

Phase diagram of the one-dimensional Anderson lattice

M. Guerrero

Department of Physics and Astronomy, University of California, Irvine, California 92717

R. M. Noack

Institut für theoretische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

(Received 5 October 1995)

We map out the phase diagram of the one-dimensional Anderson lattice by studying the ground-state magnetization as a function of band filling using the density matrix renormalization group technique. For strong coupling, we find that the quarter-filled system has an $S=0$ ground state with strong antiferromagnetic correlations. As additional electrons are put in, we find first a ferromagnetic phase, as reported by Möller and Wölfle, and then a phase in which the ground state has total spin $S=0$. Within this $S=0$ phase, we find Ruderman-Kittel-Kasuya-Yosida oscillations in the spin-spin correlation functions.

I. INTRODUCTION

In recent years, heavy fermion materials have attracted a lot of interest, from both the experimental and theoretical points of view. These systems, usually rare earth or actinide compounds, show a variety of unusual properties. At high temperatures ($T=100$ K), they behave as metals with weakly interacting magnetic moments. When the temperature is lowered, their behavior is consistent with the development of a narrow band of conduction electrons with very large effective masses m^* , up to two or three orders of magnitude larger than the bare electron mass.¹

The Anderson lattice Hamiltonian is believed to contain the essential physics needed to describe the low temperature properties of heavy fermion materials. It considers a localized orbital at each lattice site that hybridizes with an extended band of conduction electrons. Double occupation of the localized orbital is penalized by a strong Coulomb repulsion U .

Heavy fermions systems exhibit different kinds of ground states: antiferromagnetic, superconducting, paramagnetic, or semiconducting.¹ Therefore, it is important to investigate the magnetism of the ground state of the Anderson lattice as a function of the band filling.

Previous studies of this model have shown somewhat contradictory results regarding the magnetism of the ground state. Using the Gutzwiller approach, Rice and Ueda² studied the $U=\infty$ case in which doubly occupied states of the localized orbital are forbidden. They found that when the energy of the localized orbital is well below the Fermi surface, there is always a ferromagnetic instability (assuming no orbital degeneracy). However, they only considered uniform magnetic states in their solution. In contrast, the standard mean-field slave boson treatment of the problem³ gives a paramagnetic solution for any filling in the $U=\infty$ case. Reynolds, Edwards, and Hewson⁴ reformulated the Gutzwiller approach using the Kotliar and Ruckenstein slave boson treatment. They also found that a large region of the parameter space has a ferromagnetic ground state, but they concluded that the Gutzwiller solution may be too biased towards the magnetic state.

Möller and Wölfle⁵ used the Kotliar and Ruckenstein slave boson treatment to study the one-dimensional Anderson lattice. They concentrated on the symmetric case⁶ in which the energy of the localized orbital ε_f is $-U/2$, and allowed for the possibility of nonuniform magnetic states. They found that in the strong-coupling case (large U) near quarter-filling there is a very narrow antiferromagnetic region. As they increased the filling they found a transition to a ferromagnetic state, and for even larger fillings they found a ground-state magnetization with an incommensurate wave vector q . The wave vector q increases with filling and reaches π for the half-filled system, corresponding to antiferromagnetic order.

There are also some rigorous results regarding certain special cases. It has been shown that the ground state of the symmetric Anderson lattice Hamiltonian is a singlet in the half-filled case⁷ and has short-range antiferromagnetic correlations.⁸ Also, when the number of electrons is equal to the number of sites plus one (quarter-filling with one additional electron), the ground state was shown to be ferromagnetic for sufficiently large U in Ref. 9.

All the methods described above rely on some approximation scheme to solve the Hamiltonian. For example, in the slave boson techniques, a set of auxiliary bosons is introduced, in addition to the original fermions. In order to eliminate the nonphysical states of the enlarged Fock space, it is necessary to impose constraints on the boson operators. However, within a mean-field treatment, the constraints are not satisfied at each lattice site but only on average for the system as a whole. In the Gutzwiller approximation, the strong correlations are taken into account by renormalizing the hybridization matrix element by a factor that depends on the spin and on the average number of f electrons per site.

In this work we use the density matrix renormalization group (DMRG) method¹⁰ to study the phase diagram of the one-dimensional Anderson lattice model. The method gives quite accurately the properties of the exact ground state and low-lying excited states on a finite cluster, but for larger lattice sizes than, for example, Lanczos exact diagonalization calculations. The advantage over the analytic studies mentioned above is that the DMRG takes into account quantum

fluctuations, whereas the analytic methods described above treat the system within mean-field approximations. In the past, most numerical studies of the one-dimensional Anderson lattice have been limited to the symmetric half-filled case. Here we consider fillings between quarter-filling and half-filling. We investigate the symmetric case using chains of 8 and 16 sites and the $U=\infty$ case with lattices of 8 sites. Our results in the strong-coupling regime are in good agreement with Ref. 5. Near quarter-filling we find an $S=0$ ground state. As electrons are added we find first a ferromagnetic region, and then once again an $S=0$ ground state for still larger fillings. In order to determine the nature of the magnetic correlations in the phases with $S=0$, we examine the spin-spin correlation function.

Our results are consistent with the rigorous results described above and also with the phase diagram obtained in a numerical study of the Kondo lattice model.¹¹ Since the symmetric Anderson Hamiltonian can be mapped into the Kondo Hamiltonian¹² when the hybridization between the f band and the conduction band is small compared to U , the phase diagrams should be similar in this regime.

This work is organized as follows. We briefly describe the one-dimensional Anderson lattice Hamiltonian and discuss some of its properties in Sec. II. In Sec. III we present the numerical results. We study chains of 8 and 16 sites for the case in which $\varepsilon_f = -U/2$ in Sec. III A, and draw a phase diagram based on the total spin of the ground state and the nature of the spin-spin correlation functions. In Sec. III B we construct the phase diagram for $U=\infty$ using results on chains of 8 sites. Our conclusions are given in Sec. IV.

II. THE PERIODIC ANDERSON HAMILTONIAN

We consider the standard periodic Anderson Hamiltonian in one dimension:

$$H = -t \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + c_{i+1\sigma}^\dagger c_{i\sigma}) + \varepsilon_f \sum_{i\sigma} n_{i\sigma}^f + U \sum_i n_{i\uparrow}^f n_{i\downarrow}^f + V \sum_{i\sigma} (c_{i\sigma}^\dagger f_{i\sigma} + f_{i\sigma}^\dagger c_{i\sigma}), \quad (1)$$

where $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ create and annihilate conduction electrons with spin σ at lattice site i , and $f_{i\sigma}^\dagger$ and $f_{i\sigma}$ create and annihilate local f electrons. Here t is the hopping matrix element for conduction electrons between neighboring sites, ε_f is the energy of the localized f orbital, U is the on-site Coulomb repulsion of the f electrons, and V is the on-site hybridization matrix element between electrons in the f orbitals and the conduction band. For simplicity, we neglect orbital degeneracy. We denote the number of electrons by N_{el} , and N is the number of sites in the lattice. Since there are two electronic orbitals in each site, the quarter-filled case corresponds to $N_{el}=N$ and the half-filled case has $N_{el}=2N$.

For $U=0$ this Hamiltonian can be exactly diagonalized in momentum space, yielding two hybridized bands with energies λ_k^\pm

$$\lambda_k^\pm = \frac{1}{2} \left[[\varepsilon_f - 2t \cos(ka)] \pm \sqrt{[\varepsilon_f + 2t \cos(ka)]^2 + 4V^2} \right], \quad (2)$$

where a is the lattice constant. Therefore, when the number of electrons is between quarter-filling and half-filling, the lower band is occupied but the upper band is always empty, and the ground state is paramagnetic for any filling.

Now consider the case when the f level is well below the conduction band and the Coulomb repulsion U is large. With no hybridization ($V=0$), the ground state at quarter-filling has one electron at each f site and there is degeneracy in the spin configurations. When $V>0$, exchange interactions remove this degeneracy. It can be shown using perturbation theory that the effective interaction between neighboring sites favors antiferromagnetic ordering of neighboring f electrons.^{5,13} The relevant exchange process is sixth order and involves an f electron hopping to the conduction band, then to a nearest-neighbor conduction site and then into the f orbital on that site. In the intermediate state, the f orbital is doubly occupied, which is only possible if the spins of the electrons are opposite. This leads to an effective antiferromagnetic interaction.

When the filling is increased slightly, the additional electrons go into the conduction orbitals because of the strong Coulomb repulsion U in the f orbitals. In this case, there is an on-site antiferromagnetic correlation between the electron in the conduction orbital and the one in the f orbital, favoring a local singlet. To optimize the kinetic energy of the conduction electrons, it is favorable for the f electrons to have their spins oriented in the same direction.^{5,9} Therefore, if there are N_c conduction electrons compensating the f spins, one expects a ferromagnetic ground state with $S=(N-N_c)/2$. When this value of S is realized, we will call it *complete* ferromagnetism. If the value of S we find is smaller than the complete value, but still greater than the minimum (0 or 1/2), then we will refer to it as *incomplete* ferromagnetism, meaning that not all the uncompensated f electrons are aligned. These two effects give rise to a competition between ferromagnetic and antiferromagnetic ordering near quarter-filling.⁵

On the other hand, when the filling is further increased in the strong-coupling case, the interaction between f electrons, mediated by the Fermi sea, starts to play an important role. This is the well-known Ruderman-Kittel-Kasuya-Yosida¹⁴ (RKKY) interaction that induces correlations with wave vector $q=2k_F$ between the f electrons, where k_F is the Fermi wave vector of the noninteracting ($V=0$) Fermi sea of conduction electrons.

For simplicity, we concentrate here on two particular cases of the Anderson Hamiltonian: the symmetric case⁶ in which $\varepsilon_f = -U/2$ and the $U=\infty$ case. This reduces the number of independent Hamiltonian parameters by one. In the symmetric case, strong coupling (large U) means that the f level is far below the conduction band. Therefore we expect to find a competition between antiferromagnetic and ferromagnetic correlations near quarter-filling and to find RKKY correlations for larger fillings. For small U , we expect a paramagnetic ground state. In the $U=\infty$ case we set the f level ε_f to be less than or equal to 0. Again, when ε_f falls below the conduction band, we expect competition between antiferromagnetic and ferromagnetic correlations near quarter-filling, and RKKY interactions near half-filling.

III. RESULTS

A. The symmetric case

We first consider the symmetric case, $\varepsilon_f = -U/2$. We fix $t=0.5$, $V=0.375$ and vary U from 0 to 6 (all energies are in units of $2t$, which is half the bandwidth). This choice of parameters allows us to do a quantitative comparison with Ref. 5. We use the DMRG technique¹⁰ to find the energies and equal-time correlation functions of the ground state and low-lying states on finite lattices. While this technique gives energies that are, in principle, variational, it has proven to give quite accurate results for one-dimensional (1D) quantum lattice systems. The method provides a controlled way of numerically diagonalizing a finite system within a truncated Hilbert space. One can increase the accuracy by increasing the number of states kept, and can examine the convergence with the number of states. Here we typically keep up to 150 to 200 states per block, although in the numerically more difficult cases, such as the calculation of the correlation functions for the 16 site chains, we keep up to 400 states. Truncation errors, given by the sum of the density matrix eigenvalues of the discarded states, vary from 10^{-5} in the worse cases to 10^{-9} in the best cases. This discarded density matrix weight is directly correlated with the absolute error in the energy. Since the method is most accurate for a given amount of computational effort when the system has open boundary conditions (i.e., no nearest-neighbor connection between site 1 and site N), we apply open boundary conditions here.

Within the DMRG method, we fix the number of electrons N_{el} and the z component of the total spin of the system S_z and find the ground state within this subspace. In order to determine the nature of the ground state, we would like to determine the total spin, S . For a ground state of a given S_z , there are several possible values of the total spin S ($S_z \leq S \leq N_{\text{el}}/2$). In order to establish the value of S , we calculate the mean value of the operator \mathbf{S}^2 in the ground state with the lowest possible S_z (0 or 1/2 according to whether N_{el} is even or odd). In this way we can be sure that we are considering all the possible values of S . Since $\langle \mathbf{S}^2 \rangle = S(S+1)$ (setting $\hbar = 1$), we can deduce the value of S . For example, for 8 sites with $U=4$ and $N_{\text{el}}=9$, we obtain $\langle \mathbf{S}^2 \rangle = 15.748$ for the $S_z = 1/2$ ground state, implying $S = 7/2$.

In some cases, states with different values of S can be close in energy. When this happens, the wave function obtained for the ground state with a given S_z can be composed of a mixture of states with two or more S values, rather than having a definite value of S . This occurs mainly for longer chains ($N \geq 16$), for which the numerical accuracy is lower and the states are closer together in energy. In these cases, although we cannot immediately determine the value of S , we can conclude that it is not the smallest possible value. We can then study states with higher values of S_z , for which the Hilbert space is smaller (there are fewer values of S allowed) and therefore there is less mixing. Also, since we keep the same number of states in a smaller Hilbert space, the numerical accuracy is higher. For example, on a 16 site lattice with $U=2$ and $N_{\text{el}}=22$, we obtain $\langle \mathbf{S}^2 \rangle = 25.38$ for the lowest $S_z=0$ state. This indicates the S is likely to be higher than 3 but it could be either 4 or 5. We then consider the lowest

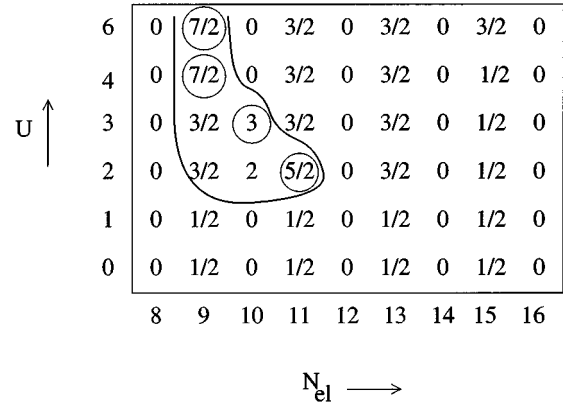


FIG. 1. Values of the spin S for different values of U and N_{el} in the ground state for 8 site chains. Parameters are $\varepsilon_f = -U/2$, $t=0.5$, and $V=0.375$. There is a narrow ferromagnetic region near quarter-filling (enclosed by a solid line). Complete ferromagnetic states are circled.

energy $S_z = 2, 3, 4$, and 5 states, and obtain $\langle \mathbf{S}^2 \rangle = 26.39, 28.35, 29.97$, and 30.00, respectively. The energies in all cases are degenerate to within the estimated accuracy of the calculation. Therefore, we conclude that $S=5$ for this case.

In Fig. 1 we present our results for the spin S of the ground state of the 8 site chain, showing the number of electrons on the horizontal axis and U on the vertical axis. At quarter-filling ($N_{\text{el}} = N = 8$), we find the ground state always has $S=0$. Also, for $U=0$ or U small, we find that the ground state is paramagnetic at all fillings, as predicted by the qualitative picture given in Sec. II. For $U \geq 2$, we find a narrow ferromagnetic region slightly above quarter-filling (enclosed with a solid line as a guide to the eye). We circle the cases of complete ferromagnetism as defined in the preceding section.

For larger fillings, we find an $S=0$ ground state for all couplings U . However, when the number of electrons is odd we obtain $S=3/2$ and not $S=1/2$ as one would expect. We attribute this to a finite size effect for the following reason: if we consider chains with 16 sites with the same density of electrons (for example, $U=4$ with 22, 26, 30 electrons), we find $S=0$ in the ground state. This alternation of $S=0$ and $S=3/2$ states was also observed in Ref. 13 in the context of the phase diagram of the Kondo lattice model. The $S=3/2$ state appears when there is an odd number of electrons in the conduction band, so that one of the conduction energy levels has a single electron. The f electrons will then interact mainly with the single unpaired electron and will tend to align ferromagnetically.¹¹ Roughly speaking, for an f electron to interact with one electron of the doubly occupied conduction band and produce a spin flip with energy gain J_{eff} , one conduction electron needs to hop to a higher energy level. When the effective Kondo coupling, J_{eff} (given by the Schrieffer-Wolff transformation¹²), is less than the spacing of the conduction electron energy levels, the f electrons can only couple with the unpaired conduction electron. In fact, as J_{eff} decreases, this effect becomes more important and, presumably for J_{eff} small enough, the ground state should have the maximum value, $S=(N-1)/2$. However, in the infinite system there is no finite separation between conduction energy levels, and the ground state should be paramagnetic for any value of J_{eff} .

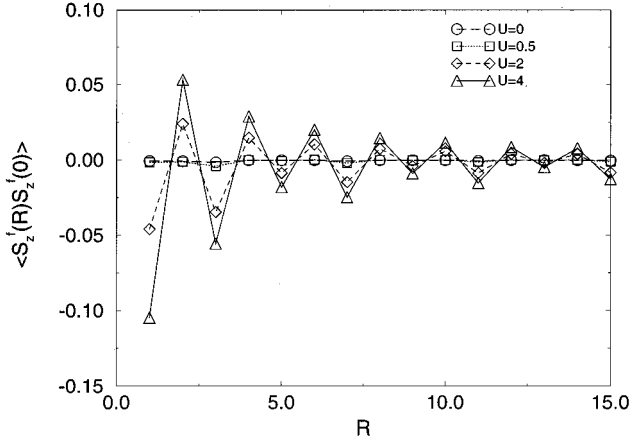


FIG. 2. The f -spin- f -spin correlation functions versus distance R apart at quarter-filling for $\varepsilon_f = -U/2$, $t=0.5$, and $V=0.375$ and different values of U . Antiferromagnetic correlations develop as U increases.

In order to better understand the nature of the correlations in the antiferromagnetic phase at quarter-filling and the transition to the ferromagnetic phase as the filling is increased, we have also carried out calculations on a 16 site lattice. At quarter-filling, the ground state is $S=0$ for all the U values we considered, but as U increases there is an onset of short-range antiferromagnetic correlations. In Fig. 2 we plot the f -spin- f -spin correlation function at quarter-filling for different values of U . For $U=0$, the correlations are very small and always negative. As U increases, they alternate in sign and increase in amplitude. This result is consistent with Ref. 5 which found a narrow antiferromagnetic region near quarter-filling. For the fully interacting system in 1D, treated exactly by the DMRG, quantum fluctuations destroy the long-range antiferromagnetic correlations found in the mean-field slave boson calculations, but short-range antiferromagnetic correlations remain.

For $U=2, 3, 4$, and 6 , we map out the extent of the ferromagnetic phase by increasing N_{el} until the ground state becomes paramagnetic. We plot the resulting phase diagram in Fig. 3. Here “C” denotes the states with complete ferromagnetism [$S = (N_{el} - N_c)/2$] and “I” denotes the states with incomplete ferromagnetism [$S < (N_{el} - N_c)/2$ but larger than the lowest possible value]. The states of incomplete ferromagnetism in the boundary region between the ferromagnetic and antiferromagnetic phases suggest that the ferromagnetic order parameter may go to zero continuously, implying a second order phase transition.

For the $U=6$ and $U=4$ points with $N_{el}=20$, the $U=3$, $N_{el}=22$, and the $U=2$, $N_{el}=18$ points in Fig. 3, the difference in energy between the $S=0$ and $S=1$ states is of the order of the numerical accuracy, making it hard to determine the total spin of the ground state. However, we include these points in the paramagnetic region because an $S=1$ ground state, although still ferromagnetic, indicates a very strong suppression of the ferromagnetism, and because the ground state is paramagnetic at the same parameters and average fillings in the 8 site chain. Also, for $U=2$, $N_{el}=19$, and $N_{el}=23$ the states are also very close in energy and it is very hard to establish the value of S in the ground state. However,

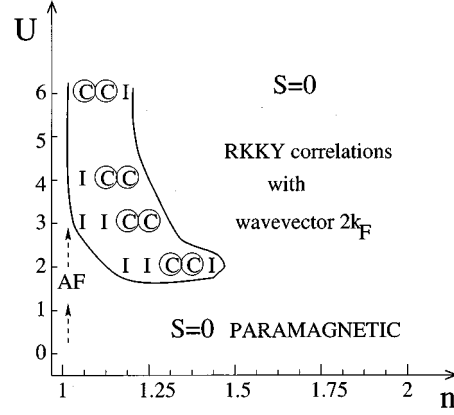


FIG. 3. The phase diagram for the 1D Anderson lattice combining results of chains of 8 and 16 sites. Parameters are $\varepsilon_f = -U/2$, $t=0.5$, $V=0.375$, and $n = N_{el}/N$. Here “C” denotes complete ferromagnetism and “I” incomplete ferromagnetism as defined in the text.

we can establish that S is greater than $1/2$ and that is smaller than $(N - N_c)/2$, so we list these points as incomplete ferromagnetism.

By comparing the results of 8 and 16 site chains for the same density of electrons $n = N_{el}/N$, one can see that the cases of complete ferromagnetism are always consistent. The incomplete ferromagnetism is systematic in the sense that for a given electron density, the incomplete ferromagnetism appears in both 8 and 16 site chains. However, the value of S does not necessarily scale with the number of sites. For example, for $U=3$ and $n = 1.125$ we find $S = 3/2$ for 8 sites and $S = 5$ for 16 sites.

For $U=4$ and $N=16$, we examine the spin-spin correlation functions at larger fillings ($N_{el}=24, 28, 32$). We calculate $C(q)$, the Fourier transform of $\langle S_z^f(R)S_z^f(0) \rangle$, where R is the distance in units of the lattice constant,¹⁵ for $N_{el}=24, 28$, and 32 . The continuous Fourier transform is calculated by zero-padding the function $\langle S_z^f(R)S_z^f(0) \rangle$ for $R > N$. In order to reduce spurious high frequency oscillations introduced by cutting off the real-space correlation function at the open boundaries, we window the data using a Bartlett windowing function¹⁶ over the interval $0 < R < N$ before transforming.

We plot $C(q)$ in Fig. 4 and we see that for each case there is a peak in $C(q)$ at $q = 2k_F$, where k_F is the Fermi wave vector of the noninteracting ($V=0$) conduction band ($k_F = \pi/4, 3\pi/8$, and $\pi/2$ for $N_{el}=24, 28$, and 32 , respectively). This form is characteristic of RKKY oscillations which are important in this $S=0$ regime. (The peaks for $N_{el}=24$ and 28 are slightly shifted from the exact value of $2k_F$; the shift is roughly 2%.)

We can compare our results with those of Ref. 5 in which the symmetric one-dimensional Anderson lattice was studied for the strong-coupling case using the Kotliar and Ruckenstein slave boson technique (the results for $U \geq 2.5$ are in their Fig. 9). In their antiferromagnetic region we find an $S=0$ ground state with short-range antiferromagnetic correlations that increase in magnitude and range as U increases. The parameter regimes in which we find complete ferromag-

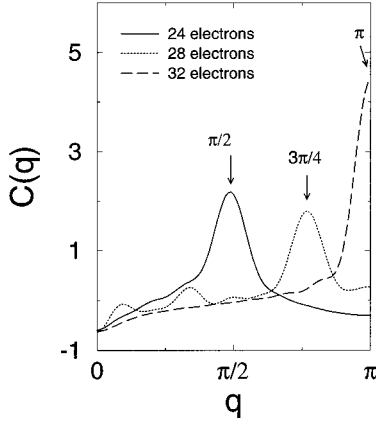


FIG. 4. The Fourier transform of the f -spin- f -spin correlation functions for $\varepsilon_f = -U/2$, $t = 0.5$, $V = 0.375$, $U = 4$, and different fillings. The peaks appear at $q = 2k_F$.

netism and incomplete ferromagnetism fall within the limits of their ferromagnetic region with the exception of our point at $U = 6$, $N_{el} = 19$ which lies in their paramagnetic region. We find incomplete ferromagnetism in the ground state at this point. This discrepancy could be due to the finite size effect described earlier in which there is a tendency towards a ferromagnetic state in the cases with an odd number of electrons in the conduction band. The ferromagnetism is always complete in Ref. 5, presumably due to the mean-field nature of their calculation. In contrast, we find a region of incomplete ferromagnetism in the boundary between the antiferromagnetic and ferromagnetic regions that suggests that the phase transition may be second order. At half-filling they find an antiferromagnetic ground state (in the strong-coupling regime). As they decrease the filling, the magnetic wave vector decreases linearly with the doping concentration from its value $q = \pi$ at half-filling. We associate this with the RKKY correlations with wave vector $2k_F$ that we find in a wide region below half-filling, since k_F is proportional to the electron density in one dimension. We therefore find that our phase diagram is in good overall agreement with that of Möller and Wölfle.⁵

B. The asymmetric $U = \infty$ case

We also study the asymmetric Anderson model at $U = \infty$, again fixing $V = 0.375$. We vary the position of the f level ε_f from 0 to -2.5 and study 8 site chains, keeping 100 states per block for the small $|\varepsilon_f|$ cases and up to 250 states per block for the larger $|\varepsilon_f|$. In Fig. 5, we tabulate the total spin S of the ground state as a function of the number of electrons N_{el} (horizontal axis) and the absolute value of ε_f (vertical axis). We consider $\varepsilon_f \leq 0$ only.

There is a clear resemblance between Figs. 5 and 1. As before, at exactly quarter-filling the ground state has $S = 0$ and there are increasing antiferromagnetic correlations as the f level falls below the bottom of the conduction band. There is a narrow ferromagnetic region near quarter-filling and then a paramagnetic region at larger fillings. The ferromagnetic region starts roughly where the f level falls below the conduction band (Kondo regime). For small values of ε_f

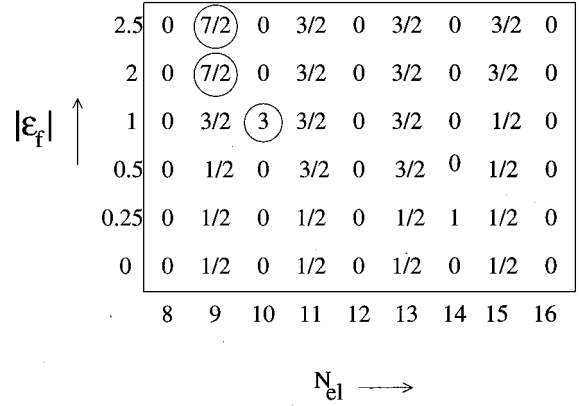


FIG. 5. Values of the spin S for different values of $|\varepsilon_f|$ and N_{el} in the ground state for $U = \infty$, $t = 0.5$, $V = 0.375$, and chains with 8 sites. There is a narrow ferromagnetic region near quarter-filling.

(mixed-valence regime), we find a paramagnetic state at all fillings. This is in contradiction with the Gutzwiller result that predicts that there will always be a ferromagnetic instability at any filling. At quarter-filling, antiferromagnetic correlations prevail, and at larger fillings, there is a region in which the ground state has $S = 0$. In this region, RKKY interactions presumably dominate the magnetic correlations, as in the symmetric case. In a previous study, it was shown that for the half-filled system, RKKY correlations are important in the Kondo regime but are strongly suppressed in the mixed-valence regime.¹⁷

In the mixed-valence region there is no ferromagnetism at any filling, in agreement with the slave boson mean-field approach. However, the slave boson treatment predicts a paramagnetic state for any value of ε_f . This suggests that the slave boson description is appropriate for the mixed-valence case, but breaks down in the Kondo regime.

IV. CONCLUSIONS

We constructed the phase diagram of the one-dimensional Anderson lattice using the density matrix renormalization group technique. The results are summarized in Fig. 3. We considered the symmetric case with $\varepsilon_f = -U/2$ and the asymmetric case with $U = \infty$. In the symmetric case for large U we found an $S = 0$ ground state with short-range antiferromagnetic correlations at quarter-filling that increase as U increases. At slightly larger fillings, there is a transition to a ferromagnetic state. The presence of a small region of incomplete ferromagnetism in the boundary suggests a second order transition. For small values of U in the symmetric case we find, as expected, a paramagnetic state at all fillings. For small values of $|\varepsilon_f|$, the phase diagram of the $U = \infty$, asymmetric case is quite similar.

In the strong-coupling limit in the symmetric case, we compared our results with Ref. 5 which studied the one-dimensional Anderson lattice using the Kotliar-Ruckenstein slave boson approach. We found good qualitative agreement with their results. The ferromagnetic region is the same in both cases. However, we find incomplete ferromagnetism in

the boundary with the $S=0$ region near quarter-filling, in contrast to the sharp transition found in Möller and Wölfle's work. Also, where they find long-range antiferromagnetic order, we obtain short-range antiferromagnetic correlations. This can be attributed to the presence of quantum fluctuations that are not taken into account in their treatment. In the strong-coupling case, our phase diagram is consistent with the phase diagram of the Kondo lattice Hamiltonian¹¹ in the small J region.

In the $U=\infty$ case, our results agree with the predictions of the standard slave boson mean-field approach³ only for small values of $|\varepsilon_f|$ (the mixed-valence case). For larger values of

$|\varepsilon_f|$, the standard slave boson technique fails to predict ferromagnetism and RKKY correlations.

ACKNOWLEDGMENTS

We would like to thank Steve White and Kazuo Ueda for helpful discussions. We also thank Clare Yu for critically reading the manuscript. This work was supported in part by ONR Grant No. N000014-91-J-1502, Los Alamos National Laboratory, and an allocation of computer time from the University of California, Irvine. Some of the numerical calculations were performed at the San Diego Supercomputer Center.

-
- ¹D. W. Hess, P. S. Riseborough, and J. L. Smith, *Encycl. Appl. Phys.* **7**, 435 (1993).
- ²T. M. Rice and K. Ueda, *Phys. Rev. Lett.* **55**, 995 (1985); *Phys. Rev. B* **34**, 6420 (1986).
- ³P. S. Riseborough, *Phys. Rev. B* **45**, 13 984 (1992).
- ⁴A. M. Reynolds, D. M. Edwards, and A. C. Hewson, *J. Phys. Condens. Matter* **4**, 7589 (1992).
- ⁵B. Möller and P. Wölfle, *Phys. Rev. B* **48**, 10 320 (1993).
- ⁶Note that technically speaking the symmetric case corresponds to $\varepsilon_f - \mu = -U/2$, where μ is the chemical potential of the noninteracting conduction electrons which varies as a function of the filling. The case $\varepsilon_f = -U/2$ corresponds to the symmetric case at half-filling for which $\mu=0$.
- ⁷K. Ueda, H. Tsunetsugu, and M. Sigrist, *Phys. Rev. Lett.* **68**, 1030 (1992).
- ⁸G. S. Shan Tian, *Phys. Rev. B* **50**, 6246 (1994).
- ⁹T. Yanagisawa, *Phys. Rev. Lett.* **70**, 2024 (1993).
- ¹⁰S. R. White, *Phys. Rev. Lett.* **68**, 3487 (1992); *Phys. Rev. B* **48**, 10 345 (1993); R. M. Noack, S. R. White, and D. J. Scalapino, in *Computer Simulations in Condensed Matter Physics VII*, edited by D. P. Landau, K. K. Mon, and H. B. Schüttler (Springer-Verlag, Heidelberg, 1994), pp. 85–98.
- ¹¹H. Tsunetsugu, M. Sigrist, and K. Ueda, *Phys. Rev. B* **47**, 8345 (1993).
- ¹²J. R. Schrieffer and P. A. Wolff, *Phys. Rev.* **149**, 491 (1966).
- ¹³C. Bastide and C. Lacroix, *J. Phys. C* **21**, 3557 (1988).
- ¹⁴M. A. Ruderman and C. Kittel, *Phys. Rev.* **96**, 99 (1954).
- ¹⁵The correlation functions $\langle S_z^f(R)S_z^f(0) \rangle$ for a certain distance R were obtained by averaging over all pairs of sites separated by a distance R . This procedure averages out the effects of local density fluctuations due to the open boundaries and results in a correlation function that is close to the infinite system one until R gets to within a few lattice spacings of the system size.
- ¹⁶W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C*, 2nd ed. (Cambridge University Press, Cambridge, 1992), p. 554.
- ¹⁷M. Guerrero and C. C. Yu, *Phys. Rev. B* **51**, 10 301 (1995).