

Momentum distribution functions in a one-dimensional extended periodic Anderson model

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We study the momentum distribution of the electrons in an extended periodic Anderson model, where the interaction, U_{cf} , between itinerant and localized electrons is taken into account. In the symmetric half-filled model, due to the increase of the interorbital interaction, the f electrons become more and more delocalized, while the itinerancy of conduction electrons decreases. Above a certain value of U_{cf} the f electrons become again localized together with the conduction electrons. In the less than half-filled case, we observe that U_{cf} causes strong correlations between the f electrons in the mixed valence regime.

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I. INTRODUCTION

Heavy-fermion and mixed valence systems are still active research fields in spite of the major achievements of the past few decades.^{1,2} The discovery of a new critical point in the pressure-temperature phase diagram of CeCu_2Ge_2 and CeCu_2Si_2 has attracted much attention both experimentally³⁻⁸ and theoretically.⁹⁻¹⁴ It is believed that the appearance of the new critical point is due to the critical valence fluctuations of the Ce ion. The simplest model, which contains the essential physics of rare-earth compounds is the periodic Anderson model:

$$\begin{aligned} \mathcal{H}_{\text{PAM}} = & -t \sum_{\langle ij \rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \\ & - V \sum_{j, \sigma} (\hat{f}_{j\sigma}^\dagger \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^\dagger \hat{f}_{j\sigma}) + \varepsilon_f \sum_{j, \sigma} \hat{n}_{j\sigma}^f \\ & + U_f \sum_j \hat{n}_{j\uparrow}^f \hat{n}_{j\downarrow}^f, \end{aligned} \quad (1)$$

where the notation is standard and $W = 4t$ is taken as the energy unit. It is known, however, that the mixed-valence regime appears always in this model as a smooth crossover, and valence fluctuations do not become critical for any choice of the parameters. A local Coulomb interaction between the conduction and localized electrons is needed for the appearance of a sharp transition and critical valence fluctuations.¹⁴ Therefore we consider the following Hamiltonian:

$$\mathcal{H} = \mathcal{H}_{\text{PAM}} + U_{cf} \sum_{j, \sigma, \sigma'} \hat{n}_{j\sigma}^f \hat{n}_{j\sigma'}^c. \quad (2)$$

Previous studies revealed how U_{cf} affects the mixed valence regime and it has been shown that a first-order valence transition and a quantum critical point may appear due to U_{cf} .^{11,15-17} The effect of U_{cf} in the Kondo regime has been also addressed both in infinite^{18,19} and one spatial dimensions.²⁰ Namely, in infinite dimensions the symmetric model for small hybridization ($V \ll W$) displays antiferromagnetic order for small U_{cf} which,

however, disappears for large U_{cf} and charge order develops. In contrast, there is no such phase transition in one dimension due to the enhanced quantum fluctuations, however, for small and large U_{cf} the spin-spin and density-density correlation function, respectively exhibits the slowest decay. Between these two regimes there is a narrow region, where the local singlet formation is significantly enhanced.

Our goal in this paper is to investigate the momentum distribution of the electrons in one dimension. It is known, that in higher dimensions they exhibit a jump at the Fermi momentum, whose size can be used to extract the energy dependence of the self-energies, from which the many-body enhancement factor of the effective mass can be obtained. Although in one dimension there is no such jump at the Fermi momentum, just a sharp change, they provide direct information about the spatial distribution of the electrons and the content of conduction and f -electron states in the quasi-particle bands, while the previous quantum information analysis²⁰ gave only an indirect description of these quantities. We address the question how they are modified by switching on U_{cf} both in the integer and mixed valence regimes. The density-matrix renormalization-group algorithm (DMRG)²¹⁻²⁵ is applied, which allows the accurate determination of ground state properties. We have used the dynamic block-state selection algorithm^{26,27} in which the threshold value of the quantum information loss, χ , is set a priori. We have taken $\chi = 10^{-5}$. A maximum of 2000 block states is needed to achieve this accuracy, and the largest truncation error was in the order of 10^{-6} . We investigated chains up to a maximum length $L = 80$ with open boundary conditions and performed 8-12 sweeps.

II. RESULTS AT HALF FILLING

The non-degenerate version of the periodic Anderson model can hold up to $n_{\text{max}} = 4$ electrons per lattice site, the average number of c and f electrons per site, n^c and n^f , respectively, can vary between zero and two. The

filling will refer to the ratio of the total electron density per site ($n^c + n^f$). In what follows we consider the symmetric half-filled model, where $n^f = 1$, and calculate the momentum distribution of conduction and f electrons which are defined as

$$n^c(k) = \frac{1}{2} \sum_{\sigma} \langle c_{k\sigma}^{\dagger} c_{k\sigma} \rangle, \quad (3)$$

$$n^f(k) = \frac{1}{2} \sum_{\sigma} \langle f_{k\sigma}^{\dagger} f_{k\sigma} \rangle. \quad (4)$$

Our DMRG calculation was performed in real space, therefore these quantities can be obtained by Fourier transforming the corresponding single particle density matrices, namely:

$$n^c(k) = \frac{1}{2} \sum_{jl\sigma} e^{ik(j-l)} \langle c_{j\sigma}^{\dagger} c_{l\sigma} \rangle, \quad (5)$$

$$n^f(k) = \frac{1}{2} \sum_{jl\sigma} e^{ik(j-l)} \langle f_{j\sigma}^{\dagger} f_{l\sigma} \rangle, \quad (6)$$

where $k = 2\pi n/L$ and $n = -L/2 - 1, \dots, L/2$. In our case these are symmetric functions, therefore we consider only the nonnegative k values.

Before going into the details of the numerical results, we briefly recall the case when $U_f = U_{cf} = 0$ which is easily solvable. Thereby the Hamiltonian can be diagonalized by an unitary transformation

$$\begin{aligned} \alpha_k^{(-)} &= -v_k c_k + u_k f_k, \\ \alpha_k^{(+)} &= u_k c_k + v_k f_k, \end{aligned} \quad (7)$$

where $\alpha_k^{(-)}$ ($\alpha_k^{(+)}$) creates a quasiparticle in the lower (upper) hybridized band with mixing amplitudes:

$$u_k^2 = \frac{1}{2} \left[1 - \frac{\varepsilon_k - \varepsilon_f}{\sqrt{(\varepsilon_k - \varepsilon_f)^2 + 4V^2}} \right], \quad (8)$$

$$v_k^2 = \frac{1}{2} \left[1 + \frac{\varepsilon_k - \varepsilon_f}{\sqrt{(\varepsilon_k - \varepsilon_f)^2 + 4V^2}} \right], \quad (9)$$

in our case $\varepsilon_k = -2t \cos k$ and the Fermi momentum is at the boundary of the Brillouin zone since the lower band is completely filled. It is easily seen that the momentum distribution functions provide information about the mixing amplitudes, namely, the portion of conduction and f states in the hybridized band:

$$\begin{aligned} n^c(k) &= v_k^2, \\ n^f(k) &= u_k^2. \end{aligned} \quad (10)$$

The momentum distribution in the noninteracting system is shown in Fig. 1 compared with the DMRG results. The small discrepancy between the two results is attributed to the open boundary condition used in DMRG. In the following we investigate how the interactions modify the above results, using again the DMRG method with

open boundary condition. We checked for short systems that the momentum distributions of the interacting system calculated with periodic and open boundary conditions are in good agreement within our error margin.

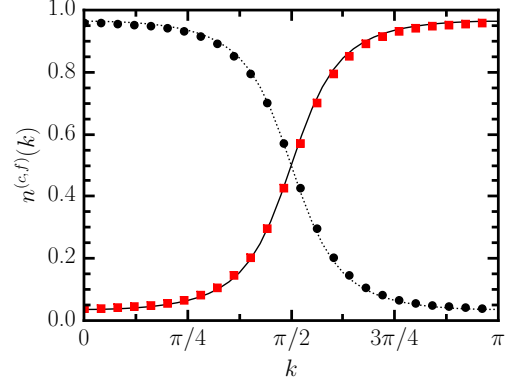


FIG. 1. Momentum distribution functions of the conduction and f electrons in the noninteracting case ($U_f = U_{cf} = 0$, $V/W = 0.1$, $\varepsilon_f = 0$). The solid and dotted lines are obtained from Eq. (8) and (9), respectively. The symbols \bullet , \blacksquare denote the DMRG results for $L = 50$.

It has been pointed out^{20,28} that strong U_f leads to localization of the f electrons, since the number of doubly occupied f levels is negligible and the ground state is a collective singlet. This is what we see in Fig. 2 (a), namely, $n^f(k)$ hardly depends on k in the Kondo regime, while the distribution of conduction electrons is just slightly affected by U_f . The quantum information

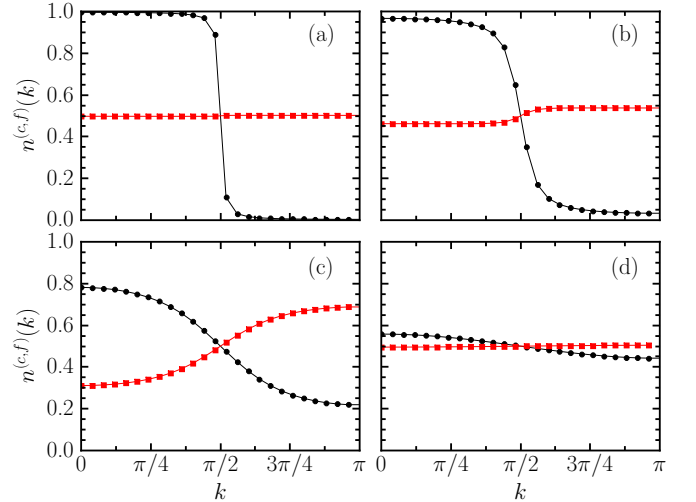


FIG. 2. Momentum distribution functions of the conduction (\bullet) and f (\blacksquare) electrons for $L = 50$ and $n = 2$. Panel (a), (b), (c) and (d) correspond to $U_{cf}/W = 0, 1.5, 1.7$ and 3 , furthermore $U_f/W = 3$, $V/W = 0.1$ and $\varepsilon_f = -U_f/2$ in all cases. The lines are guides to the eye.

analysis²⁰ showed that as U_{cf} is switched on more and more doubly occupied f sites are created, therefore the f electrons become less localized in real space. Finally,

when U_{cf} is large the c and f electrons tend to avoid each other and the sites are occupied by two c or two f electrons in an alternating fashion. Now we examine how these features are reflected in the momentum distributions. As U_{cf} is switched on, the wave number dependence of the conduction electrons become weaker and weaker and therefore less itinerant in real space, while the distribution of the f electrons becomes more and more dispersive as it can be seen in Fig. 2 (b) and (c). Above $U_{cf} \approx U_f/2 + W/4$ both distributions hardly depend on the wave number as it is observed in Fig. 2 (d). That is, the behavior of the momentum distributions agrees well with the results of the entropy analysis.

III. AWAY FROM HALF FILLING

In the previous section we considered the half-filled case. Now we discuss what happens when the ground state is metallic, and fix the electron density at $n = 1.75$. It has been shown,^{15,16} that a stable mixed valence regime appears around $n^f = 2 - n$ in the presence of U_{cf} , and strong enough U_{cf} leads to a first-order transition between the Kondo and mixed valence states as ε_f is varied. One can observe in Fig. 3, that for strong U_{cf} a stable mixed valence regime appears indeed, and the change of the valence becomes sharp. In the follow-

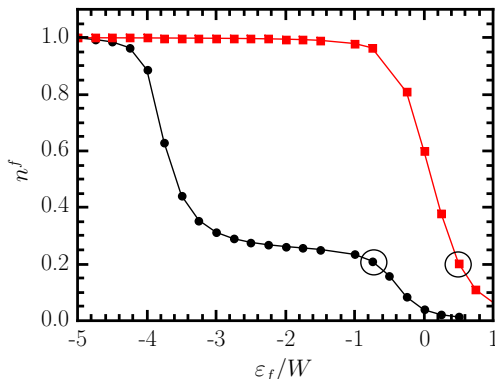


FIG. 3. The f -level occupancy as a function of ε_f for $L = 80$, $U_{cf} = 0$ (■) and $U_{cf}/W = 4$ (●), furthermore $U_f/W = 10$, $V/W = 0.2$. The circled data points are used in the comparison in Fig. 4. The lines are guides to the eye.

ing we investigate how the momentum distribution of the electrons change due to U_{cf} in the mixed valence regime. This is shown in Fig. 4, where ε_f , indicated by the circles around the data points in Fig. 3, was chosen such that the occupancy of the f level is nearly the same in the two cases. One can clearly see that both $n^c(k)$ and $n^f(k)$ change drastically around the Fermi momentum when $U_{cf} = 0$. This is not surprising since our system is a Luttinger liquid, where a logarithmic singularity is expected to occur at the Fermi momentum. For a finite U_{cf} a significant amount of the conduction and f electrons is scattered above the Fermi momentum and the

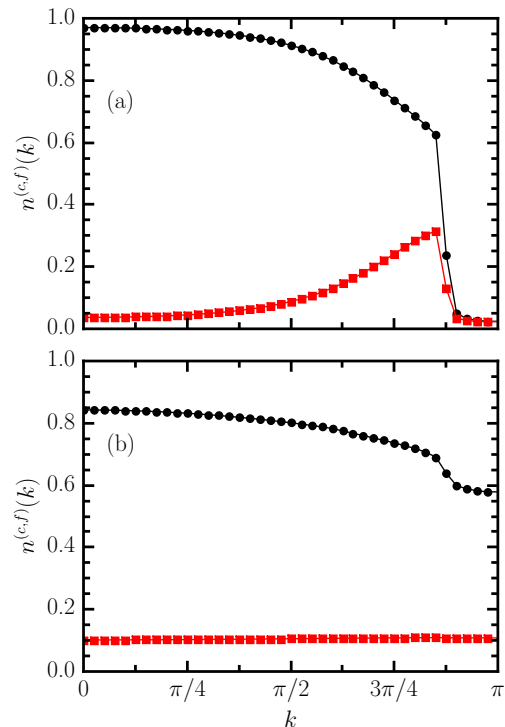


FIG. 4. Momentum distribution functions of the conduction (●) and f (■) electrons for $L = 80$ and $n = 1.75$. Panel (a), (b) correspond to $U_{cf}/W = 0$, $\varepsilon_f/W = 0.5$ and $U_{cf}/W = 4$, $\varepsilon_f/W = -0.75$, respectively, furthermore $U_f/W = 10$, $V/W = 0.2$ in all cases. The lines are guides to the eye.

k -dependence of the electron densities is significantly reduced in both cases, which indicates a strongly correlated mixed valence state. It is worth noting that the distribution functions do not tend to zero above the Fermi momentum for strong U_{cf} . These results agree well with what has been obtained in infinite dimensions using the Gutzwiller wave function,¹⁶ the main difference is the absence of the discontinuity at the Fermi momentum due to the one-dimensional property of the model.

IV. CONCLUSIONS

We have investigated an extended periodic Anderson model with an additional Coulomb interaction using the DMRG algorithm to better understand its effect on the momentum distribution of the electrons. In the half-filled, symmetric model (in the Kondo regime), switching on U_{cf} results in the increased itinerancy of the f electrons, however, above a certain value of U_{cf} it tends to localize f electrons again. The itinerancy of the conduction electrons is gradually reduced as U_{cf} is increased. These results agree well with what has been obtained by quantum information analysis.²⁰ We also investigated what happens when the system is less than half-filled, that is the ground state is metallic. It has been revealed that in the mixed valence regime U_{cf} makes both the con-

duction and f electrons more correlated. These findings agree qualitatively well with the properties of the infinite dimensional model, although, as expected for a one-dimensional model, there is no sharp Fermi edge. This could be analyzed further using the momentum space

version of the DMRG method.^{29–32}

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