

Many-body band structure and Fermi surface of the Kondo lattice

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We present a theory for the single-particle excitations and Fermi surface of the Kondo lattice. Thereby we construct an effective Hamiltonian describing the creation and propagation of single-particle-like charge fluctuations on a ‘‘resonating-valence-bond background’’ of local singlets. The theory may be viewed as a Fermionic version of linear spin-wave theory and is of comparable simplicity so that the calculations for the strong-coupling limit can be performed analytically. We calculate the single-particle spectral function for the ‘‘pure’’ Kondo lattice as well as for several extended versions: with a Coulomb repulsion between conduction and f electrons, Coulomb repulsion between conduction electrons, and a ‘‘breathing’’ f orbital. In all cases we study the evolution of the spectrum in going from the Kondo insulator to the heavy electron metal. We compare our results to exact diagonalization of small clusters and find remarkable agreement in nearly all cases studied. In the metallic case the f electrons participate in the Fermi surface volume even when they are replaced by localized Kondo spins and the number of bands, their dispersion and spectral character, and the nontrivial (i.e., nonrigid bandlike) doping dependence including a pronounced transfer of spectral weight are reproduced at least semiquantitatively by the theory. [S0163-1829(98)02236-X]

I. INTRODUCTION

The theoretical description of the Kondo lattice remains an outstanding problem of solid-state physics. This model, or variations of it, may be viewed as the appropriate one for understanding such intensively investigated classes of materials as the heavy electron metals,¹⁻³ Kondo insulators,⁴ and possibly the recently discovered⁵ transition-metal hydride-based switchable mirror compounds.^{6,7} The simplest model that incorporates the essential physics may be written as

$$\begin{aligned}
 H = & \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} + V \sum_{i,\sigma} (c_{i,\sigma}^{\dagger} f_{i,\sigma} + \text{H.c.}) \\
 & - \epsilon_f \sum_{i,\sigma} f_{i,\sigma}^{\dagger} f_{i,\sigma} + U_f \sum_i f_{i,\uparrow}^{\dagger} f_{i,\uparrow} f_{i,\downarrow}^{\dagger} f_{i,\downarrow} \\
 & + U_{fc} \sum_{i,\sigma,\sigma'} f_{i,\sigma}^{\dagger} f_{i,\sigma} c_{i,\sigma'}^{\dagger} c_{i,\sigma'} + U_c \sum_i c_{i,\uparrow}^{\dagger} c_{i,\uparrow} c_{i,\downarrow}^{\dagger} c_{i,\downarrow}.
 \end{aligned} \tag{1}$$

Here we consider the minimal model, where each unit cell contains two orbitals, one of them for the mobile conduction electrons the other for the strongly correlated f electrons. Then, $c_{i,\sigma}^{\dagger}$ ($f_{i,\sigma}^{\dagger}$) creates a conduction electron (f electron) in cell i , and $\epsilon_{\mathbf{k}} = 1/N \sum_{i,j} e^{i\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_i)} t_{i,j}$ is the Fourier transform of the intercell hopping integral $t_{i,j}$ for c electrons. For later reference we have already included a Coulomb repulsion U_{fc} between f and conduction electrons in the same cell, and a Coulomb repulsion U_c between conduction electrons. The latter two parameters are usually taken to be zero, but as will be seen below our formalism allows us to take them into account without any additional effort. In the so-called sym-

metric case, $U_f = 2\epsilon_f$, and the limit $U_f \rightarrow \infty$ (1) can be reduced to its strong-coupling limit⁸

$$H_{sc} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} + J \sum_i \mathbf{S}_{i,c} \cdot \mathbf{S}_{i,f}, \tag{2}$$

where $\mathbf{S}_{i,c}$ ($\mathbf{S}_{i,f}$) denotes the spin operator for conduction electrons (f electrons) in cell i and $J = 4V^2/U_f$.

While the impurity versions of these models, which retain only a single f site in a sea of conduction electrons, are well understood^{2,3,9-12} and are even amenable to exact solutions,^{13,14} much less is known about the lattice models. One problem that by many is believed to be at the heart of the solution is the way in which the more or less localized f electrons, which in the strong-coupling theory are replaced by mere spin degrees of freedom, participate in the formation of the Fermi surface and the heavy quasiparticle bands. Experiments on heavy Fermion compounds,¹⁵ computer simulations of Kondo lattices,^{16,17} and theoretical considerations^{18,19} suggest that despite their frozen charge degrees of freedom, the f electrons participate in the Fermi surface volume as if they were uncorrelated. In other words, the experimental Fermi surface volume corresponds to the case $U_f = U_{fc} = U_c = 0$. The limiting cases $V = 0$ or $J = 0$, which obviously do not allow for participation of the f electrons in the Fermi surface, therefore represent singular points, so that a perturbation expansion in the (small) parameters V or J may not be expected to give meaningful results. Rather, the interaction between f spins and conduction electrons must be incorporated in a nonperturbative way, in a manner similar to that of the single-impurity Kondo effect.¹⁴ It is the purpose of the present manuscript to present a minimum effort theory for the Kondo lattice that is based on this

basic requirement and shows how the nominal participation of the localized electrons in the Fermi surface can be understood even in the complete absence of any true hybridization. We describe the system by an effective Hamiltonian for the fermionlike charge fluctuations on top of a strong-coupling ground state, and show that this treatment leads to remarkable agreement with numerical results at least on energy scales that are relevant to high-energy spectroscopy. We would also like to point out that the method of calculation is similar in spirit to the cell-perturbation method developed by Jefferson and co-workers.²⁰ A preliminary report has been published elsewhere.²¹

II. CONSTRUCTION OF THE EFFECTIVE HAMILTONIAN

As our starting point we choose the case of vanishing intercell hopping $t_{i,j}$ (i.e., $\epsilon_k=0$). The lattice problem then reduces to single-cell problems so that we first discuss the eigenstates of a single cell with one, two, and three electrons. The two-electron ground state is a singlet with wave function

$$|\Psi_0^{(2)}\rangle = \left[\alpha f_{\uparrow}^{\dagger} f_{\downarrow}^{\dagger} + \frac{\beta}{\sqrt{2}} (c_{\uparrow}^{\dagger} f_{\uparrow}^{\dagger} + f_{\uparrow}^{\dagger} c_{\uparrow}^{\dagger}) + \gamma c_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger} \right] |\text{vac}\rangle \quad (3)$$

(we have suppressed the site index on the fermion creation operators). The ground-state wave function and energy is then obtained by diagonalizing the 3×3 matrix,

$$H_2 = \begin{pmatrix} -2\epsilon_f + U_f & \sqrt{2}V & 0 \\ \sqrt{2}V & -\epsilon_f + U_{fc} & \sqrt{2}V \\ 0 & \sqrt{2}V & U_c \end{pmatrix}. \quad (4)$$

For the strong-coupling model (2) the problem becomes trivial with $\alpha = \gamma = 0$, $\beta = 1$, the energy of the two-electron ground state is $-(3J/4)$.

The single- or three-electron states can be written as

$$|\Psi_{\nu,\sigma}^{(1)}\rangle = (\beta'_{\nu} f_{\sigma}^{\dagger} + \gamma'_{\nu} c_{\sigma}^{\dagger}) |\text{vac}\rangle,$$

$$|\Psi_{\mu,\sigma}^{(3)}\rangle = (\alpha''_{\mu} c_{\sigma}^{\dagger} f_{\uparrow}^{\dagger} f_{\downarrow}^{\dagger} + \beta''_{\mu} c_{\uparrow}^{\dagger} c_{\downarrow}^{\dagger} f_{\sigma}^{\dagger}) |\text{vac}\rangle, \quad (5)$$

and the wave functions and energies are obtained by diagonalizing the matrices

$$H_1 = \begin{pmatrix} -\epsilon_f & V \\ V & 0 \end{pmatrix} \quad (6)$$

and

$$H_3 = \begin{pmatrix} -2\epsilon_f + U_f + 2U_{fc} & -V \\ -V & -\epsilon_f + U_c + 2U_{fc} \end{pmatrix}. \quad (7)$$

For the strong-coupling limit the index ν takes only one value and we have $\gamma = \alpha = 0$, and $\beta = \beta' = 1$. Both the single- and three-electron states have zero energy in this case.

For later reference, we also define the photoemission and inverse photoemission (IPES) matrix elements (here $\alpha = c, f$)

$$r_{\alpha,\nu,\sigma} = \langle \Psi_{\nu,\sigma}^{(1)} | \alpha_{\sigma} | \Psi_0^{(2)} \rangle, \\ s_{\alpha,\mu,\sigma} = \langle \Psi_{\mu,\sigma}^{(3)} | \alpha_{\sigma}^{\dagger} | \Psi_0^{(2)} \rangle. \quad (8)$$

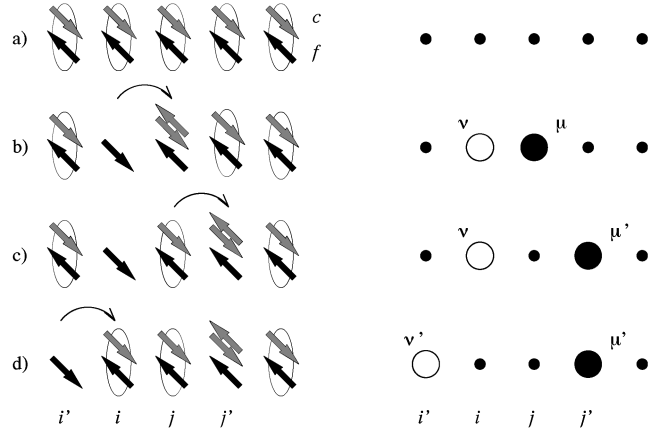


FIG. 1. Charge fluctuations and their propagation (left panel) and their representation in terms of model fermions (right panel).

They can be expressed in terms of the wave functions defined above, e.g.,

$$\langle \Psi_{\nu,\sigma}^{(1)} | c_{\sigma} | \Psi_0^{(2)} \rangle = \text{sign}(\sigma) \left(\gamma \gamma'_{\nu} + \frac{\beta \beta'_{\nu}}{\sqrt{2}} \right),$$

$$\langle \Psi_{\mu,\sigma}^{(3)} | c_{\sigma}^{\dagger} | \Psi_0^{(2)} \rangle = \alpha \alpha''_{\mu} - \frac{\beta \beta''_{\mu}}{\sqrt{2}}, \quad (9)$$

where the additional sign in the first equation is due to our convention for ordering the two spin directions in Eq. (3).²²

We now return to the lattice problem and consider the case of half-filling (i.e., two electrons/unit cell, corresponding to the Kondo insulator). For vanishing $t_{i,j}$ the lattice ground state is simply the product of N single-cell ground states of type (3) (see the state labeled *a* in Fig. 1). In the following, this state will be referred to as the vacuum. Then, switching on $t_{i,j}$ produces charge fluctuations in the vacuum state: an electron can hop from cell *i* to another cell *j*, leaving the cell *i* in a single-electron eigenstate with number ν , and the cell *j* in a three-electron eigenstate with number μ (see state *b* in Fig. 1). In a further step an electron from the threefold occupied cell *j* can hop to another neighbor *j'* leaving cell *j* in a two-hole eigenstate and *j'* in a three-hole state (see Fig. 1, state *c*) or, alternatively, an electron can hop from another neighbor *i'* into cell *i*, leaving *i* in a two-electron state, *i* in a single electron state. Finally, an electron from *j* can hop into *i*, leaving both *i* and *j* in two-electron states. In this picture the intercell kinetic energy may be viewed of as a perturbation that has a twofold effect: the pair creation of charge fluctuations and the propagation of these. It therefore plays a completely analogous role as the transverse part of the Heisenberg exchange in the linear spin-wave theory for the Heisenberg antiferromagnet, and in the following we want to exploit this analogy. To that end we make the additional assumption that a cell containing two electrons must always be in the two-electron ground state $|\Psi_0^{(2)}\rangle$. This means that after a charge fluctuation has passed through a given cell, the cell must return to the two-electron ground state. In other words, under this constraint the propagating charge fluctuations do not leave a trace of excited

cells—their propagation becomes coherent. Ways to relax this constraint and take into account incoherent processes will be discussed below.

As a last important step, we note that the pair creation process in Fig. 1 changes the energy by $E_\nu + E_\mu - 2E_0$ (which is nothing but the conductivity gap of a single cell), and that the switching of, e.g., a holelike charge fluctuation from species ν to species ν' changes the energy by $E_{\nu'}^{(1)} - E_\nu^{(1)}$. To keep track of these changes in energy, we interpret the difference $\epsilon_\nu = E_\nu^{(1)} - E_0^{(2)}$ as the “energy of formation” of the hole species ν (and analogously for electronlike fluctuations).

We now define our restricted set of basis states:

$$|n_1\nu_1, n_2\nu_2, \dots, n_N\nu_N\rangle = \prod_{i=1}^{i=N} |\Psi_{\nu_i}^{(n_i)}\rangle \quad (10)$$

with the side condition that $n_i=2$ automatically implies $\nu_i=0$. In the following, we will diagonalize the Hamiltonian in the subspace of the states (10). To that end, we represent the basis states (10) in terms of “model fermions:” if a cell with number i is in the two-hole ground state we say it is empty; if the cell is in the ν th single-electron state with z -spin σ we model this by the presence of a holelike fermion, created by $a_{i,\nu,\sigma}^\dagger$; and if there are three electrons forming the μ th single-cell state with z -spin σ we say that the cell is occupied by an electronlike model fermion, created by $b_{i,\mu,\sigma}^\dagger$. Then, solving H in the restricted basis (10) obviously is equivalent to diagonalizing the Hamiltonian $H_{eff} = \mathcal{P}H\mathcal{P}$ where

$$\begin{aligned} H = & \sum_{i,\sigma} \sum_{\nu} \epsilon_\nu a_{i,\nu,\sigma}^\dagger a_{i,\nu,\sigma} + \sum_{i,\sigma} \sum_{\mu} \epsilon_\mu b_{i,\mu,\sigma}^\dagger b_{i,\mu,\sigma} \\ & + \sum_{i,j,\sigma} \sum_{\nu,\mu} (t_{i,\nu,j,\mu} b_{j,\mu,\sigma}^\dagger a_{i,\nu,\sigma}^\dagger + \text{H.c.}) \\ & + \sum_{i,j,\sigma} \sum_{\nu,\nu'} \tilde{t}_{i,\nu,j,\nu'} a_{j,\nu,\sigma}^\dagger a_{i,\nu',\sigma} \\ & + \sum_{i,j,\sigma} \sum_{\mu,\mu'} \tilde{t}_{i,\mu,j,\mu'} b_{j,\mu,\sigma}^\dagger b_{i,\mu',\sigma} \end{aligned} \quad (11)$$

with

$$\begin{aligned} t_{i,\nu,j,\mu} &= t_{i,j} r_{c,\nu,\sigma} s_{c,\mu,\sigma}, \\ \tilde{t}_{i,\nu,j,\nu'} &= -t_{i,j} r_{c,\nu',\sigma}^* r_{c,\nu,\sigma}, \\ \tilde{t}_{i,\mu,j,\mu'} &= t_{i,j} s_{c,\mu',\sigma}^* s_{c,\mu,\sigma}. \end{aligned} \quad (12)$$

Here \mathcal{P} projects onto the subspace of states where no site is occupied by more than one fermion. This kinematic constraint reflects the fact that the state of a given cell must be unique. Due to the product nature of the basis states (10), the evaluation of the matrix elements of the intercell kinetic energy (12) reduces to the calculation of matrix elements between products of no more than two single cell states. The matrix elements on the right-hand side (r.h.s.) of Eq. (12) are therefore simply products of the c -like photoemission and inverse photoemission matrix elements for a single cell (8);

this corresponds to the quite intuitive picture that the propagation of a c electron is equivalent to photoemission in one cell, and inverse photoemission in the neighboring one. The respective matrix elements give the renormalization of the inter-cell hopping due to intracell (i.e. local) correlation effects. Also, as long as the interaction between electrons contains only intra-cell terms the entire strong-correlation physics obviously is completely taken care of by the calculation of the single-cell states, and only enters via the single-cell energies $\epsilon_\nu = E_\nu^{(1)} - E_0^{(2)}$ and $\epsilon_\mu = E_\mu^{(3)} - E_0^{(2)}$. Thus, while we are presently only using Coulomb repulsions as intracell interactions, Hund’s rule exchange or electron-phonon coupling could also be treated in the same way.

Having computed the matrix elements and excitation energies the most obvious next step then is (in analogy to linear spin-wave theory) to relax the constraint enforced by \mathcal{P} , whereupon the Hamiltonian (11) is readily solved by Bogoliubov transformation. This gives us the energies and dispersion, and for the full Kondo lattice Hamiltonian we obtain four bands (we have two holelike and two electronlike model Fermions), whereas for the strong-coupling version we have only two. For the latter case, Eq. (11) takes the form

$$\begin{aligned} H_{eff} = & \frac{1}{2} \sum_{k,\sigma} \left[\left(-\epsilon_k + \frac{3J}{2} \right) a_{k,\sigma}^\dagger a_{k,\sigma} + \left(\epsilon_k + \frac{3J}{2} \right) b_{k,\sigma}^\dagger b_{k,\sigma} \right] \\ & - \frac{1}{2} \sum_{k,\sigma} \text{sign}(\sigma) \epsilon_k (b_{k,\sigma}^\dagger a_{-k,\bar{\sigma}}^\dagger + \text{H.c.}). \end{aligned} \quad (13)$$

This is readily solved by the ansatz

$$\begin{aligned} \gamma_{k,1,\sigma} &= u_{k,\sigma} b_{k,\sigma} + v_{k,\sigma} a_{-k,\bar{\sigma}}^\dagger, \\ \gamma_{k,2,\sigma} &= -v_{k,\sigma} b_{k,\sigma} + u_{k,\sigma} a_{-k,\bar{\sigma}}^\dagger \end{aligned} \quad (14)$$

and, introducing $\Delta = 3J/2$, we obtain the quasiparticle dispersion

$$E_\pm(\mathbf{k}) = (1/2) [\epsilon_k \pm \sqrt{\epsilon_k^2 + \Delta^2}], \quad (15)$$

shown in Fig. 2(a). At half-filling, particle-hole symmetry requires the chemical potential to be zero, so that the lower of the two bands (15) is completely filled, the upper one completely empty. We note that formally Eq. (15) is completely equivalent to the hybridization of a dispersionless effective f level in the band center with a free-electron band with dispersion ϵ_k , the strength of the nominal mixing element being Δ . This results in the heavy, i.e., almost dispersionless bands immediately above and below the Fermi energy in Fig. 2—the slope of these bands decreases strongly with decreasing J . It should be noted, however, that the resulting energy gap of Δ does *not* arise from the formation of a bonding and antibonding combination of c -like and f -like Bloch states, as in the hybridization model; rather, this gap originates from the energy cost to break two intracell singlets in the first step of a charge fluctuation. This gap, therefore, is of a very similar nature to that of the energy gap in a superconductor: the minimum energy for moving an electron from some site i to a distant site j (which by definition is the single-particle gap of the system) is two times the energy required to break a pair (which may be either a Kondo singlet or a Cooper pair: the first pair is broken at site i , because

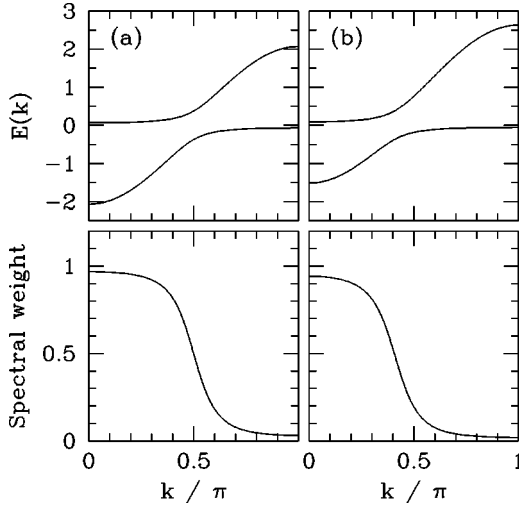


FIG. 2. Quasiparticle dispersion (top panels) and dispersion of the c -like spectral weight along the lower band (bottom panels) for the 1D strong-coupling model with $J=0.5$, $\epsilon_k = -2\cos(k)$. The density of conduction electrons is 1 in (a) and 0.8 in (b).

one member of the pair is removed—the second pair is broken at site j because the surplus electron interferes with the pair formation around this site.

III. SINGLE-PARTICLE GREEN S FUNCTION

To compute the full single-particle spectral function we need to resolve the ordinary electron creation and annihilation operators in terms of the model fermions, a and b . Taking into account our basic assumption, namely, that a single cell with two electrons can only be in its ground state, we can expand the electron annihilation operator (where $\alpha = c, f$)

$$\alpha_{i,\sigma} = \sum_{\nu} u_{\nu} |\Psi_{\nu,\sigma}^{(1)}\rangle \langle \Psi_0^{(2)}| + \sum_{\mu} v_{\mu} |\Psi_0^{(2)}\rangle \langle \Psi_{\mu,\sigma}^{(3)}|,$$

$$\alpha_{i,\sigma}^{\dagger} = \sum_{\nu} v_{\nu}^* |\Psi_{\nu,\sigma}^{(3)}\rangle \langle \Psi_0^{(2)}| + \sum_{\mu} u_{\mu}^* |\Psi_0^{(2)}\rangle \langle \Psi_{\mu,\sigma}^{(1)}| \quad (16)$$

Taking matrix elements of both sides we readily find that $u_{\nu} = r_{\alpha,\nu,\sigma}$, $v_{\mu} = s_{\alpha,\mu,\sigma}^*$. Next, we can replace, e.g., $|\Psi_{\nu,\sigma}^{(1)}\rangle \langle \Psi_0^{(2)}| \rightarrow a_{i,\nu,\sigma}^{\dagger}$ and thus have the desired resolution of the photoemission operator. Specializing to the strong-coupling limit, the annihilation operator for c electrons takes the form

$$c_{k,\sigma} = \frac{1}{\sqrt{2}} [\text{sign}(\sigma) a_{-k,\sigma}^{\dagger} - b_{k,\sigma}]. \quad (17)$$

Using Eq. (14) we can now resolve the annihilation operator in terms of the quasiparticles, obtain its matrix element, and square it to obtain the spectral weight in the lower (i.e., occupied) band as

$$W = \frac{1}{2} [1 - 2\text{sign}(\sigma) u_{k,\sigma} v_{k,\sigma}]. \quad (18)$$

Let us assume that $\epsilon_k \gg \Delta$ and let k be in the outer part of the Brillouin zone; i.e., we assume that we are deep in the heavy portion of the occupied band [see Fig. 2(a)]. Then, we find

$$W = \frac{1}{4} (\Delta/\epsilon_k)^2 \ll 1,$$

i.e., the heavy band does have an extremely small spectral weight [see the lower part of Fig. 2(a)]. This will turn out to be of considerable importance, as we will demonstrate.

To proceed to the doped case, we need an expression for the electron number operator. While at first sight this may appear a triviality, we will now see that one thereby runs into a rather deep-rooted problem, which reflects the special features of the strong-correlation problem. In the vacuum state the number of electrons (counting c and f electrons) is $2N$ and the presence of an a -fermion (b fermion) decreases (increases) the electron number by 1, so that for the full Kondo lattice the electron number operator should be simply

$$N_e = \sum_{k,\nu,\sigma} a_{k,\nu,\sigma} a_{k,\nu,\sigma}^{\dagger} + \sum_{k,\mu,\sigma} b_{k,\mu,\sigma}^{\dagger} b_{k,\mu,\sigma} - 2N$$

$$= \sum_{k,\sigma} \sum_{\mu=1}^4 \gamma_{k,\mu,\sigma}^{\dagger} \gamma_{k,\mu,\sigma} - 2N. \quad (19)$$

For the strong-coupling limit, we obtain, in an analogous fashion,

$$N_e = \sum_{k,\sigma} \sum_{\mu=1}^2 \gamma_{k,\mu,\sigma}^{\dagger} \gamma_{k,\mu,\sigma}. \quad (20)$$

The extra $-2N$ on the r.h.s. of Eq. (19) simply cancels the lowest of the four bands obtained in the full Kondo lattice. As will be seen below, this is a practically dispersionless lower Hubbard band for the f electrons, which is absent in the strong-coupling limit (or better: pushed to $-\infty$). The Fermi surfaces of both models thus are completely equivalent, and e.g. for the case of hole doping in one dimension one would obtain a Fermi momentum $k_F = (\pi/2)(\rho_c + 1)$ (where $\rho_c < 1$ denotes the density of conduction electrons) in the lower hybridization band. This implies that we have a Fermi surface that satisfies a nominal Luttinger theorem, i.e., the f electrons are treated as participating in the Fermi surface. The physical origin, however, is the fact that we have a density $1 - \rho_c$ of holes in the singlet background, which forms the vacuum for our treatment. This results in a hole pocket centered on $k = \pi$ with Fermi momentum $(\pi/2)(1 - \rho_c)$. The resulting Fermi surface then is *nominally* equivalent to a Luttinger Fermi surface *including* the f electrons and obviously this equivalence holds true irrespectively of dimensionality and Fermi surface topology. We believe that this is the reason why the f electrons *seem to* participate in the Fermi surface volume despite the fact that they are localized. At half-filling, we do not have a half-filled band of single-particle-like mixtures of c and f electrons—such a picture is obviously completely wrong for the strong-coupling model. Rather, the half-filled ground state should be viewed as an array of local singlets, where each f spin captures one conduction electron to form an immobile singlet. The system has a single particle gap because removing an electron and reinserting it at a far-away site breaks two of the local singlets, in a completely analogous fashion as in a

superconductor. Unlike a superconductor, the two members of each pair do belong to different species, whereby the number of one of the species, the f electrons, is essentially independent of the total electron density. Removing electrons from the system thus produces holes in the singlet background and leaves behind unpaired f electrons. Unlike the actual f electrons, which are largely immobile (completely immobile for the strong-coupling model) the holes are mobile, because an f electron can form a pair with a c electron from a nearby pair, thereby leaving another f electron unpaired.

However, there is still a major complication: the electron number must also equal the \mathbf{k} and ω integrated photoemission weight, which is given by the expectation value of the operator

$$N'_e = \sum_{\mathbf{k}, \sigma} (c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} + f_{\mathbf{k}, \sigma}^\dagger f_{\mathbf{k}, \sigma}). \quad (21)$$

Inserting the expansion (16) of the c and f electrons in terms of the model Fermions into this expression it is easy to see that in general $N_e \neq N'_e$. For example, in the strong-coupling limit we find, using Eq. (17)

$$N'_e = \frac{1}{2} \sum_{\mathbf{k}, \sigma} [(a_{\mathbf{k}, \sigma} a_{\mathbf{k}, \sigma}^\dagger + b_{\mathbf{k}, \sigma}^\dagger b_{\mathbf{k}, \sigma}) - \text{sign}(\sigma)(b_{\mathbf{k}, \sigma}^\dagger a_{-\mathbf{k}, \sigma}^\dagger + a_{-\mathbf{k}, \sigma} b_{\mathbf{k}, \sigma})] + N. \quad (22)$$

We thus arrive at the, at first sight, devastating conclusion that counting the electrons in real space on one hand and integrating the spectral weight in \mathbf{k} space on the other gives us different results for the electron number. On the other hand, this is not an indication for a qualitative flaw in our theory, but has a very clear and simple physical origin, namely, the fact that in a strongly correlated electron system spectral weight and band structure are completely decoupled. As an example, let us consider the band structure shown in Fig. 2(a). If one simply were to introduce a chemical potential corresponding to the real-space electron count (20) the Fermi energy would necessarily cut into the heavy part of the lower band. Let us assume that the only effect of doping were that k_F progressively cuts deeper into the heavy band portion of the otherwise completely rigid quasiparticle band structure calculated above. Trivially, for the one-dimensional chain the number of occupied momenta, N_{occ} would change with k_F as

$$\frac{\partial N_{occ}}{\partial k_F} = 4.$$

On the other hand, the integrated photoemission weight, N_{PES} , would change as

$$\frac{\partial N_{PES}}{\partial k_F} = 4W = \left(\frac{\Delta}{\epsilon_{k_F}} \right)^2.$$

Introducing a simple chemical potential following Eq. (20) into an otherwise rigid quasiparticle band structure thus inevitably leads to the breakdown of the sum rule for the integrated photoemission weight. The breakdown of rigid-band behavior and the failure of a simple electron count are therefore a completely natural consequence of the special

feature of strongly correlated electrons, namely, that they may have quasiparticle weights that substantially deviate from unity.

In order to cope with this problem, we try the simplest possible solution and enforce the consistency of the ordinary electron count and spectral weight integration by adding both expressions (20) and (22) for the electron number to the Hamiltonian, each one with a separate Lagrangian multiplier:

$$H \rightarrow H - \mu N_e - \lambda N'_e. \quad (23)$$

The notion of two chemical potentials may seem awkward at first sight, but as will be shown now, this approach results in a remarkable consistency with the numerical results. Let us again consider the strong-coupling limit. The spectral weight operator N_e takes the same form as the kinetic energy, but with the replacement $\epsilon_{\mathbf{k}} \rightarrow 1$ or, equivalently, $t_{i,j} \rightarrow 1$. The Hamiltonian thus becomes

$$H_{eff} = \frac{1}{2} \sum_{\mathbf{k}, \sigma} \left[-(\epsilon_{\mathbf{k}} - \lambda) + \frac{3J}{2} + 2\mu \right] a_{\mathbf{k}, \sigma}^\dagger a_{\mathbf{k}, \sigma} + \left[(\epsilon_{\mathbf{k}} - \lambda) + \frac{3J}{2} - 2\mu \right] b_{\mathbf{k}, \sigma}^\dagger b_{\mathbf{k}, \sigma} - \frac{1}{2} \sum_{\mathbf{k}, \sigma} \text{sign}(\sigma) (\epsilon_{\mathbf{k}} - \lambda) (b_{\mathbf{k}, \sigma}^\dagger a_{\mathbf{k}, \sigma}^\dagger + \text{H.c.}), \quad (24)$$

so that, using again Eq. (14), we find the dispersion

$$E_{\pm}(\mathbf{k}) = \frac{1}{2} [(\epsilon_{\mathbf{k}} - \lambda) \pm \sqrt{(\epsilon_{\mathbf{k}} - \lambda)^2 + \Delta^2}] - \mu. \quad (25)$$

Using the representation of the spectral operators, we obtain the momentum distribution/spin direction of the conduction electrons:

$$n_{\mathbf{k}}^c = \frac{1}{2} \left(1 - \frac{\epsilon_{\mathbf{k}} - \lambda}{\sqrt{(\epsilon_{\mathbf{k}} - \lambda)^2 + \Delta^2}} \right). \quad (26)$$

Then, for $|\epsilon_{\mathbf{k}} - \lambda| \gg \Delta$ we may replace the denominator on the r.h.s. by $-|\epsilon_{\mathbf{k}} - \lambda|$ and obtain $n_{\mathbf{k}}^c = \frac{1}{2} [1 - \text{sign}(\epsilon_{\mathbf{k}} - \lambda)]$. This is simply the free-electron result. For $\epsilon_{\mathbf{k}} - \lambda = 0$, on the other hand, we find $n_{\mathbf{k}}^c = 1/2$. Let us now discuss these results. To begin with, the real-space chemical potential μ acts like a standard chemical potential, which cuts into the heavy band and, as discussed above, produces a Fermi surface consistent with the nominal Luttinger theorem. On the other hand, the chemical potential for the spectral weight λ gives rise to a pseudo-Fermi-surface for the conduction electrons, where $n_{\mathbf{k}}^c$ drops sharply but continuously from a value ≈ 1 to nearly 0 [see Fig. 2(b)]. Since the integrated c distribution must equal the number of conduction electrons, it is clear that $\lambda \approx \epsilon(k_F^0)$, with k_F^0 the Fermi momentum for *unhybridized* conduction electrons. Carrying on the formal analogy of Eq. (25) with a hybridization gap picture, λ obviously plays the role of an on-site energy of the effective f level, and therefore the line $\epsilon_{\mathbf{k}} = \lambda$ marks the locus in \mathbf{k} space where the strongly dispersive conduction band bends over into the nearly flat heavy band [see Fig. 2(b)] In other words, the band structure of the Kondo lattice is equivalent to an effective f level, which is pinned near the frozen core Fermi energy for conduction electrons of density ρ_c , and which

mixes into the conduction band with a matrix element of strength $3J/4$. We note that this is very much what one would expect intuitively: in the limit $t \gg J$ the kinetic energy of the c electrons is by far the dominant energy contribution of the system. This can be expressed as

$$\langle H_{kin} \rangle = \int dk n_k^c \epsilon_k$$

and obviously the minimum value compatible with the Pauli principle is obtained by the free-electron distribution for the conduction electrons. Then, in order to recover a (small) additional energy $\sim J$ from the Kondo hybridization, the system will not sacrifice much kinetic energy, i.e., $n^c(\mathbf{k})$ will stay close to its free-electron shape. We also note that a similar shape for $n^c(\mathbf{k})$ was obtained previously by Shiba and Fazekas²³ in a variational treatment.

As can be seen from Eq. (26) the steepness of the drop of $n_c(\mathbf{k})$ at k_F^0 depends on the pair breaking energy $\Delta \propto J$. For (unphysical) values $J \sim t$ the drop is almost completely smeared out, and only upon decreasing J the pseudo-Fermi-surface becomes sharper and sharper (see Ref. 21). The behavior of $n_c(\mathbf{k})$ found in Ref. 21 is in almost quantitative agreement with the density matrix renormalization group results of Moukuri and Caron,¹⁶ which shows the quality of our simple analytical calculation.

Having discussed the strong-coupling version, we now turn to the full Kondo-lattice problem. Thereby we encounter a new problem. In the strong-coupling version, we have introduced the pseudo-chemical-potential λ in order to enforce the consistency of real-space electron count and integrated photoemission weight; clearly we will have to do the same thing for the full Kondo lattice. For the full model, however, there is an additional distinction to be made because now we have c -like and f -like spectral weight, and we need to make sure that the total spectral weight is distributed between the two species in a proper version. We will see that this compels us to introduce yet another Lagrange multiplier that essentially governs the ratio of c -like to f -like weight.

To that end, let us first construct an operator that counts the total number of α -type electrons (where $\alpha = c, f$). To begin with, we define the expectation values of the electron numbers in the single-cell states:

$$n_\alpha^{(i,\nu)} = \langle \Psi_{\nu,\sigma}^{(i)} | n_{\alpha,\uparrow} + n_{\alpha,\downarrow} | \Psi_{\nu,\sigma}^{(i)} \rangle.$$

These expectation values are readily computed from the single-cell wave functions, e.g., $n_f^{(2,0)} = 2\alpha^2 + \beta^2$. By analogy with Eq. (22) we may thus write down the following operator to count the total number of α electrons:

$$\begin{aligned} N_\alpha = & N n_\alpha^{(2,0)} + \sum_{k,\nu,\sigma} (n_\alpha^{(1,\nu)} - n_\alpha^{(2,0)}) a_{k,\nu,\sigma}^\dagger a_{k,\nu,\sigma} \\ & + \sum_{k,\mu,\sigma} (n_\alpha^{(3,\mu)} - n_\alpha^{(2,0)}) b_{k,\mu,\sigma}^\dagger b_{k,\mu,\sigma}. \end{aligned} \quad (27)$$

Using $n_f^{(i,\nu)} + n_c^{(i,\nu)} = i$ we find $N_c + N_f = N_e$, with N_e given by Eq. (19) (as it has to be). On the other hand, by using the resolutions (16) of the α operators we can form the operators $N'_\alpha = \sum_{k,\sigma} \alpha_{k,\sigma}^\dagger \alpha_{k,\sigma}$, which give the integrated spectral weight for the α electrons alone. We then replace the Hamiltonian,

$$H \rightarrow H - \mu N_e - \lambda (N'_c + N'_f) - \lambda_f (N_f - N'_f). \quad (28)$$

We determine λ from the condition $\langle N'_c + N'_f \rangle = N_e$ (λ thus has precisely the same meaning as for the strong-coupling limit discussed above) and λ_f from the requirement $\langle N_f - N'_f \rangle = 0$. This implies that automatically also $\langle N_c - N'_c \rangle = 0$, therefore we have reached ‘‘specieswise’’ consistency between real-space electron count and integrated spectral weight.

IV. COMPARISON WITH EXACT DIAGONALIZATION

Using the eigenenergies obtained by diagonalizing the effective Hamiltonian (28) with the self-consistently determined values of the Lagrange multipliers λ and λ_f we obtain the band dispersions. Combining the resolutions (16) of the c and f operators in terms of the model fermions and the eigenvectors obtained by diagonalizing Eq. (28) we can compute the photoemission and inverse photoemission matrix elements, so that we can obtain the photoemission spectrum

$$A_\alpha^{(-)}(\mathbf{k}, \omega) = \frac{1}{\pi} \text{Im} \left\langle \Psi_0 \left| \alpha_{k,\sigma}^\dagger \frac{1}{\omega + (H - E_0) - i0^+} \alpha_{k,\sigma} \right| \Psi_0 \right\rangle$$

and the inverse photoemission spectrum

$$A_\alpha^{(+)}(\mathbf{k}, \omega) = \frac{1}{\pi} \text{Im} \left\langle \Psi_0 \left| \alpha_{k,\sigma} \frac{1}{\omega - (H - E_0) - i0^+} \alpha_{k,\sigma}^\dagger \right| \Psi_0 \right\rangle,$$

where $\alpha = c, f$. Thereby $|\Psi_0\rangle$ denotes the ground-state wave function, E_0 the ground-state energy. We have carried out this calculation for several one-dimensional versions of the Kondo lattice and in the following we compare them to the results of Lanczos diagonalization. For the Lanczos studies we used a six-unit-cell chain. To simulate longer chains, we combine spectra calculated with periodic and antiperiodic boundary conditions (see Ref. 17 for a detailed discussion). While there is no rigorous justification for this procedure, inspection of the numerical spectra shows that one can obtain remarkably smooth band structures in this way.

To begin with, Fig. 3 shows the Lanczos result for the single-particle spectral function for a one-dimensional chain of the ‘‘pure’’ Kondo lattice, i.e., $U_{fc} = U_c = 0$, Figure 4 shows the result obtained from the theory (similar Lanczos spectra with slightly different parameters have also been obtained by Tsutsui *et al.*¹⁷) To begin with, in contrast to any band theory approach, our theoretical spectrum correctly reproduces the four well-distinguishable bands in the numerical spectra: the practically dispersionless upper and lower Hubbard band, which have almost pure f character, and the two hybridization bands, which resemble the strong-coupling result (15). The basic idea of our approach, namely, to broaden the ionization and affinity states of a single cell into bands, thus obviously works quite well. The spectra nicely show the pseudo-fermi-surface for the c electrons: while the true Fermi momentum in the doped case is at $k_F = 5\pi/6$, where the heavy band intersects E_F (although this is not easily recognized in the theoretical spectra), there is a pronounced transfer of c -like spectral weight from below to above E_F at $k_F^0 = \pi/2$. This means that doping shifts the drop of the momentum distribution for the c electrons (which is

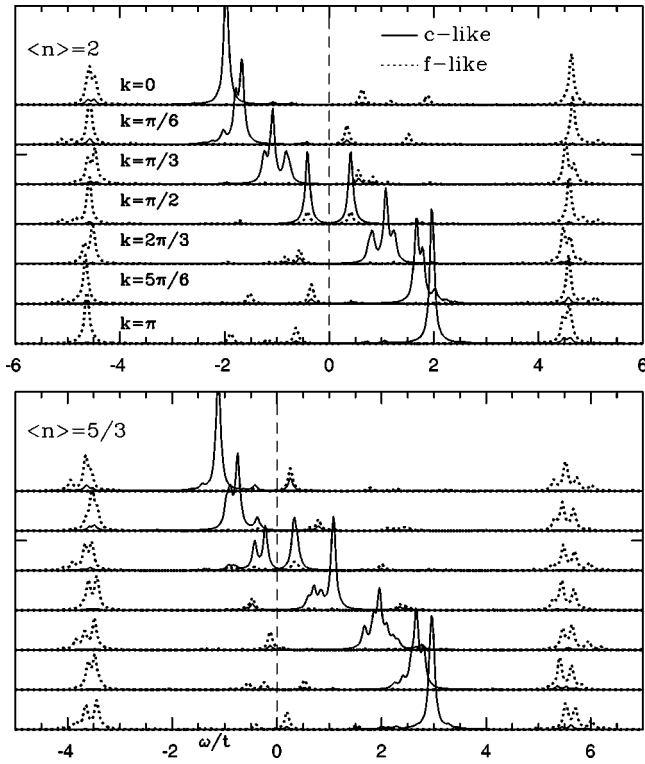


FIG. 3. Single-particle spectral function for the 1D Kondo lattice, obtained by Lanczos diagonalization of a six-unit-cell system. Full lines (dashed lines) correspond to c -like (f -like) spectral weight. The vertical dashed line gives the Fermi energy E_F , peaks to the right (left) of this line correspond to electron creation (annihilation). Parameter values are $U=8$, $\epsilon_f=4$, $V=1$, $\epsilon(k)=-2 \cos(k)$.

nothing but the integrated c weight below E_F) from $\pi/2$ to $\pi/3$ —this is precisely the pseudo-Fermi-surface discussed above for the strong-coupling limit (see Fig. 2). The theoretical spectra somewhat overestimate the weight of the heavy f -like portions in the hybridization bands; moreover, the position of the f -like Hubbard bands is shifted to slightly too high (binding) energies. On the other hand, the Fermiology is reproduced quite well. It is interesting to note that qualitatively identical results for smaller values of U_f and ϵ_f and lower electron filling have been obtained by Tahvildar-Zadeh *et al.*²⁴ using the $D \rightarrow \infty$ technique—quite obviously there is overall agreement between different numerical approaches, for quite different parameters values and fillings (and our analytical results).

Figure 5 shows a more asymmetric case; more precisely, we set $\epsilon_f=U$. As expected, the upper Hubbard band for the f electrons is virtually absent. Interestingly, the theoretical spectrum shows a very weak band at $\approx 3t$ above the Fermi energy, the intensity of which shows a weak increase with doping. The Lanczos spectrum for half-filling shows some diffuse f weight roughly in this area, and even some indication of peaks in the doped case. Next, the dispersion of the hybridization bands shows a quite pronounced asymmetry between photoemission and inverse photoemission, which is nicely reproduced by the theory (see Fig. 6). The explanation is simple: due to the reduced energy of the pure f state $f_{\uparrow}^{\dagger}f_{\uparrow}^{\dagger}|\text{vac}\rangle$ the weight of this state in the single-cell ground state for two electrons $|\Psi_0^{(2)}\rangle$ must increase. The weight of

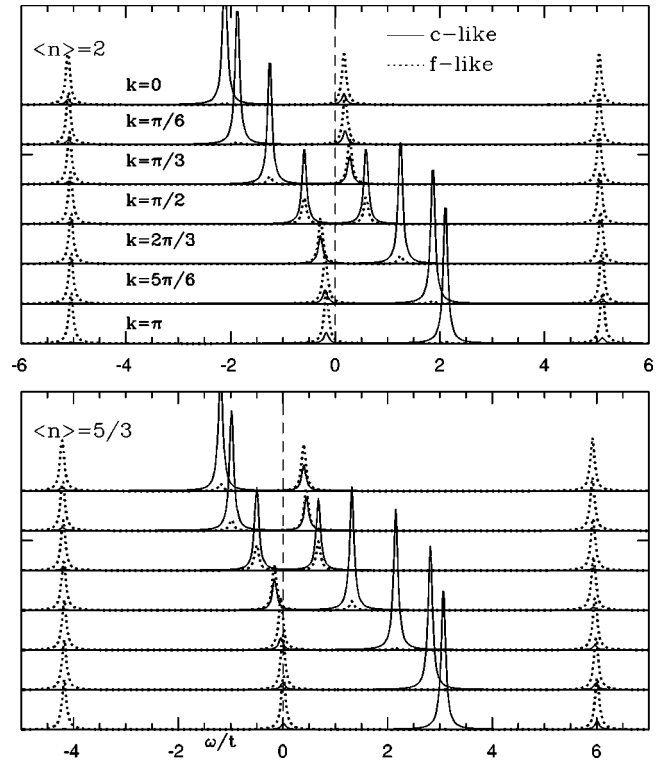


FIG. 4. Theoretical spectrum for the same parameter values as Fig. 3.

the two remaining states therefore must decrease, so that the overall probability of finding a c electron in the ground state is reduced (this manifests itself also in the significantly smaller integrated c weight in the photoemission spectrum).

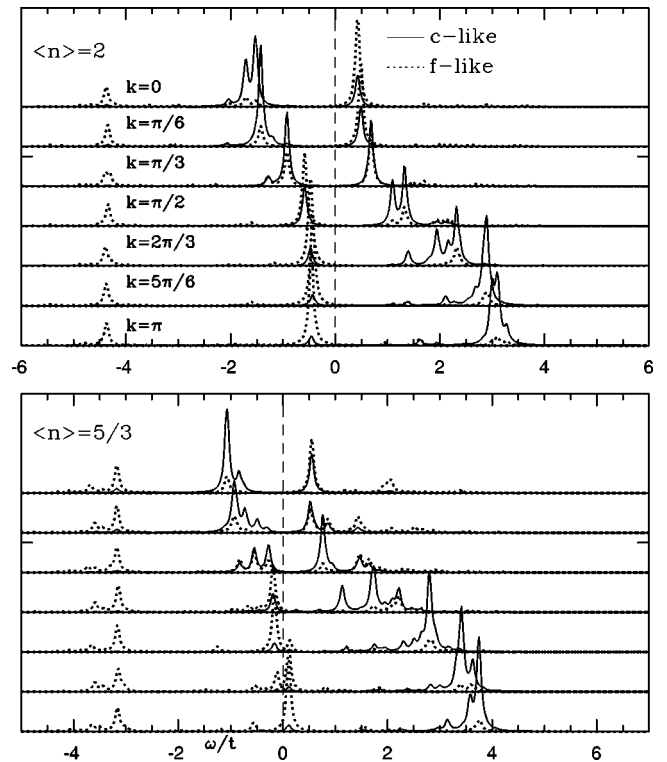


FIG. 5. Lanczos spectrum for $U_f=4$; all other parameter values as in Fig. 3.

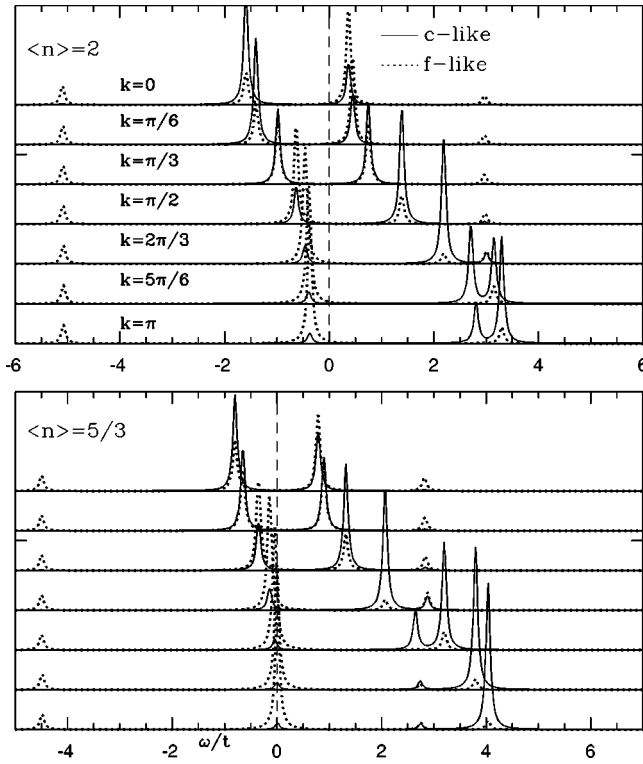


FIG. 6. Theoretical spectrum for the parameter values as in Fig. 5.

Since only the c electrons can hop between cells, the bandwidth seen in photoemission therefore will be reduced. Next, since the c weight that disappears from the photoemission part must reappear in the inverse photoemission spectrum, it follows from analogous considerations that the dispersion in the IPES part will be enhanced. As in the symmetric case, doping causes a shift of the chemical potential into the lower hybridization band, but there is now also some change of the spectral character of the upper hybridization band near $k = \pi$: there the c character increases, the f character decreases with doping, and the theoretical spectra obviously do correctly reproduce this trend.

Next, we study a more complicated form of the hopping term for conduction electrons. More precisely, we introduce a hopping integral between second-nearest neighbors, and to have a pronounced effect we choose this to be of equal magnitude, but opposite sign to the nearest-neighbor hopping. In other words, the conduction electrons now have the dispersion relation

$$\epsilon_k = -2t(\cos(k) - \cos(2k)). \quad (29)$$

For the band fillings under consideration, a system of noninteracting electrons thus would have four Fermi points rather than 2, and we want to see if our simple ‘‘rule of thumb’’ deduced above for the band structure in the strong-coupling limit continues to be valid also in this more complicated situation. Namely, the band structure of the Kondo lattice should be qualitatively given by the one obtained for mixing with a dispersionless f level, that is, pinned to the ‘‘frozen core’’ Fermi energy of the nonhybridizing conduction band, see Fig. 2. Then, Fig. 7 shows the Lanczos result for the single-particle spectral function and Fig. 8 shows the theo-

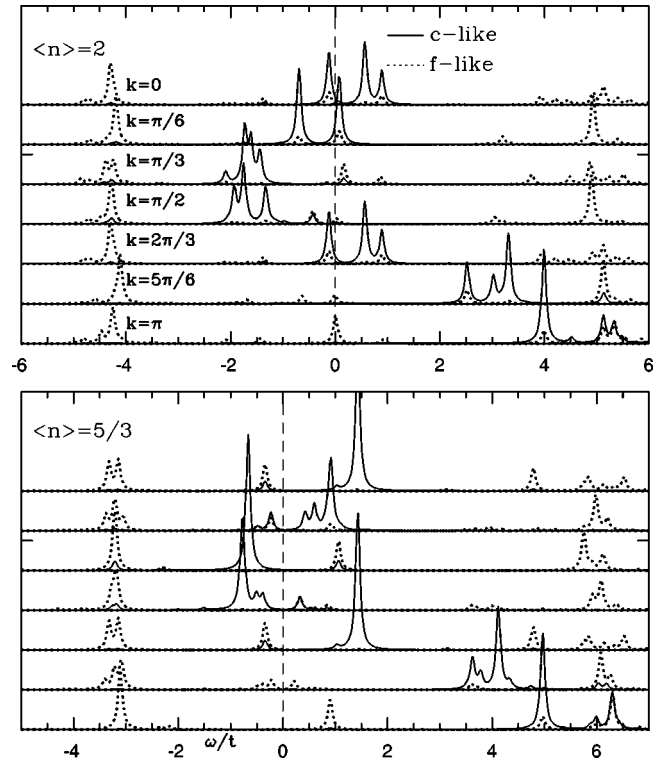


FIG. 7. Lanczos spectrum for conduction electrons with the dispersion (29); all other parameter values as in Fig. 3.

retical data. It is quite obvious that the theory remains valid also in this case. The relatively complicated band structure predicted by the rule of thumb can indeed be seen quite well in the Lanczos spectra: the s -shaped conduction band, with a

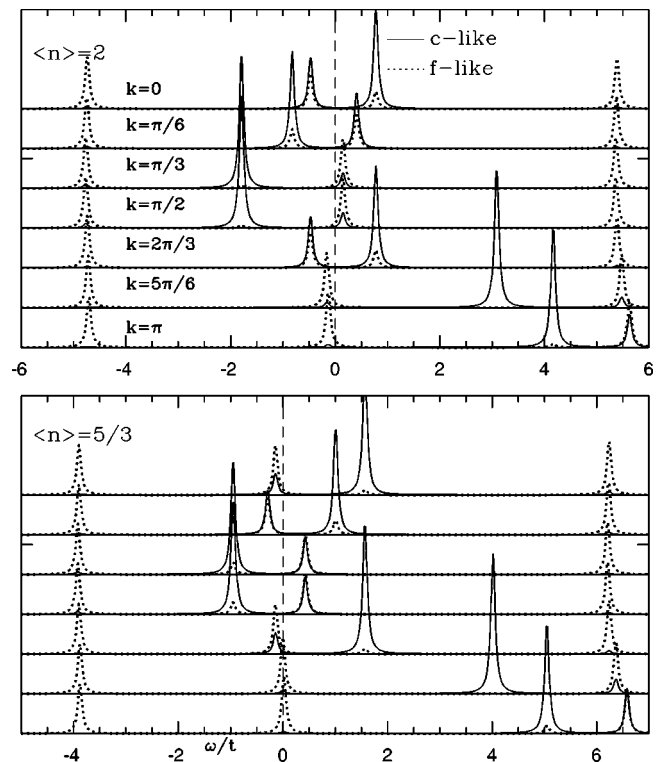


FIG. 8. Theoretical spectrum for the parameter values as in Fig. 7.

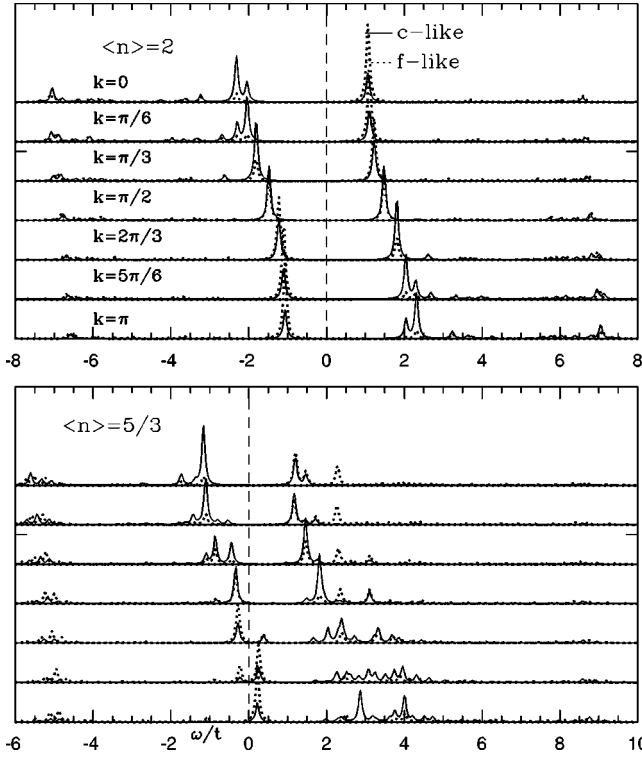


FIG. 9. Lanczos spectrum with $U_{fc}=4$; all other parameter values as in Fig. 3.

local maximum at $k=0$, which crosses from inverse photoemission and back again and thereby mixes with the dispersionless, low-intensity f band (it should be noted that the low-intensity f -like peaks at $5\pi/6$ and π in the Lanczos spectra for $\langle n \rangle = 2$ are actually on the photoemission side). With doping away from half-filling the heavy band near $k=\pi$ develops a Fermi edge, and the two pseudo-Fermi-surfaces for the c electrons at $\pi/6$ and $2\pi/3$ shift as expected for free, nonhybridizing c electrons. In the doped case, the flat low-intensity band that skims below E_F and crosses E_F at $k_F=5\pi/6$ can be identified particularly well. Also the heavy part in the inverse photoemission at $k=\pi/3$ and $\pi/2$, which is predicted by the theory can be identified reasonably well. Again, the theoretical spectra somewhat overestimate the spectral weight of these heavy band portions, and the relative position of the lower Hubbard band is not completely correct. Our simple picture of the Fermiology, however, obviously remains valid also with this more complicated Fermi-surface topology.

We proceed to the case of nonvanishing U_{fc} , i.e., a Coulomb repulsion between f and conduction electrons. The Lanczos spectra for this case are shown in Fig. 9, the theoretical spectra in Fig. 10. The main effects of U_{fc} is to open a wider gap at half-filling, to enhance the weight of the heavy bands, and to shift the Hubbard bands to higher energy. All in all, the total width of the spectrum is now $\approx 12 = U_f + U_{fc}$ rather than U_f as it used to be in the preceding cases. As compared to the preceding cases, the Hubbard bands, moreover, acquire an appreciable dispersion, and doping causes a pronounced spectral weight transfer from the upper to the lower Hubbard band. The widening of the gap at half-filling appears hard to understand at first sight, because U_{fc} by itself does not increase the energy cost for a charge

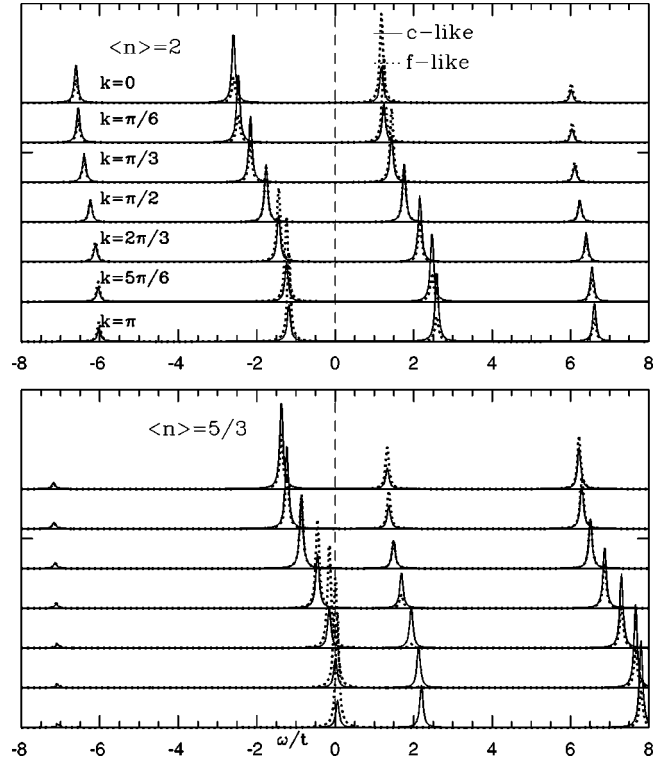


FIG. 10. Theoretical spectrum for the parameter values as in Fig. 9.

fluctuation: transferring a c electron from one cell to another (see the process of Fig. 1, $a \rightarrow b$) does not change the energy due to f - c repulsion as long as the f occupation is nearly constant at 1 (which is almost certainly the case for the large ϵ_f we are using). It is straightforward to see, however, that the opening of the gap is due to a loss of kinetic energy: switching on U_{fc} increases the energy of the state $(1/\sqrt{2})(c^\dagger f^\dagger + f^\dagger c^\dagger)$ by U_{fc} , so that the energy difference relative to the other two basis states is decreased by this amount [see the Hamilton matrix (4)]. This means that charge fluctuations in the two-electron ground state are enhanced, thus the kinetic energy for this state becomes more negative. On the other hand, this mechanism for enhancing the charge fluctuations is operative neither for one nor for three electrons in a cell [see the respective Hamilton matrices Eqs. (6) and (7)], so that there is no gain in kinetic energy in these cases. The charge fluctuation thus is accompanied by a net loss of kinetic energy, which in turn results in a larger charge gap. Moreover, it follows from expression (26) for the c -type spectral weight of the lower hybridization band that the distance in k space over which the weight drops is approximately given by Δ_c/v_F , with Δ_c the charge gap and v_F the Fermi velocity. It is thus immediately obvious that an increase of the charge gap (for whatever reason) will give a ‘‘more homogeneous’’ c weight along the hybridization bands. While at half-filling the agreement between Lanczos and theoretical spectra is very good, the situation changes for the doped case. The lower of the two hybridization bands is still well described, but the weights and dispersions of the other bands, as well as the weight shift between the Hubbard bands, are not reproduced well. Actually the Lanczos spectra show a rather strong reduction of the gap between the two central bands upon doping—we believe that this indicates a

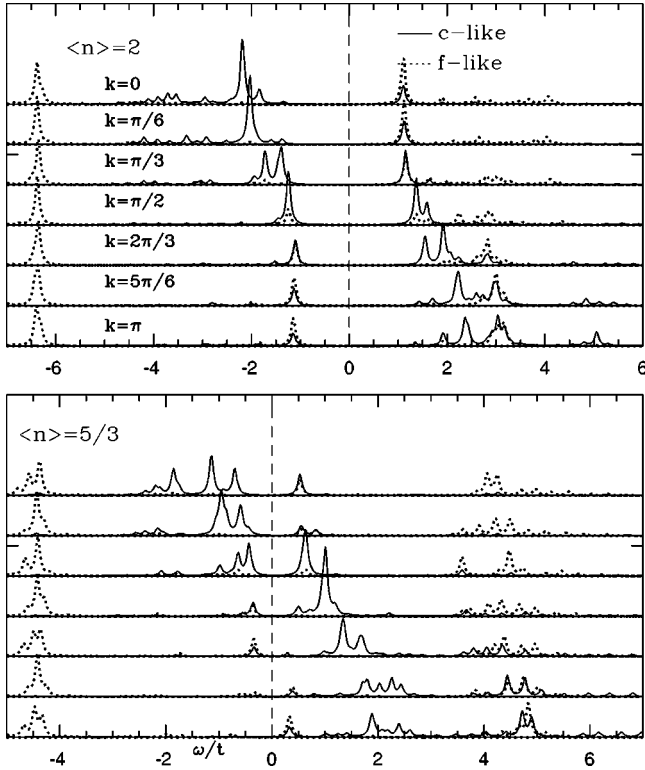


FIG. 11. Lanczos spectrum with $U_c=4$; all other parameter values as in Fig. 3.

rather profound doping-induced reconstruction of the electronic structure and since our theory corresponds more or less to an “expansion around the Kondo insulator” it may not be expected to reproduce this.

The situation is actually quite similar if we introduce a Coulomb repulsion between conduction electrons,^{25–27} U_c , see Figs. 11 and 12. Again, this opens a wider quasiparticle gap in the spectrum and the hybridization bands now have a predominant c character over their entire width. At half-filling the upper hybridization band intersects and mixes with the upper Hubbard band for the f electrons. The upper and lower Hubbard bands for the f electrons remain unaffected and are dispersionless; the lower one has practically pure f -like character. At half-filling, there is again good agreement between Lanczos and theory but for the doped case the situation is again different. The Lanczos spectra show a rather dramatic collapse of the gap between the hybridization bands; the upper hybridization band, which intersected the upper Hubbard band at half-filling, is now at least $2t$ below. Again, this suggests a strong doping-induced reconstruction of the entire electronic structure, and our theory naturally fails to reproduce this.

The effect of U_c at half-filling can be understood already in the context of the strong-coupling model limit, where we simply would have to replace $\Delta \rightarrow \Delta + U_c$. The more homogeneous c character of the hybridization bands then follows in an analogous fashion as for U_{fc} .

As a last example, we turn to a somewhat exotic version of the Kondo lattice model, where the magnitude of the c - f hybridization depends on the occupation of the f level. More precisely, we replace

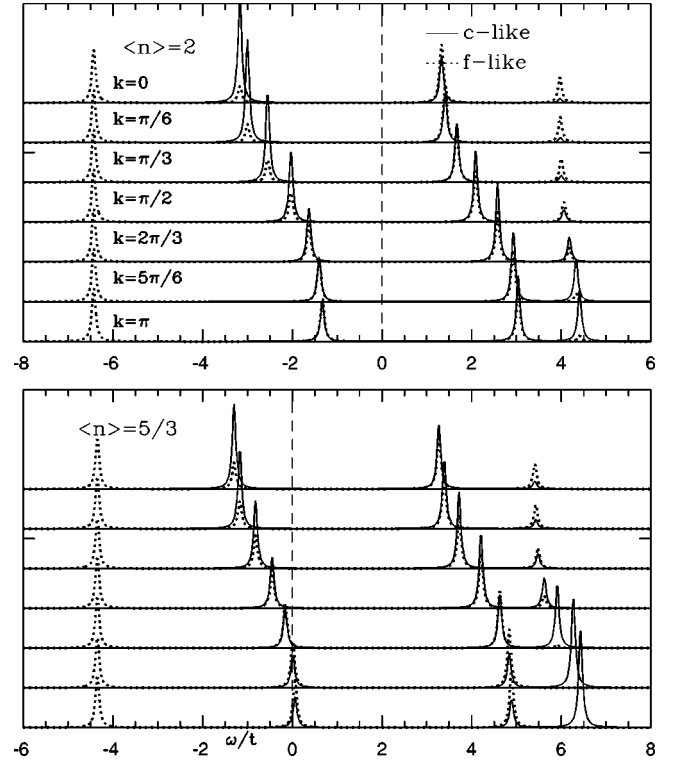


FIG. 12. Theoretical spectra for the parameters of Fig. 11; all other parameter values as in Fig. 3.

$$Vc_{i,\sigma}^\dagger f_{i,\sigma} \rightarrow V_1 c_{i,\sigma}^\dagger f_{i,\sigma} f_{i,\bar{\sigma}}^\dagger f_{i,\bar{\sigma}} + V_2 c_{i,\sigma}^\dagger f_{i,\sigma} f_{i,\bar{\sigma}} f_{i,\bar{\sigma}}^\dagger$$

with $V_1 \gg V_2$. Such a model may be relevant⁷ to describe the recently discovered⁵ transition-metal hydrides with switchable mirror properties, such as YH_3 . In this case, the yttrium $4d$ electrons would play the role of the conduction electrons; the hydrogen corresponds to the f electrons. The conditional hopping term is supposed to describe the relaxation of the orbital wave function on hydrogen as a function of electron occupation.⁷ This is manifested, e.g., by the dramatically larger radius of the free H^- ion as compared to the neutral free H atom (for a detailed discussion see Ref. 7; for a discussion of such an “orbital Kondo effect” in the context of cuprate superconductors see Refs. 28,29). Here we are not so much interested in the details of the correspondence with YH_3 , but rather in the applicability of our theory to this model. The conditional hopping is easily incorporated by replacing the Hamiltonian (4) for two electrons in a cell by

$$H_2 = \begin{pmatrix} -2\epsilon_f + U_f & \sqrt{2}V_1 & 0 \\ \sqrt{2}V_1 & -\epsilon_f + U_{fc} & \sqrt{2}V_2 \\ 0 & \sqrt{2}V_2 & U_c \end{pmatrix} \quad (30)$$

and analogous replacements in the single- and three-electron subspaces. It is quite obvious that the conditional hopping will lead to a dramatic increase of the charge gap: in our picture, the magnitude of the gap is determined by the energy difference between two cells with two electrons on one hand, and on the other, a cell with one electron and another with three electrons. Then, the electron in the singly occupied cell can mix with the conduction band only by using the (much smaller) hybridization integral V_2 , which corresponds to the

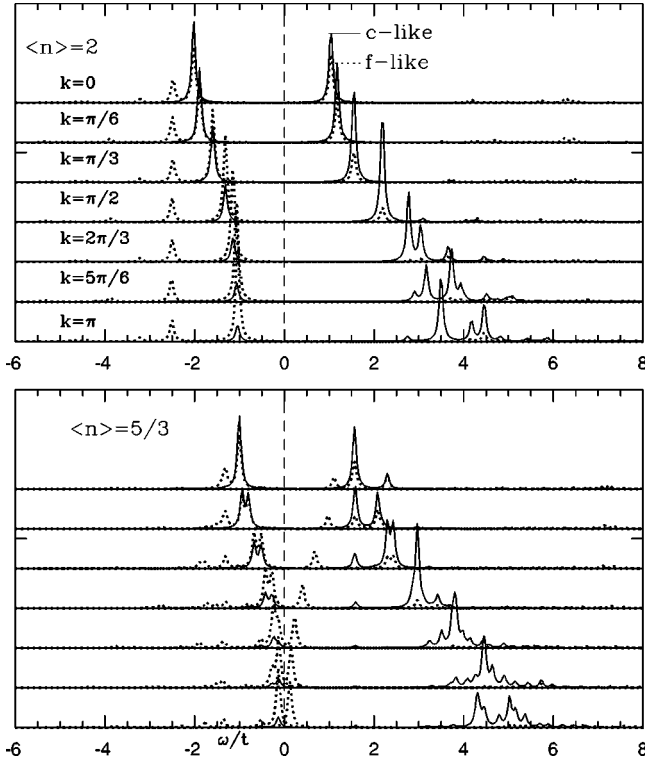


FIG. 13. Lanczos spectrum for the breathing f orbital. Parameter values are $U = \epsilon_f = 2$, $V_1 = 2.0$, $V_2 = 0.2$, $\epsilon_k = -2\cos(k)$.

collapsed f orbital. Only the single hole in the cell occupied by three electrons can delocalize using the large hopping integral V_1 . A charge fluctuation thus will result in a huge loss of *kinetic energy* and thus open a substantial gap in the band structure (the effect is thus similar, but much stronger than the U_{fc} discussed above). This gap will be opened even in the complete absence of any Coulomb repulsion on the f orbital, so that the breathing f orbital can lead to strong-correlationlike behavior even if there is no really strong Coulomb repulsion at play. In fact, comparing the Lanczos and theoretical results (Figs. 13 and 14) one can note first of all a good agreement between the two, and in addition a very substantial correlation gap in the spectrum. Also, there are low-intensity ‘‘Hubbard bands,’’ the positions and spectral weights of which are reproduced quite well by the theory. An interesting feature in the Lanczos data is the extra f -like band in the inverse photoemission spectrum that disperses from just above E_F at $k = \pi$ to $\approx 2t$ above E_F at $k = 0$, and that is completely absent in the theory. We believe that this band is a consequence of superconducting pairing correlations in the doped ground state. As discussed by various researchers, the breathing f orbital presents a very strong pairing mechanism^{28,29} for electrons in the doped material, in that the electrons will always pair up around one f site to hybridize by the large hopping parameter V_1 . In the spectral function the presence of such pairing correlations will manifest itself as a Bogoliubov-type ‘‘mirror image’’ of the top-most band, i.e., the replacement

$$\tilde{\epsilon}_k - \mu \rightarrow \pm \sqrt{(\tilde{\epsilon}_k - \mu)^2 + \Delta_{sc}^2},$$

where $\tilde{\epsilon}_k$ is the ‘‘nonsuperconducting dispersion’’ of the lower hybridization band (which should correspond to the

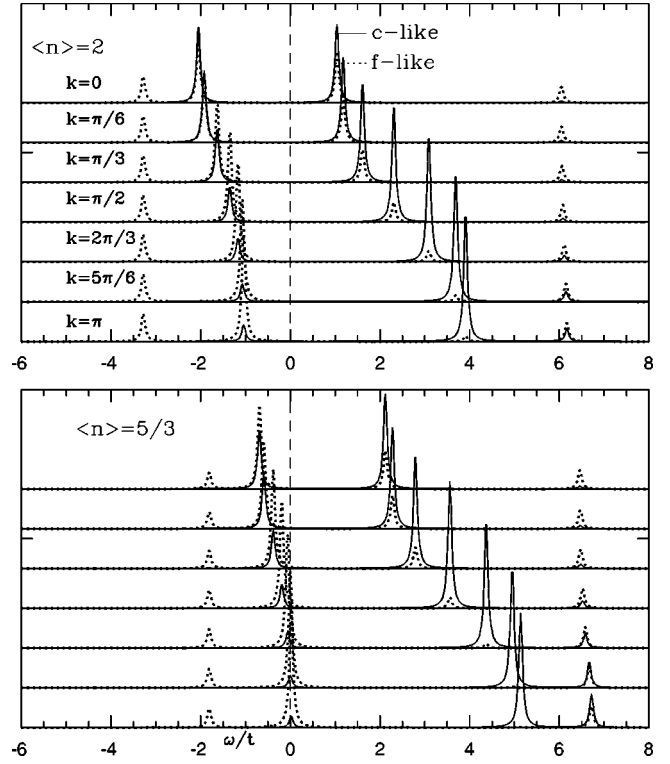


FIG. 14. Theoretical spectra for the parameters of Fig. 13.

one given by our theory) and Δ_{sc} the superconducting gap. The latter appears to be quite small in the numerical spectra. We defer a detailed discussion of superconductivity to a separate publication, but we note that our theory does not encompass superconductivity, so that the absence of this band in the theoretical spectra can be no surprise.

Summarizing this section, our theory gives a remarkably good description of sometimes rather complicated and unexpected features of a wide variety of extended versions of the Kondo lattice. Moreover, it allows us in all cases to extract simple physical pictures in order to understand the overall trends. The main inaccuracy concerns the positions of the f -like Hubbard bands, but we believe that this is not a severe deficiency because this is an extreme high-energy feature. In the cases of extra intracell repulsions the Lanczos spectra showed some indications of a doping-induced reconstruction of the electronic structure—this could not be reproduced by our theory. Also, superconductivity in the doped ‘‘breathing f model’’ naturally could not be described.

V. CONCLUSION

In summary, we have presented a ‘‘nearly analytical’’ theory for the Kondo lattice. In simplest terms it may be viewed as a Fermionic version of linear spin-wave theory, in that we constructed an effective Hamiltonian describing the pair creation and propagation of Fermionic charge fluctuations on a strong-coupling resonating-valence-bond-type vacuum. This gives us a systematic way to broaden the ionization and affinity states of a single cell into bands, reminiscent of the cell perturbation theory developed by Jefferson and co-workers.²⁰ For quite a number of different versions of the Kondo-lattice model, the theoretical results for the single particle spectral function were found to be in overall excel-

lent agreement with exact diagonalization of small clusters, as far as the dispersion of energy and spectral weight is concerned. It is a particularly encouraging fact the rather non-trivial evolution of the spectra with electron density in many cases is reproduced in detail. This gives us some confidence that despite some uncontrolled approximations the theory is already very close to the correct picture. Given its extraordinary simplicity (all results are obtained by an elementary Bogoliubov transformation) we believe that the theory should easily be amenable to systematic improvement to describe as yet neglected processes.

The emerging picture of the Kondo insulator then is quite different from that of a conventional band insulator, and in fact more reminiscent of a superconductor: the ground state at half-filling corresponds to an array of (overlapping) local singlets, where each Kondo spin forms a bound state with one conduction electron. The system has a single-particle gap for precisely the same reason as in a superconductor: removing a conduction electron from some site i and reinserting it at a remote site j breaks two f - c pairs; thus there is an increase in energy of twice the binding energy of a single pair.

A key ingredient for the construction of the effective Hamiltonian was the existence of a unique RVB-type “singlet background,” which sets the stage for the pair creation and propagation of the fermionic charge fluctuations. The basic idea of the present work, therefore, is not restricted to the Kondo lattice. Rather, once such an “RVB vacuum” has been identified, an essentially analogous construction can be carried out also for other strongly correlated systems. The most obvious example is the doped t - J ladder, where the “rung singlet RVB state” may replace the product of single-cell states, and for which a very similar construction can indeed be carried out.³⁰

Perhaps the most important approximation we have made is the neglect of any excited states of two electrons in a cell. This means that we have neglected single-cell states where one conduction electron and one f electron couple to a triplet. Such states do in fact have a very small excitation energy $\propto V^2/U$. As we have already mentioned, this restriction forbids the propagating charge fluctuations to “radiate off” tripletlike spin excitations and thus makes their propagation completely coherent. The good agreement with the numerics, and also the relatively “coherent” nature of the Lanczos spectra themselves (in which the incoherent high-energy continua familiar from the t - J or Hubbard model³¹ are almost completely absent), give us some confidence that despite their low energy, the neglect of the singlet triplet excitations is a good approximation as far as the single-particle properties are concerned. Moreover, it is quite easy to incor-

porate these singlet-triplet excitations into the present theory:²¹ the three components of a triplet state in cell i can be grouped into an SO(3) vector \mathbf{t}_i . Then, we would model the cell i being in the α th triplet state by the presence of a *Bosonic* excitation, created by $t_{i,\alpha}^\dagger$. In addition to a term describing the on-site energies of these triplets we would obtain terms that describe the coupling between the Fermionic charge fluctuations and the Bosonic spin fluctuations. Their form can be inferred from rotational invariance: for example, $\mathbf{t}_i^\dagger \cdot (a_{i,\tau}^\dagger \boldsymbol{\sigma}_{\tau,\tau'} a_{j,\tau'})$ (with $\boldsymbol{\sigma}$ the vector of Pauli matrices) describes the hopping of a hole from $i \rightarrow j$ while creating a spin excitation in cell i ; the terms $(\mathbf{t}_j^\dagger \cdot \mathbf{t}_i) \cdot \sum_\tau a_{i,\tau}^\dagger a_{j,\tau}$ and $(a_{i,\tau}^\dagger \boldsymbol{\sigma}_{\tau,\tau'} a_{j,\tau'}) \cdot (\mathbf{t}_j^\dagger \times \mathbf{t}_i)$ represent two different ways for a spin excitation to exchange its position with a hole. The actual prefactors of these terms can be computed in an entirely analogous fashion as the hopping integrals for the charge fluctuations themselves, and these terms can be incorporated into the formalism by using standard Green’s-function techniques. Details will be reported elsewhere.³² Since already the simplest version of the theory apparently gives a quite good description of the physics, one may expect that such an extension is actually “convergent” and gives a good description of the spin dynamics as well.

As a final remark, we note that the “vacuum” in the case of the simple Kondo lattice was a unique product of singlet states, and that the charge fluctuations did have precisely the quantum numbers of electrons or holes. For systems with a larger unit cell, however, one can envisage situations where this is very different: one example would be a twofold orbitally degenerate f -level mixing with a nondegenerate c orbital.³³ For one electron/orbital the number of electrons/unit cell then would be 3, and the (Fermionic) charge fluctuations would correspond to cells with an even number of electrons. Thereby Hund’s rule coupling between the degenerate f orbitals would favor high-spin states, so that one might actually obtain “high-spin quasiparticles.” From the good success for the simple Kondo lattice one might expect that the present formalism would continue to give a good description even in this more complicated situation.

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