-particle spectra will be the topic of section 4 including a discussion of the Fermi-liquid properties and the impact of the vertex-corrections. In section 5, we will develop a theory of the magnetic vertex correction exact up to $O(1/N^3)$ and compare the calculated static magnetic susceptibility with the Bethe-Ansatz results. Spin-fluctuation spectra will also be covered. The two critical cases, the intermediate-valance and the resonant level case, will be thoroughly examined in section 6. In section 7, a summary and an outlook on further applications will be given.

II. THEORY

In direct perturbation theory a well established set of diagrammatical rules has been established to evaluate self-energy contributions to the local propagator $P_M(z)$. In Fig. the lowest order contributions up to $V^8$ to the self-energy $\Sigma_0(z)$ of propagator $P_0(z)$ of the un-occupied state are shown. Contributions (b) and (c) are one-particle irreducible but contain self-energy insertions and are already included in the skeleton diagram (a). In order
there exist only one skeleton diagram, whereas there are exactly two in order \( V^8 \). To include these higher order corrections, a well-established concept of vertex functions is used. In our case, a vertex function is defined by cutting the electron and the local propagator line at the uppermost vertex in each skeleton diagram and by summing up all contributions of the remaining lower parts of the skeletons. The concept of vertex-function has already been successfully applied in an NCA-theory (Non-Crossing-Approximation) for the finite-\( U \) Anderson model. The resulting dimension-less factor \( \Delta^f_m(x, y) \) renormalizes the bare hybridisation vertex \( V \) of an absorbed band electron in an energy dependent way; \( x \) is the ingoing and \( y \) the outgoing energy of the local propagator. The corresponding vertex-function \( \Delta^O_m(x, y) \) for an emitted band electron is obtained from the vertex function of an absorbed electron \( \Delta^f_m(x, y) \) by symmetry: \( \Delta^O_m(x, y) = \Delta^f_m(y, x) \). Therefore we only calculate \( \Delta_m(x, y) \equiv \Delta^f_m(x, y) \). In a formal way all skeleton diagrams are summed up by using the exact vertex-function in:

\[
\Sigma_0(z) = V^2 \sum_{km} f(\epsilon_k) \Delta_m(z, z + \epsilon_k) P_m(z + \epsilon_k) \\
\Sigma_m(z) = V^2 \sum_k f(-\epsilon_k) \Delta_m(z - \epsilon_k, z) P_m(z - \epsilon_k) .
\]

Approximations are made by the selection of contributions to \( \Delta_m \). The NCA, for example, is recovered by setting \( \Delta_m(x, y) = 1 \).

In order to derive the integral equation for the vertex function exactly up to \( O(1/N^2) \) the lower parts of the skeleton diagrams (d) and (e) have to be included in addition to skeleton diagram (a). Skeleton (f) can be neglected, since it is of the order \( O(1/N^3) \). The corresponding generating functional is shown diagrammatically in Fig. 3. An infinite number of skeletons are resummed by replacing the bare hybridisation vertex by the renormalized one \( V \cdot \Delta_m(x, y) \) in each diagram in order to include as many higher order terms as possible. This yields a self-consistent equation for the vertex function displayed in Fig. 4. In the case of zero magnetic field all \( P_m \) are equal, and the vertex function is reduced to
\[ \Delta(x, y) \equiv \Delta_m(x, y) = \\
1 - |V|^4 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} du dv \rho(u) \rho(v) f(u) f(-v) G(x, x + u, x + u - v) \]
\[ \cdot \Delta(x + u - v, y + u - v) H(y, y - v, y + u - v) . \] (3)

Here we have chosen \( \rho(\epsilon) \) to be the density-of-states (DOS) of the conduction electrons and the auxiliary functions \( G, H \) and \( K \)

\[ G(x, x + u, x + u - v) = \Delta(x, x + u) P_m(x + u) \] (4)

\[ \Delta(x + u - v, x + u) P_0(x + u - v) \]

\[ H(y, y - u, y + u - v) = P_m(y + u - v) \]
\[ \cdot (\Delta(y - v, y + u - v) P_0(y - v) \Delta(y - v, y) \]
\[ - K(y + u - v, y, y + u) ) \]

\[ K(y + u - v, y, y + u) = N|V|^2 \int_{-\infty}^{\infty} dl \rho(l) f(-l) \Delta(y + u - v - l, y + u - v) \]
\[ \cdot P_0(y + u - v - l) \Delta(y + u - v - l, y + u - l) \]
\[ \cdot P_m(y + u - l) \Delta(y - l, y + u - l) \]
\[ \cdot P_0(y - l) \Delta(y - l, y) . \] (6)

The negative sign in Eqn.(3) takes into account the odd number of crossing electron lines in the skeleton (d) while in diagram (e) an even number of crossing lines can be found. The approximation defined by Eqn. (1) to (6) will be called \( PNCA_\infty \) in the following (\( \infty \) stands for \( U = \infty \)).

In the one-particle Green’s function \( F_m(i\omega_n) \) the vertex correction also comes into play in a natural way:\

\[ F_m(i\omega_n) = \frac{1}{Z_f} \oint_C \frac{dz}{2\pi i} e^{-\beta z} \Delta_m(z, z + i\omega_n) P_0(z) P_m(z + i\omega_n) . \] (7)

This equation can e.g. be obtained by cutting one band electron line in the functional \( \Phi[P_M] \) of Fig. 3. Thereby, no ambiguity is left in the analytic expression. The contour \( C \) encircles the all singularities of the kernel in a counterclockwise fashion. Analytic continuation of the Green’s function gives
\[ F_m(\omega + i\delta) = \int_{-\infty}^{\infty} dw' P_m(\omega + w') (\Re \Delta_x(\omega, \omega + w') \xi_0(w') + \Re \xi_0(\omega, \omega + w')) \]
\[- \int_{-\infty}^{\infty} dw' P_0^*(w' - \omega) (\Re \Delta_y(w' - \omega, \omega) \xi_m(w') + \Re \xi_m(w' - \omega, \omega')). \]

We have introduced the real auxiliary functions
\[ \xi_M(\omega) \equiv -\frac{1}{\pi Z_f} e^{-\beta\omega} \Im P_M(\omega + i\delta) \]
and the complex auxiliary functions
\[ \Re \Delta_x(\omega, \omega + i\omega_n) \equiv \frac{1}{2}[\Delta(\omega + i\delta, \omega + i\omega_n) + \Delta(\omega - i\delta, \omega + i\omega_n)] \]
\[ \Im \Delta_x(\omega, \omega + i\omega_n) \equiv \frac{1}{2\pi}[\Delta(\omega + i\delta, \omega + i\omega_n) - \Delta(\omega - i\delta, \omega + i\omega_n)] \]
\[ \Re \Delta_y(\omega - i\omega_n, \omega) \equiv \frac{1}{2}[\Delta(\omega - i\delta, \omega + i\omega_n) + \Delta(\omega - i\omega_n, \omega - i\delta)] \]
\[ \Im \Delta_y(\omega - i\omega_n, \omega) \equiv \frac{1}{2\pi}[\Delta(\omega - i\omega_n, \omega - i\delta) - \Delta(\omega - i\omega_n, \omega - i\delta)] \]
\[ \xi_{\Delta_x}(x, y) \equiv - \frac{1}{\pi Z_f} e^{-\beta x} \Im \Delta_x(x, y) \]
\[ \xi_{\Delta_y}(x, y) \equiv - \frac{1}{\pi Z_f} e^{-\beta y} \Im \Delta_y(x, y) . \]

The functions \( \xi_M(\omega) \) introduced above have a simple physical meaning as defect propagator: integration over the whole frequency range yields the occupation probability \( < \hat{X}_{MM} > \) of the local state \( M \). The complex functions \( \Re(\Im) \Delta_{x,y}(\omega) \) and \( \xi_{\Delta_{x,y}}(x, y) \) enable the evaluation of Eqn. (7) for real frequencies and thus serve purely numerical purposes.

**III. LOCAL PROPAGATORS, THRESHOLD EXPONENTS AND SPECIFIC HEAT**

On a cluster of work-stations, we brought a numerical iteration procedure for the above system of integral equations to full convergence using dynamically defined logarithmic meshes for the threefold integration in (3). Besides the modulus \( ||P_M^{(i)} - P_M^{(i+1)}|| \) (\( i \) labels the step of iteration), which reaches a value of typical \( 10^{-16} \) at the end, the sum rules
\[ \int_C \frac{dz}{2\pi i} P_M(z) = 1 ; \int_C \frac{dz}{2\pi i} \Sigma_m(z) = |V|^2 \sum_{km} \left( < M|\hat{n}_m^f|M > |1 - f(\epsilon_{km})| \right) \]
\[ < M|(1 - \hat{n}_m^f)|M > f(\epsilon_{km}) \]
have been checked to estimate the quality of the numerical calculations. The deviation between left and right side is in the range of typically 1-4 % and scales with the inverse number of mesh points. For all numerical studies all energies are measured in units of the Anderson width $\Delta = \pi V^2 N_F$ ($V^2$ is the square of the hybridisation matrix element and $N_F$ the band DOS at the chemical potential). The featureless symmetric conduction band DOS has been chosen to be $\rho^c(\omega) = \frac{1}{2\Gamma(1.25)} \exp(-\omega/W^4)$ to reduce band edge effects. The half band width is set to $W = 10\Delta$. In most cases the temperature will be measured in units of the corresponding Kondo-energy

$$T_K = W \left( \frac{\Delta}{\pi W} \right)^{\frac{1}{W}} \exp \left( -\frac{\pi |\epsilon_f|}{N \Delta} \right).$$

(12)

For the investigation of the Kondo-regime $\epsilon_f = -3\Delta$ and $N = 2$ is chosen, since the largest impact of the vertex function is to be expected for small $N$. In Fig. 3 the spectral density $\rho_0(\omega) \equiv \frac{1}{\pi} \text{Im} P_0(\omega - i\delta)$ is displayed in the vicinity of the threshold for three different temperatures $T = 0.5, 1, 2T_K$. Note the fact that the energy scale has been shifted by the threshold energy $E_s$. The transformation $Z_f = \oint \frac{dz}{2\pi i} e^{-\beta z} P_M(z) \equiv e^{-\beta E_s} \tilde{Z}_f$ defining a renormalized local partition function $\tilde{Z}_f = \oint \frac{dz}{2\pi i} e^{-\beta z} \tilde{P}_M(z)$ and a local propagator $\tilde{P}_M(z) \equiv P_M(z + E_s)$, ensures that the numerically calculated $\tilde{Z}_f$ stays of the order $O(1)$ during the variation of temperature. Also the defect propagators $\xi_M$ can be calculated very accurately down to very low temperatures.

With decreasing temperature the threshold behaviour of the propagator $P_0$ in $\text{PNCA}_\infty$ exhibits a weaker increase than the corresponding $NCA$ propagator. We regard this as a strong hint toward a reduced threshold exponent $\alpha_0$ compared with the $NCA$ due to the influence of the vertex corrections. On the other hand, the inset indicates quite clearly an excellent agreement on the high energy part of the spectrum in both approximations as to be expected. The spectral density $\rho_m(\omega)$, shown in Fig. 3b for the same set of model parameters and temperatures, reveals an additional difference between the two approximations. $P_0^{\text{PNCA}}$ and $P_m^{\text{PNCA}}$ develop their common threshold energy $E_s$ already at finite temperature while in $NCA$ an identical $E_s$ for both propagators is found only at $T = 0$. This gives rise to a
temperature dependent position of the ASR in the one-particle spectra in NCA, as we will see in the next section.

To obtain a first estimate for threshold exponents we fit the ionic spectrum in the low frequency range $0 < \omega < T_K$ to a trial function $h_M(\omega) = a(T) \cdot \omega^{-\alpha_M(T)}$ at different temperatures. This procedure has been checked for the NCA and provides the exactly known NCA exponents $\alpha_0 = \frac{N}{N+1}$ and $\alpha_m = \frac{1}{N+1}$ within an accuracy of 5%. While no temperature dependence is found for the exponent $\alpha_0 = 0.44 \pm 0.02$, Fig. 5a, the different values of $\alpha_m(T)$ have been used to to extrapolate $\alpha_m(0) = 0.27 \pm 0.01$ for the present parameters $N = 2, \epsilon_f = -3\Delta$ giving $n_f = 0.87$, Fig. 5b.

There is still no agreement in the literature about the exact exponents for $N \geq 2$. The proposal of Menge and Müller-Hartmann\cite{Menge:1989}

\begin{equation}
\alpha_0 = \frac{n_f^2}{N} \quad \alpha_m = \frac{n_f}{N} (2 - n_f)
\end{equation}

indicates a dependence of the exponents not only of the degeneracy $N$ but also on the occupation number $n_f$ in all regimes. This proposal has been recently backed by a analysis of pseudo-boson and fermion propagators provided by the numerical renormalisation group\cite{Bauer:1993}. On the other side, an analysis of parquet-equations for the Kondo limit of the model ($n_f = 1$) claims that the exponents

\begin{equation}
\alpha_0 = \frac{N - 2}{N + 1 - \frac{2}{N^2}} \quad \alpha_m = \frac{1 - \frac{1}{N^2}}{N + 1 - \frac{2}{N^2}}
\end{equation}

should be exact in order $O(1/N^2)$\cite{Hartmann:1993}. We did not investigate the threshold behaviour on the full scale of the model parameters. Therefore we cannot rule out any of the proposals, even though the PNCA$_\infty$ exponents in the Kondo-regime come very close to Gruneberg’s and Keiter’s results.

Since we have convinced ourselves that the high energy parts of the spectra remain unchanged, we can still use the NCA to obtain specific heat data for a wide temperature range. On the other hand, the low energy corrections turn out to be essential for the calculation of correlation functions. In Figs. 6 and 7 origin and scaling behaviour of the
two different contributions to the specific heat are clearly demonstrated. In (a) the effective
hybridisation is tuned leading to a renormalized Anderson width $\Delta^*$ and in (b) the position
of the bare $f$-electron level has been varied for $N = 2$. While the first maximum in each
curve of the specific heat turns out to be an universal function of $T/T_K$, the position of the
second rather determined by the $f$-level energy and its width by $\Delta^*$. Therefore, the first peak
is generated by spin excitations on the Kondo-scale $T \sim T_K$, whereas the second contains
charge excitations from the broadened $f$-level into unoccupied band states. With increasing
degeneracy the maximum due to spin excitations is enhanced essentially linearly with $N^4$, since
their contribution is proportional to the number of channels, as it is already know from
Bethe-Ansatz calculations\cite{17}. The charge excitations peak is rather decreased and smeared
out by broadening of the $f$-level proportional to $N \Delta$. Its position and broadening is in good
agreement with Bethe-Ansatz\cite{14} and numerical renormalisation group calculations\cite{15}, but the
height comes out somewhat smaller. This could be due to absence of the doubly occupied
state for $U = \infty$. Of course, the appearance of the charge excitations is more of academic
interest for the low temperature behaviour, but may be important for spectroscopic studies.

**IV. ONE-PARTICLE SPECTRA**

The generalized Friedel’s sum rule

$$n_f(T) = \frac{1}{\pi} \sum_m \int_{-\infty}^{\infty} d\omega \left( \partial_\omega f(\omega) \right) \delta_m(\omega) + \frac{1}{2\pi i} \sum_m \oint_C dz f(z) F_m(z) \partial_z \Sigma_m(z) \equiv \kappa(T)$$

relates the local occupation number $n_f$ to the generalized phase shifts $\delta_m(\omega) \equiv
-\Im m \ln [-F_m^{-1}(i\delta)]$. $\kappa$ essentially measures the asymmetry of the $f$-electron spectrum and
can be interpreted as the negative change of the number of band electrons in the presence of
the impurity\cite{1}. In the limit $T = 0$, Eqn. (15) is used in combination with local Fermi-liquid
relations to derive the density of states rule:

$$\rho^{(f)}(0, T = 0) = \frac{1}{\pi \Delta} \sin^2 \left( \frac{\pi(n_f - \kappa)}{N} \right). \quad (16)$$
This formula predicts a scattering resonance with a maximum height of \( \frac{1}{\pi \Delta} \) near the chemical potential \( ((n_f - \kappa) \approx 1) \) for \( N = 2 \) and \( T = 0 \), the ASR, which moves away from \( \mu \) increasing degeneracies \( N \). Fig. 8 shows the one-particle spectra of \( PNCA_\infty \) and \( NCA \) for five values of temperatures. The most significant differences between both approximations concern the position and height of the ASR. The position in \( NCA \) is found strongly temperature dependent and the height exceeds the unitarity limit of \( 1/(\pi \Delta) \) already at temperatures slightly below \( T_K \). We can trace back the temperature dependence to the mismatch of the threshold energies of \( P_0 \) and \( P_m \), which merge only at \( T = 0 \). The violation of Eqn. (16) clearly indicates the importance of the vertex corrections. On the other hand, the \( PNCA_\infty \)-ASR grows with decreasing temperature at a stable position close to the chemical potential. It violates only slightly the density of states sum rule and its agreement with Friedel’s sum rule (13) is found to be within 7% as indicated in table 4.

By focusing our attention on Fig. 9, we gain insight on the impact of vertex corrections on the ASR. The \( PNCA_\infty \) result (solid curve) is compared to the \( NCA \) result (dashed curve) for the fixed temperature \( T = 0.5T_K \) and additionally to a curve where the \( NCA \) propagators \( P_M(z) \) have been used to evaluate the renormalized hybridisation \( V \cdot \Delta(x, y) \) via Eqn. (3). In the later convergence is achieved after two steps of iteration. The resulting ASR, calculated after each step, has been shifted towards the chemical potential, but stays enhanced compared to the \( PNCA_\infty \)-ASR. The reduction of height of the ASR is clearly connected to the modified threshold exponents as is also revealed by an inspection of the iteration procedure. This stressed the importance of vertex corrections in the local propagators \( P_M(z) \).

The plots in figure 10 attract attention to the local Fermi-liquid properties as seen in the imaginary part of the self-energy of the Green’s function:

\[
\Im m \Sigma_{fm}(\omega - i\delta) = \Delta + C_\omega \omega^2 + C_T T^2 .
\] (17)

From the symmetric Anderson model it is know that \( C_\omega = \Delta/T_{K}^2 \) and \( C_T = \Delta \frac{\pi^2}{T_K} \). In the strongly asymmetric case \( (U = \infty) \) under consideration here, only the scaling \( C_\omega = \Delta/T_{K}^2 \) can be found. The quadratic expansion coefficient for the temperature exhibits a rather
strong dependence on the degeneracy $N$ as been shown in Fig. [10], originating from the shift of the ASR away from the chemical potential, while in the completely symmetric case the phase shift $\delta_m$ remains $\pi/2$ independently of $N$. On the base of our PNCA$_\infty$-results we suggest a new analytic investigation of Fermi liquid relations for the asymmetric case.

V. MAGNETIC SUSCEPTIBILITY AND SPIN-FLUCTUATIONS

Magnetic excitations are measured by the magnetic susceptibility:

$$\chi(i\nu_n) = -\frac{1}{Z} \oint_C \frac{dz}{2\pi i} e^{-\beta z} \text{Tr} \left[ \frac{1}{z - H} \frac{1}{z + i\nu_n - H} \right] = \chi(-i\nu_n) \; , \quad (18)$$

where $i\nu_n = \frac{2\pi in}{\beta}$ is a bosonic Matsubara-frequency. Focusing our attention on the operator the local magnetization in the SIAM, $\hat{M}_z \equiv g\mu_B \sum_m m \cdot \hat{X}_{m,m}$, we rewrite $\chi_f(i\nu_n)$ in analogy to $F_m$:

$$\chi_f(i\nu_n) = -\frac{N\mu_j^2}{3} \frac{1}{Z} \oint_C \frac{dz}{2\pi i} e^{-\beta z} P_m(z) P_m(z + i\nu_n) \Gamma(z, z + i\nu_n) \; , \quad (19)$$

defining $\mu_j^2 \equiv j(j+1)(g\mu_B)^2$. The new magnetic vertex function $\Gamma(x, y)$ formally includes all higher order contributions arising from diagrams with crossing band electron lines; in NCA $\Gamma(x, y) = 1$. It turns out to be symmetric in its complex energy arguments in order to maintain the symmetry $\chi(i\nu_n) = \chi(-i\nu_n)$. Using the standard set of diagrammatical rules\(^5\), we obtain $\Gamma(x, y)$ exactly up to order $O(1/N^3)$ shown in Fig. [11]. $O(1/N^2)$ contributions compensate each other. On the other hand, diagram (c) and (d) in Fig. [11] transform into each other by exchanging the energy arguments. Therefore, we only have to insert

$$\Gamma_c(x, y) = -|V|^4 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} du dv \rho(u) \rho(v) f(-l) f(-u) f(v)$$

$\cdot P_0(x - u) \Delta(x - u, x) \quad \cdot P_m(x - u + v) \Delta(x - u, x - u + v)$$

$\cdot \Gamma(x - u + v, y - u + v) \quad \cdot P_m(y - u + v) j(y + u - v, y, y + u)$

$$\quad \cdot P_m(y - u + v) j(y + u - v, y, y + u)$$

(20)
into the magnetic vertex function of the $PNCA_{\infty}$-theory

$$\Gamma(x, y) = 1 + \Gamma_c(x, y) + \Gamma_c(y, x), \quad (21)$$

and to solve Eqn. (20) and (21) self-consistently. Eqn.(19) then leads to a local dynamical susceptibility $\chi_f$, which is exact in $O(1/N^2)$.

The quality of the approximation has been checked by comparison of the static magnetic susceptibility $\chi_f(T) \equiv \lim_{\nu \to 0} \chi(\nu)$ to the exact Bethe-Ansatz results\textsuperscript{17}, Fig. 12. The $PNCA_{\infty}$ susceptibility shows a surprisingly good agreement with the exact results, even though the Bethe-Ansatz susceptibility has been obtained for the Coqblin-Schrieffer model. In particular, the characteristic maximum for degeneracies $N \geq 3$ has been reproduced in $PNCA_{\infty}$. On the other hand in $NCA$ not even a saturation of $\chi_f$ occurs for $0.1T_K < T < T_K$ and $N = 2$. The deficiencies of the $NCA$ do not show up so strongly at e.g. $N = 6$ or at higher temperatures $T > T_K$, where vertex corrections become less important.

The scattering function $S(\nu)$ for neutron scattering experiments is linked to the magnetic susceptibility by the dissipation-fluctuation theorem:

$$S(\omega) \sim \frac{1}{1 - \exp(-\beta \omega) \Im m\chi(\omega)} \quad (22)$$

The right hand side approaches the spin-fluctuation spectrum $\sigma(\omega) \equiv \chi(\omega)/\omega$ for small $\omega$. In Fig. 13 the spin-fluctuation spectra of the $PNCA_{\infty}$ and the $NCA$ are compared for three different degeneracies $N$ at a fixed temperature $T = 0.2T_K$. The pronounced maxima of $\sigma^{PNCA}(\omega)$ for $N > 3$ resemble the maxima in the static susceptibility discussed before. They appear on the same energy scale $\omega(T) \approx 0.5T_K$. It is also interesting to note that even though no maximum is found for $N = 2$ a rather broad inelastic peak can be reported in $\sigma^{PNCA}(\omega)$ which is not seen in the $NCA$ spectrum. Of course, this features disappears well above $T_K$ for both approximations leaving a single elastic peak at $\omega = 0$ in the spectra. The low frequency behaviour of $\Im m\chi(\omega)$ can be interpolated by $\omega/(\Gamma_{\text{neut}}^2 + \omega^2)$. $\Gamma_{\text{neut}}$ is the neutron scattering linewidth which is experimentally defined by the position of the maximum. Here, it is convenient to use
\[
\frac{1}{\Gamma^2_{\text{neut}}} = \lim_{\omega \to 0} \frac{\Im m \chi(\omega)}{\omega} .
\]

In Fig. 14, the reduced linewidth \(\Gamma_{\text{neut}}/T_K\) is displayed versus temperature for \(N = 2, 4, 6\) in \(PNCA_\infty\). The linewidth is nearly temperature independent in the local Fermi-liquid regime at \(T < T_K\). It develops a weak minimum at \(T \approx 0.5T_K\) which is slightly enhanced by increasing degeneracy and behaves like \(\sqrt{T}\) for high temperatures.

**VI. CRITICAL EXAMINATION OF THE \(PNCA_\infty\)**

In the last three sections we discussed \(PNCA_\infty\) results obtained for the Kondo regime of the model. In this section we will focus our attention on the case \(N = 1\) and the mixed-valance regime. For \(N = 1\) all diagrams are of the same order in the sense of an \(1/N\)-expansion scheme. Nevertheless, this classification is questionable here, since there is no Kondo effect left although the diagram topology remains unchanged. The one-particle Green’s function is exactly known:

\[
F(z) = \frac{1}{z - \epsilon_f - \frac{V^2}{\#k} \sum_k \frac{1}{z - \epsilon_k}} ;
\]

(#\(k\) denotes the number of band electron states). In figure 15 the one-particle spectra of the \(NCA\) and the \(PNCA_\infty\) are compared with the exact result for two values of \(\epsilon_f\). While the \(P_M(z)\) have been determined very accurately, oscillations of the defect propagators \(\xi(\omega) = \exp(-\beta\omega)\frac{1}{\pi Z_f} \Im m P_M(\omega)\) during the iteration procedure cause oscillations in the \(PNCA_\infty\)-spectra around the exact solution, i.e. convergence is not fully obtained in this case. These oscillations contribute about 3\% to the residual deviations of the \(PNCA_\infty\). In the most critical case, \(\epsilon_f = -\Delta\), the \(NCA\)-pathology is strongly pathological near \(\mu\), but the \(PNCA_\infty\) is much less so. For \(\epsilon_f = -3\Delta\) only a very weak pathology at \(\mu = 0\) remains, while the \(NCA\) still produces an unphysical resonance at the chemical potential.

A rather strange two peak structure is found in the spectrum for the case of the intermediate valence regime \(\epsilon_f = -\Delta\) and \(N = 2\), shown in Fig. 16a: the first peak nearly at \(\mu = 0\) exceeds clearly the density of states rule \((16)\ \rho(0) = 0.21\) for \(n_f \approx 0.6\), which
would be the height of the minimum in between both peaks. We suppose that the true spectrum will monotonically decrease from the minimum position onwards for decreasing energy. The first peak clearly reflects a $PNCA_\infty$-pathology already seen in Fig. 15a. Despite this spurious structure, the overall violation of the DOS-sum rule is reduced from almost 60% in $NCA$ down to 15% in $PNCA_\infty$. In part (b) of the figure, $\epsilon_f$ is chosen to be $+\Delta$. Again, only a weak pathology is found in this case, and the spectrum can be reasonably fitted using a Lorentzian with a width of $0.95\Delta$. This resembles the fact that there is no blocking effect in this regime, whereas the local correlations still reduce the spectral weight to $<X_{00}> + <X_{mm}> = 0.87 < 1$.

VII. CONCLUSION AND OUTLOOK

We have demonstrated that our new $PNCA_\infty$-approximation to the Anderson-model improves the low energy properties in the Kondo-regime quite remarkably, whereas the satisfactory behaviour of the old $NCA$-approximation at higher energies is maintained. Vertex corrections do have in fact a large impact on the low energy excitations: position and height of the ASR for $N = 2$ is shifted towards the chemical potential as consistent with Friedel’s sum rule. Also the magnetic susceptibility agrees surprisingly well with the Bethe-Ansatz results. We plan to apply this method also to the finite-$U$ Anderson-model and the extended Anderson model, which includes a direct exchange interaction between $f$- and conduction electrons. The self-consistent set of equations have been derived already. Our perturbational approach to the Anderson-model has opened the prospect of studying the low temperature properties of Heavy Fermion systems in much more detail before. Quite generally, the so-called LNCA scheme can be applied, which provides a very successful perturbational treatment of the Anderson lattice. Within this theory based on a picture of independent effective sides plus quasi-particle interactions collective effects like superconducting or magnetic ground states can be calculated in a systematic way. In order to underline this perspective we present the temperature dependent pseudo-gap formation in
the $f$-spectrum of the Anderson lattice with $N = 2$ and $\epsilon_f = -3$ in Fig. 17. The temperatures are given in units of the corresponding impurity Kondo temperature which deviates moderately from the characteristic temperature of the lattice $T^*$. While the LNCA-scheme combined with the local $NCA$ is limited to temperatures larger than $T_K$ due to violations of the local Fermi-liquid properties, the so-called $L$-$PNCA_\infty$, which uses the $PNCA_\infty$ to solve the effective site, reaches much lower temperatures. Since now the ASR of the impurity is located only very slightly above the chemical potential in accordance with Friedel’s sum rule, the pseudo-gap is formed around $\omega = 0$ in the $L$-$PNCA_\infty$. In a forthcoming publication we will investigate the temperature dependent quasi-particle band-structure and the impact on the transport coefficients and optical conductivity in greater detail.

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### TABLES

Friedel’s Sum Rule and the $NCA$-Theory:

| $T/T_K$ | $n_f$  | $\sum m \frac{\delta_m}{\pi}$ | $\kappa_{res}$ |
|---------|--------|-------------------------------|----------------|
| 0.1     | .8682  | .5863                         | .2819          |
| 0.2     | .8682  | .6114                         | .2567          |
| 0.3     | .8682  | .6379                         | .2303          |

(a)

Friedel’s Sum Rule and the $PNCA_{\infty}$-Theory:

| $T/T_K$ | $n_f$  | $\sum m \frac{\delta_m}{\pi}$ | $\kappa_{res}$ |
|---------|--------|-------------------------------|----------------|
| 0.1     | .8445  | .9023                         | -.0577         |
| 0.2     | .8525  | .9140                         | -.0615         |
| 0.3     | .8565  | .9207                         | -.0641         |

(b)

TABLE I. Parameter: $N = 2, \epsilon_f = -3\Delta, W = 10$
FIGURES

FIG. 1. Diagrammatic contributions to the self-energy $\Sigma_0(z)$ of the unoccupied propagator $P_0$ up to $V^8$.

FIG. 2. Diagrammatical representation of the self-consistency equation of the vertex function $\Delta_m(x, y)$ in $O(1/N^2)$.

FIG. 3. Generating functional for the self-energies and the Green’s functions up to order $O(1/N^2)$. The $PNCA_\infty$ contains additional higher order contributions.

FIG. 4. Comparison of the spectra of $P_0(\omega)$ (a) and $P_m(\omega)$ (b) in NCA and $PNCA_\infty$ at $T = 0.5, 1.0, 2.0T_K$. The increase in height at $\omega = 0$ is correlated with a decrease of temperature. Parameters: $N = 2, 0, 2, 5, T_K$. The increase in height at $\omega = 0$ is correlated with a decrease of temperature. Parameters: $N = 2, 0, 2, 5, T_K$.

FIG. 5. Threshold behaviour of the spectrum of $P_0(z)$ (a) and an estimation for the threshold exponent $\alpha_m$ (b). Parameters as before.

FIG. 6. Specific heat contribution of the impurity vs temperature $T/T_K$ for (a) different values of the effective Anderson width $\Delta^* = \pi|V^*|^2\rho_0, \epsilon_f = -3\Delta_0$, and (b) different values of $\epsilon_f$. Parameters: $N = 2, 0, 2, 5, T_K$.

FIG. 7. Specific heat contribution of the impurity vs temperature $T/\Delta_0$ for (a) different values of the effective Anderson width $\Delta^* = \pi|V^*|^2\rho_0, \epsilon_f = -3\Delta_0$, and (b) different values of $\epsilon_f$. Parameters: $N = 2, 0, 2, 5, T_K$.

FIG. 8. Temperature dependency of the ASR in (a) $PNCA_\infty$ and (b) in NCA. Parameters: as before.

FIG. 9. Impact of the vertex correction on the one particle spectrum. Parameters: as before.

FIG. 10. Minimum of the self-energy versus temperature for $N = 2, 4, 6$. Parameters: $\epsilon_f(N = 2) = -3\Delta, \epsilon_f(N = 4) = -5\Delta, \epsilon_f(N = 6) = -6.7\Delta, W = 10\Delta$. 

18
FIG. 11. Diagrammatic representation of the self-consistency condition of the magnetic vertex function $\Gamma(x,y)$.

FIG. 12. Static magnetic susceptibility calculated (a) in NCA, (b) in $PNCA_\infty$ for the single impurity Anderson model and (c) for the Coqblin-Schrieffer models using the Bethe Ansatz. The NCA results are normalized with respect to the $PNCA_\infty$ values at $T = 0$. Parameters: as in Fig. 10

FIG. 13. $\Im \chi(\omega)/\omega$ vs $\omega/T_K$ for $N = 2, 4, 6$, calculated at $T = 0.2T_K$ (a) in $PNCA_\infty$ and (b) in NCA. Parameters: as in Fig. 10

FIG. 14. Neutron scattering linewidth $\Gamma_{neut}$ vs. $T/T_K$ calculated in $PNCA_\infty$ for different $N$. Parameters: as in Fig. 10

FIG. 15. One-particle spectra in NCA and $PNCA_\infty$ compared with the exact solution for (a) $\epsilon_f = -\Delta, T = 1/15\Delta$ and (b) $\epsilon_f = -3\Delta, T = 1/60\Delta$. Parameter: $N = 1$.

FIG. 16. One-particle spectra in NCA und $PNCA_\infty$ for (a) $\epsilon_f = -\Delta$ and (b) $\epsilon_f = +\Delta$, the intermediate valence regime. Parameters: $N = 2, T = \frac{1}{15}\Delta$.

FIG. 17. $f$-spectra of the periodic Anderson model in the vicinity of the chemical potential (a) in $L-PNCA_\infty$ and (b) in LNCA for three temperature $T = 0.75, 1.0, 2.0T_K$. Parameters $N = 2, \epsilon_f = -3\Delta, W = 10\Delta$. 

19