Spin fluctuations of a random vacuum state: 
a new approach to the Kondo lattice

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Abstract

We address the Kondo lattice with one conduction band by introducing a representation of the \( s = 1/2 \) local moments consisting in an \( s = 1 \) triplet of spin fluctuations of a vacuum state. The excitation of these fluctuations by the electronic field results in the creation of new fermionic modes. It is shown that, in the one-electron case, the zero-temperature spectrum of these excitations consists in two \( s = 1/2 \) doublet bands and an \( s = 3/2 \) quadruplet. One of the doublets is seen to be a slight modification of the bare initial electronic band for low values of the exchange coupling, while the other bands correspond to complex, coherent recombinations of the bare electron and spin fluctuations displaying large effective masses.

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I. INTRODUCTION

Heavy-fermion metals display a rich phenomenology produced by the interaction between conduction electrons and partially filled \( f \)-bands from (typically) Ce or U.\(^1\) Its high-temperature properties are those of a collection of weakly interacting local moments and conduction electrons with quite ordinary masses. At low temperatures, however, they exhibit Fermi liquid behaviour with values of the linear specific heat and temperature-independent Pauli spin susceptibility corresponding to huge quasiparticle masses. This Fermi liquid becomes, in many systems, antiferromagnetic, superconducting, or both.

The high-temperature behaviour described above, suggests that these systems should be represented by the *Kondo lattice model* (KLM), in which the conduction electrons are coupled to the local moments through an exchange interaction. This model is the limit of the more general *Anderson lattice model* (ALM) when the fluctuations in the number of \( f \)-electrons per Ce or U site can be neglected.\(^3\)

A number of techniques have been proposed for dealing with these models (especially the ALM).\(^4\) Of particular importance have been the mean-field\(^6\) and variational\(^7\) approximations. In both cases, the Hamiltonian of the ALM is essentially transformed into an effective Hamiltonian in which the \( f \)-electrons are uncorrelated, shifted close to the Fermi level and hybridize weakly with the conduction electrons. This high density of states at the Fermi level would explain the high values of the linear coefficient of the specific heat and the magnetic susceptibility. The formulation of these theories relies heavily on the fact that the occupation of the \( f \)-orbitals is not exactly integer.

In this article, we present a new approach to the description of the heavy-fermion state. By selecting the KLM, we are effectively asserting that the phenomenology of these systems is associated with the interaction of conduction electrons and local moments and that the \( f \)-charge fluctuations do not play an essential role. The general philosophy of our approach bears strong parallelisms with the physical discussion of the Kondo model, namely, the interaction of a single magnetic impurity with conduction electrons through an antiferromagnetic
exchange coupling. In this model, the excess magnetic susceptibility is seen to depart, at a characteristic ($T_k$) temperature, from the Curie-Weiss law, smoothly approaching a constant limit as $T \to 0$. This is because at $T = 0$, the local spin forms a collective singlet state with the spins of the conduction band with a binding energy of essentially $K_B T_k$. Thus, for temperatures below $T_k$, the resonant scattering of the conduction electrons acts as an effective temperature for the local moment giving rise to the mentioned $T$-dependence of the magnetic susceptibility.

Analogously, in the treatment of the KLM presented in this paper, heavy fermions appear as collective, many-particle states made up of electrons and spin fluctuations. Nevertheless, while the Kondo resonance is an $s = 0$ singlet, our collective excitations are fermions. Another difference is that, while the Kondo resonance can form only for antiferromagnetic couplings, the situation in the KLM is the same for both ferro and antiferromagnetic couplings. This is important since heavy-fermion metals like CeAl$_3$ are known to have ferromagnetic couplings.

The key idea of this article is the introduction of a new, very physical representation of the algebra of the local moments. Let us suppose for a moment that the conduction electrons are absent. If we consider a lattice of $N$ sites with a local $s = 1/2$ spin at each site, the Hilbert space of the system is spanned by a basis of $2^N$ states corresponding to all the possible spin arrangements constructed from the up and down states of the local spin at each lattice site. Since each of these $2^N$ states has the same energy when conduction electrons are absent, the global state of the system can be regarded as a linear combination of the $2^N$ basic vectors, each of them carrying the same probability and an arbitrary, random phase. This is what we call the *random vacuum state* (RVS). We show that by repeatedly applying the spin operators $\sqrt{2}S^+_{f_i}$, $\sqrt{2}S^-_{f_i}$, and $2S^z_{f_i}$ to this vacuum state we obtain, in the thermodynamic limit, a set of orthonormal vectors that span a new representation of the algebra of the local moments. The states of this new Hilbert space can be interpreted as spin fluctuations of the RVS. This new representation, initially constructed using physical considerations, can be presented at the end in an axiomatic fashion as a perfectly consistent,
rigorous mathematical structure.

Thus, with this representation, when conduction electrons are incorporated into the system, their interaction with the local moments can be viewed as an electronic excitation of spin fluctuations of a vacuum state. In this process, the conduction electrons get dressed with spin fluctuations giving rise to new fermionic excitations. For low relative values of the exchange coupling (the actual physical situation), we find two types of excitations. One type corresponds to slight modifications of the initial bare conduction electrons. The other modes are complex, many-particle combinations of electrons and spin fluctuations displaying large effective masses.

We provide a systematic technique to calculate the energy and wave function of these excitations. The method essentially consists in determining variationally the best approximation to the actual wave function within the space in which the bare electron dresses with \( n \) spin fluctuations at most. The larger we take \( n \), the better the approximation.

In this basic, qualitative article, we consider the lowest \((n = 1)\) approximation for the system with a single conduction electron only. Although the lowest approximation proves to be inadequate for the precise determination of the heavy-fermion bands, it does reveal the qualitative picture presented in this paper. The precise calculation of the heavy-fermion modes for low relative values of the exchange coupling will require to consider higher orders \((n > 1)\) of approximation and promises to be a hard technical task.

In Section II, we present the detailed construction of the algebra of spin fluctuations. The determination of the translational and spin rotational symmetries of the system within this new representation is carried out in Section III. The use of these symmetries will be essential for the construction and characterization of the fermionic excitations.

In Section IV we address the simple case of a single conduction electron interacting with the lattice of local moments and study how this bare electron gets dressed with spin fluctuations. The inspection of the atomic limit (band width \( \to 0 \)) leads to the conclusion that the spectrum of the system contains two \( s = 1/2 \) doublet bands and an \( s = 3/2 \) quadruplet. These bands are then calculated in the lowest approximation to determine their qualitative
features away from the atomic limit. As we already mentioned, this approximation indicates that for small values of the coupling, one of the doublets is a minor modification of the bare conduction band, while in the other doublet and in the quadruplet, the conduction electron strongly combines with spin fluctuations forming bands with large effective masses. We also find in this analysis, that the two doublets hybridize only above a certain critical value of the coupling.

The natural extension of this picture to the case of a system with a finite electronic density would require to treat the bare conduction electrons as a Fermi sea with electrons and holes as elementary excitations with positive energies. These electrons and holes will be the ones giving rise to collective modes when they combine with spin fluctuations. The existence of collective states with negative energies would lead to the condensation of some of these modes in the ground state, forming the heavy-fermion gas that is observed experimentally. The detailed study of the Kondo lattice with a finite density of conduction electrons within the framework of the approach introduced in this article is intended to be the focus of our future endeavours.

II. SPIN FLUCTUATIONS OF A RANDOM VACUUM STATE

We shall study a KLM consisting in a conduction band coupled to a lattice of $s = 1/2$ local moments by an exchange interaction. The Hamiltonian is given by

$$H = \varepsilon_k c_{k\alpha}^\dagger c_{k\alpha} + JS_{ei}S_{fi},$$

where $S_{ei}$ and $S_{fi}$ are the spin of the conduction electrons and the local spin at site $i$ respectively. As in many equations throughout this paper, sum over repeated indexes is implicitly understood. $S_{ei}$ is given in terms of the electronic operators in the site (Wannier) representation by

$$S_{ei} = \frac{1}{2}c_{i\alpha}^\dagger \sigma_{\alpha\beta} c_{i\beta}.$$
If $R_i$ is the position of the $i$-site, the $c_{i\alpha}^\dagger$-operators are given, for a lattice with $N$ sites, by

$$c_{i\alpha}^\dagger = N^{-1/2} \sum_k e^{-iR_i \cdot k} c_{k\alpha}^\dagger.$$  

(3)

The fundamental operators $c_{k\alpha}$, $S_{fi}$ are characterized by the following algebraic properties:

$$\{c_{k\alpha}, c_{k'\beta}^\dagger\} = \delta_{kk'} \delta_{\alpha\beta} , \{c_{k\alpha}, c_{k'\beta}\} = 0 ,$$  

(4)

$$[S_{fi}^\alpha, S_{fj}^\beta] = i\delta_{ij} \epsilon_{\alpha\beta\gamma} S_{fi}^\gamma ,$$  

(5)

$$S_{fi}^\dagger = S_{fi} ,$$  

(6)

$$S_{fi}^2 = 3/4 ,$$  

(7)

$$[c_{k\alpha}, S_{fi}] = 0 .$$  

(8)

As we said before, the fundamental idea of this paper is a novel treatment of the local moments: We shall first consider these degrees of freedom only, adding the conduction electrons at the end.

We can satisfy (4) and (6) by writing

$$S_{fi} = \frac{1}{2} f_{i\alpha}^\dagger \sigma_{\alpha\beta} f_{i\beta}^\dagger ,$$  

(9)

where $f_{i\alpha}^\dagger$ and $f_{i\alpha}$ are creation and annihilation operators of $f$-electrons satisfying cannonical anticommutation relations. From Eq. (9) we get

$$S_{fi}^2 = \frac{3}{4} f_{i\alpha}^\dagger f_{i\alpha} + \frac{3}{2} f_{i\uparrow}^\dagger f_{i\uparrow}^\dagger f_{i\uparrow} f_{i\downarrow} ,$$  

(10)

which implies that $S_{fi}^2 = 0$ if the $i$-site is empty or doubly occupied and $S_{fi}^2 = 3/4$ if it is singly occupied. Therefore, as it is physically obvious, the condition (7) is equivalent to demanding that each site be occupied by one and only one $f$-electron.

Thus, the Hilbert space in which the $S_{fi}$-operators act, should be the set of all vectors of the form
\[
\sum_{\alpha_i = \uparrow, \downarrow} C_{\alpha_1, \ldots, \alpha_N} f_{1\alpha_1}^\dagger f_{2\alpha_2}^\dagger \cdots f_{N\alpha_N}^\dagger |0\rangle. \tag{11}
\]

Since the spin operators \( S_{fi} \) preserve the number of \( f \)-electrons at each site, they are well-defined in this space. It will be convenient for future developments, however, to work with the following equivalent set of operators:

\[
s_{1,i} \equiv \sqrt{2} \left( S_{fi}^x + i S_{fi}^y \right) = \sqrt{2} f_{i\uparrow}^\dagger f_{i\downarrow},
\]
\[
s_{0,i} \equiv 2 S_{fi}^z = f_{i\uparrow}^\dagger f_{i\uparrow} - f_{i\downarrow}^\dagger f_{i\downarrow},
\]
\[
s_{-1,i} \equiv \sqrt{2} \left( S_{fi}^x - i S_{fi}^y \right) = \sqrt{2} f_{i\downarrow}^\dagger f_{i\uparrow}. \tag{12}
\]

The initial \( S_{fi} \)-operators can always be recovered using the inverse transformation:

\[
S_{fi}^x = \frac{1}{2\sqrt{2}} (s_{1,i} + s_{-1,i}), \quad S_{fi}^y = -\frac{i}{2\sqrt{2}} (s_{1,i} - s_{-1,i}), \quad S_{fi}^z = \frac{1}{2} s_{0,i}. \tag{13}
\]

It is straightforward to see that the operators (12) acting on the space (11) satisfy the following multiplication table:

\[
\begin{align*}
s_{0,i}s_{1,i} &= s_{1,i} \quad & s_{0,i}s_{-1,i} &= -s_{-1,i} \\
s_{1,i}s_{0,i} &= -s_{1,i} \quad & s_{-1,i}s_{0,i} &= s_{-1,i} \\
s_{1,i}s_{-1,i} &= 1 + s_{0,i} \quad & s_{1,i}^2 &= s_{-1,i}^2 = 0 \\
s_{-1,i}s_{1,i} &= 1 - s_{0,i} \quad & s_{0,i}^2 &= 1
\end{align*} \tag{14}
\]

as well as the properties

\[
\begin{align*}
s_{1,i}^\dagger &= s_{-1,i}, \quad s_{0,i}^\dagger &= s_{0,i},
\end{align*} \tag{15}
\]

\[
[s_{l,i}, s_{l',j}] = 0 \quad \forall i \neq j. \tag{16}
\]

Eqs. (14)–(16) can also be regarded as the defining conditions of the algebra since, as it can be readily checked, they imply Eqs. (5)–(7).

Let us now think in more physical terms: Since the local moments do not interact among themselves, all the spin configurations will have the same energy when the conduction
electrons are absent. Thus, the physical state of the system can be regarded, in this situation, as a random linear combination of the $2^N$ possible spin configurations, namely,

$$|RV S⟩ = \frac{1}{\sqrt{2^N}} \sum_{α_i=↑,↓} e^{iR_{α_1...α_N}} f_{1α_1}^\dagger ... f_{Nα_N}^\dagger |0⟩,$$

where the phases $R_{α_1...α_N}$ are taken at random. We will call this state the random vacuum state (RVS).

We can now apply to this state our fundamental $s_{1,i}$-operators. As it is obvious from Eq. (12), their effect is to excite spin fluctuations in the vacuum state. $s_{1,i}$ annihilates all the components with spin up at site $i$ and flips the $i$-spin of the others; the result is a normalized state with the $i$-spin up. $s_{-1,i}$ does exactly the contrary and $s_{0,i}$ introduces a relative phase shift of $\pi$ between the $i$-spin up and down components.

By repeatedly applying the operators $s_{l,j}$ to the RVS, we generate new states like, for example,

$$|ψ⟩ = s_{1,2}s_{0,5}s_{1,15}|RV S⟩.$$

(18)

We shall loosely say that $|ψ⟩$ has spin fluctuations at sites 2, 5, and 15. When applying $s_{l,i}$ to a state that already has in its expression an operator in the same lattice site, we can use the multiplication table (14) to produce a state with one $s_{l,i}$-operator at most. For example,

$$s_{-1,15}|ψ⟩ = s_{1,2}s_{0,5}|RV S⟩ - s_{1,2}s_{0,5}s_{0,15}|RV S⟩.$$

(19)

We can construct $4^N$ different combinations of spin fluctuations by leaving each site either empty or with one of the three possible fluctuations. The linear combinations of these states form a vector space in which the $s_{l,j}$-operators are perfectly defined through Eqs. (14) and (16).

Using the randomness of the vacuum state, it is straightforward to prove that the $4^N$ basic states constructed above are orthonormal in the thermodynamic limit. For example, the scalar product of $s_{0,1}|RV S⟩$ and $s_{1,1}|RV S⟩$ is given by
which is essentially the average of $2^{N-1}$ random phases and, therefore, vanishes as $N \to \infty$.

The result for the general case can be obtained in an analogous way.

It should be emphasized that the exact orthonormality holds only in the thermodynamic limit ($N \to \infty$). Actually, for $N$ finite, it would be mathematically impossible to have a set of $4^N$ exactly orthonormal states in a vector space of dimension $2^N$.

At this point, the physical ideas introduced in this section and in particular the concept of RVS can be regarded as guiding physical tools in the construction of our new algebraic structure. Now that this structure has been established, we can completely ignore the concept of RVS and present, as we do next, the obtained representation of the algebra of the local moments in an axiomatic, mathematically rigorous way:

1. Vector space: It is the set of all states of the form

$$\sum_{l_i=-1,0,1,2} C_{l_1l_2...l_N} u_{l_1,1} u_{l_2,2} ... u_{l_N,N} |\Phi\rangle,$$

where $C_{l_1l_2...l_N} \in \mathbb{C}$, $u_{2,i} = 1$, and $u_{l_i,i} = s_{l_i,i}$ for $l_i = -1, 0, 1$.

2. Operators $s_{l,i}$: Their action on the vector space is given by the multiplication table (14) and Eq. (16).

3. Scalar product: It is defined by declaring that the basis of the space formed by the $4^N$ vectors $u_{l_1,1} u_{l_2,2} ... u_{l_N,N} |\Phi\rangle$ is orthonormal.

These three points define a Hilbert space with operators $s_{l,i}$ satisfying Eqs. (14)–(16) or, equivalently, with operators $S_{fi}$ [given by Eq. (13)] satisfying the defining conditions of the algebra (3)–(7).

The inclusion of the conduction electrons is straightforward: The basis for the complete Hilbert space is obtained by applying electronic creation operators to the basis of spin fluctuations presented above, and the action of the operators $c_{k\alpha}^\dagger$, $c_{k\alpha}$ on the states is given
by the canonical anticommutation relations (4), Eq. (8) (where we can substitute \( s_{fi} \) by \( s_{l,i} \)), and the condition \( c_{k\alpha} |\Phi\rangle = 0 \) \( \forall k, \alpha \).

Finally, the Hamiltonian is given, in terms of the basic operators of this new representation, by:

\[
H = \varepsilon_k c_{k\alpha}^\dagger c_{k\alpha} + \frac{J}{4} \left[ (c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}) s_{0,i} + \sqrt{2} c_{i\uparrow}^\dagger c_{i\downarrow} s_{-1,i} + \sqrt{2} c_{i\uparrow}^\dagger c_{i\uparrow} s_{1,i} \right].
\]  

III. TRANSLATIONAL AND SPIN ROTATIONAL SYMMETRIES

In this section, we determine the translational and spin rotational symmetries of the system within this new representation. These symmetries will be used in the following sections to characterize the spectrum of excitations of the system. A unitary operator is completely determined by specifying how it transforms the basic operators \( c_{k\alpha}^\dagger, s_{l,i} \) and its action on the vacuum state: this is what we do next to introduce the symmetries.

A. Lattice translations

It is physically evident that, if \( \mathbf{a}_\gamma (\gamma = 1, 2, 3) \) are three primitive vectors of the real lattice, their associated translation operators \( T_{\mathbf{a}_\gamma} \) should satisfy:

\[
T_{\mathbf{a}_\gamma} c_{\mathbf{R}_i,\alpha}^\dagger T_{\mathbf{a}_\gamma}^\dagger = c_{\mathbf{R}_i+\mathbf{a}_\gamma,\alpha}^\dagger,
\]

(23)

\[
T_{\mathbf{a}_\gamma} s_{l,\mathbf{R}_i} T_{\mathbf{a}_\gamma}^\dagger = s_{l,\mathbf{R}_i+\mathbf{a}_\gamma},
\]

(24)

\[
T_{\mathbf{a}_\gamma} |\Phi\rangle = |\Phi\rangle.
\]

(25)

These equations define unitary operators that leave the Hamiltonian invariant and thus represent the basic translational symmetries of the system.

To exploit this symmetry it is convenient to Fourier transform all operators to the momentum representation:

\[
c_{k\alpha}^\dagger = N^{-1/2} \sum_i e^{i\mathbf{R}_i \cdot \mathbf{k}} c_{i\alpha}^\dagger,
\]

(26)

\[
s_{l,k} = N^{-1/2} \sum_i e^{i\mathbf{R}_i \cdot \mathbf{k}} s_{l,i},
\]

(27)
where $k$ is always in the first Brillouin zone. Lattice translations just multiply these operators by a phase factor:

$$T_{\alpha}c_{\gamma}^\dagger T_{\alpha}^\dagger = e^{-ika\gamma}c_{\alpha\gamma}^\dagger,$$

$$T_{\alpha}s_{l,k}T_{\alpha}^\dagger = e^{-ika\gamma}s_{l,k}.$$

The $s_{l,k}$ operators satisfy the following equations, which will be of much use in the next sections:

$$[s_{0,k}, s_{\pm 1,k'}] = \pm 2N^{-1/2}s_{\pm 1,k+k'},$$

$$[s_{1,k}, s_{-1,k'}] = 2N^{-1/2}s_{0,k+k'},$$

$$[s_{l,k}, s_{l',k'}] = 0,$$

$$s_{l,k}^\dagger = s_{-l,-k}.$$

Finally, the Hamiltonian is given, in the momentum representation, by

$$H = \varepsilon_k c_{k\alpha}^\dagger c_{k\alpha} + \frac{J}{4N^{1/2}} \left[ (c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow})s_{0,k'-k} + \sqrt{2}c_{k\uparrow}^\dagger c_{k'\downarrow}s_{-1,k'-k} + \sqrt{2}c_{k\downarrow}^\dagger c_{k'\uparrow}s_{1,k'-k} \right].$$

**B. Spin rotations**

The spin rotational symmetry is quite subtle. The total-spin operators of the system are given by

$$\Sigma = \sum_{i} S_{ei} + S_{fi},$$

and satisfy

$$[\Sigma^\alpha, \Sigma^\beta] = i\epsilon_{\alpha\beta\gamma}\Sigma^\gamma,$$

$$\Sigma^\dagger = \Sigma,$$

$$[H, \Sigma] = 0.$$
These are the properties that characterize the generators of a unitary representation of $SU(2)$ that leaves the Hamiltonian invariant. There is, however, an important problem: the operators $\Sigma$ do not annihilate the vacuum state and, therefore, the unitary transformations generated by them would not leave $|\Phi\rangle$ invariant. Since (in the absence of magnetic order) we do not physically expect the spin rotational symmetry to be broken, $\Sigma$ cannot be taken as the generators of this symmetry. We should thus look for another set of operators $S$ satisfying Eqs. (36)–(38) plus the condition

$$S|\Phi\rangle = 0.$$  \hspace{1cm} (39)

As we already saw, every vector in the Hilbert space constructed in Section II can be written as $V|\Phi\rangle$, where $V$ is a linear combination of products of operators $c_{i\alpha}^\dagger$ and $s_{l,j}$. The effect of a transformation $\exp(i\alpha \Sigma)$ on a state would be

$$e^{i\alpha \Sigma}V|\Phi\rangle = e^{i\alpha \Sigma}Ve^{-i\alpha \Sigma}\left[e^{i\alpha \Sigma}|\Phi\rangle\right],$$  \hspace{1cm} (40)

where

$$e^{i\alpha \Sigma}|\Phi\rangle \neq |\Phi\rangle.$$  \hspace{1cm} (41)

The obvious thing to do to satisfy Eqs. (36)–(38) plus the condition (39), is to demand that $\exp(i\alpha S)$ transform $V$ in the same way as $\exp(i\alpha \Sigma)$ but leave $|\Phi\rangle$ invariant, namely,

$$e^{i\alpha S}V|\Phi\rangle = e^{i\alpha \Sigma}Ve^{-i\alpha \Sigma}|\Phi\rangle,$$  \hspace{1cm} (42)

which implies that the action of $S$ on the Hilbert space is given by

$$SV|\Phi\rangle = [\Sigma, V]|\Phi\rangle.$$  \hspace{1cm} (43)

It is quite straightforward to prove that the linear operators $S$ defined by Eq. (43) satisfy Eqs. (36)–(38) and will, therefore, be taken as the generators of the spin rotational symmetry of the system. This implies, in particular, that the conduction electrons $c_{k\alpha}^\dagger|\Phi\rangle$ ($\alpha = \uparrow, \downarrow$) and the spin fluctuations $s_{l,k}|\Phi\rangle$ ($l = -1, 0, 1$) form, respectively, an $s = 1/2$ doublet and an $s = 1$ triplet under spin rotations, as is physically expected.
IV. KONDO LATTICE WITH ONE CONDUCTION ELECTRON

We shall consider, in this section, the case of a single conduction electron interacting with the lattice of local moments. This system is interesting because it is simpler than the general case and reveals very clearly the appearance of heavy fermions as collective states of the bare conduction electron and spin fluctuations.

We shall first examine the atomic limit (band width → 0) to determine that the spectrum of the system consists in two $s = 1/2$ doublet bands and an $s = 3/2$ quadruplet. Then, we will study the structure of these bands away from the atomic limit using the lowest approximation in which the conduction electron can only dress with one spin fluctuation at most. Finally, we will see that this study reveals the formation of collective, heavy-fermion states for low relative values of the exchange coupling.

The KLM is particularly simple in the atomic limit; it is just the sum of local Hamiltonians associated to each lattice site:

$$H = \sum_i H_i \quad (H_i = J S_{ei} S_{fi}) .$$

(44)

Thus, in this limit, the one-electron problem reduces to diagonalizing $H_i$ in the space of the local degrees of freedom with a single electron present. In the representation introduced in Section II, this space is generated by the following eight vectors:

$$c_{i\alpha}^\dagger |\Phi\rangle \quad \alpha = \uparrow, \downarrow ,$$

(45)

$$c_{i\alpha}^\dagger s_{l,i} |\Phi\rangle \quad \alpha = \uparrow, \downarrow , \quad l = -1, 0, 1 ;$$

(46)

(a state with more than one spin fluctuation accompanying the conduction electron at site $i$ can be developed by the multiplication table (14) into a linear combination of these states).

Since the spin operators $S$ are well-defined in this local space and commute with $H_i$, they can be used to diagonalize the local Hamiltonian. The diagonalization of $S^2$ is straightforward: the vectors (45) form an $s = 1/2$ doublet while the six vectors (46) are the product of an $s = 1/2$ by an $s = 1$ representations and can be decomposed into an $s = 1/2$ doublet
and an $s = 3/2$ quadruplet. The energy of the quadruplet is seen to be $J/4$ while the
diagonalization of $H_4$ in the subspace of $s = 1/2$ leads to two doublets with energies $J/4$
and $-3J/4$. The states in each multiplet can be determined, for example, by repeatedly
applying the lowering operator $(S^- = S^x - is^y)$ to the states with the highest eigenvalue of
$S^z$ $(s^z = s)$. The explicit expressions of these vectors are given below.

1. Quadruplet ($E = J/4$):

\[
|\frac{J}{4}, \frac{3}{2}, \frac{3}{2}, i\rangle = c_{i\uparrow}^\dagger s_{1,i}\Phi, \tag{47}
\]

\[
|\frac{J}{4}, \frac{3}{2}, \frac{1}{2}, i\rangle = \frac{1}{\sqrt{3}} S^-|\frac{J}{4}, \frac{3}{2}, \frac{3}{2}, i\rangle = \frac{1}{\sqrt{3}} (c_{i\uparrow}^\dagger s_{1,i} - \sqrt{2}c_{i\downarrow}^\dagger s_{0,i})|\Phi\rangle, \tag{48}
\]

\[
|\frac{J}{4}, \frac{3}{2}, -\frac{1}{2}, i\rangle = -\frac{1}{2} S^-|\frac{J}{4}, \frac{3}{2}, \frac{1}{2}, i\rangle = \frac{1}{\sqrt{3}} (c_{i\uparrow}^\dagger s_{1,i} + \sqrt{2}c_{i\downarrow}^\dagger s_{0,i})|\Phi\rangle, \tag{49}
\]

\[
|\frac{J}{4}, \frac{3}{2}, -\frac{3}{2}, i\rangle = \frac{1}{\sqrt{3}} S^-|\frac{J}{4}, \frac{3}{2}, -\frac{1}{2}, i\rangle = c_{i\downarrow}^\dagger s_{-1,i}|\Phi\rangle. \tag{50}
\]

2. $E = J/4$ doublet:

\[
|\frac{J}{4}, \frac{1}{2}, \frac{1}{2}, i\rangle = \frac{\sqrt{3}}{6} (3c_{i\uparrow}^\dagger + c_{i\downarrow}^\dagger s_{0,i} + \sqrt{2}c_{i\downarrow}^\dagger s_{1,i})|\Phi\rangle, \tag{51}
\]

\[
|\frac{J}{4}, \frac{1}{2}, -\frac{1}{2}, i\rangle = S^-|\frac{J}{4}, \frac{1}{2}, \frac{1}{2}, i\rangle = \frac{\sqrt{3}}{6} (3c_{i\downarrow}^\dagger - c_{i\uparrow}^\dagger s_{0,i} + \sqrt{2}c_{i\downarrow}^\dagger s_{-1,i})|\Phi\rangle. \tag{52}
\]

3. $E = -3J/4$ doublet:

\[
|\frac{-3J}{4}, \frac{1}{2}, \frac{1}{2}, i\rangle = \frac{1}{2} (c_{i\uparrow}^\dagger - c_{i\downarrow}^\dagger s_{0,i} - \sqrt{2}c_{i\downarrow}^\dagger s_{1,i})|\Phi\rangle, \tag{53}
\]

\[
|\frac{-3J}{4}, \frac{1}{2}, -\frac{1}{2}, i\rangle = S^-|\frac{-3J}{4}, \frac{1}{2}, \frac{1}{2}, i\rangle = \frac{1}{2} (c_{i\uparrow}^\dagger + c_{i\downarrow}^\dagger s_{0,i} - \sqrt{2}c_{i\downarrow}^\dagger s_{-1,i})|\Phi\rangle. \tag{54}
\]

Thus, the Fourier transform of these vectors, namely,

\[
|E, s, s^z, \mathbf{k}\rangle = N^{-1/2} \sum_i c^{\mathbf{R}, \mathbf{k}} |E, s, s^z, i\rangle \tag{55}
\]

(with $\mathbf{k}$ in the first Brillouin zone), are exact eigenstates of the operators $H$, $S^2$, $S^z$, and $T_a$, in
the atomic limit, with eigenvalues $E$, $s(s+1)$, $s^z$, and $\exp(-ik_a)$ respectively. These operators form a complete set in the sense that each vector is characterized by a definite
set of eigenvalues. Since $S^2$, $S^z$, and $T_{a\gamma}$ always commute with $H$, they can be used to characterize the spectrum of the system away from the atomic limit as well. This simplifies enormously the calculation of the spectrum: we just have to diagonalize $H$ in the subspace of vectors with definite eigenvalues of these operators.

Thus, from the analysis of the atomic limit and the symmetries of the system, we conclude that the spectrum contains two $s = 1/2$ doublet bands and an $s = 3/2$ quadruplet. We shall now propose how to calculate these bands away from the atomic limit. Since all the members in a spin multiplet have the same energy, we only need to calculate the energy of one of them; we shall select the one with $s^z = s$.

The most general state of the one-electron system is a linear combination of terms containing a single $c_{\kappa\alpha}^\dagger$-operator multiplied by several spin fluctuations corresponding to various lattice sites. The approximation that we propose to calculate the spectrum of excitations consists in determining variationally the best approximation to the actual eigenstates of $H$ within the subspace in which only a maximum of $n$ spin fluctuations can accompany the conduction electron.

One should start by writing the most general vector in this subspace with definite eigenvalues of $T_{a\gamma}$, $S^2$, and $S^z$. We shall denote this state (with $s^z = s$) by $|\xi, s, s, k\rangle = V_{\xi, s, k}|\Phi\rangle$, where $\xi$ represents the parameters of this general vector. The diagonalization of $T_{a\gamma}$ is straightforward if we consider all the degrees of freedom in momentum space, and the spin eigenstate conditions are equivalent to

$$S^+|\xi, s, s, k\rangle = \left[\Sigma^+, V_{\xi, s, k}\right]|\Phi\rangle = 0,$$

(56)

$$S^z|\xi, s, s, k\rangle = \left[\Sigma^z, V_{\xi, s, k}\right]|\Phi\rangle = s|\xi, s, s, k\rangle.$$  

(57)

The action of $H$ on $|\xi, s, s, k\rangle$ can be written as

$$H|\xi, s, s, k\rangle = E_k|\xi, s, s, k\rangle + |\perp\rangle,$$

(58)

where $|\perp\rangle$ is a vector orthogonal to $|\xi, s, s, k\rangle$. Obviously, the best approximation to the actual eigenstate will be the normalized vector for which $\langle\perp | \perp\rangle$ is minimized. Thus, the optimal $\xi$-parameters should be determined by demanding that
\[ \langle \downarrow | \downarrow \rangle = \langle \xi, s, s, k | H^2 | \xi, s, s, k \rangle - E_k^2 \]  

is minimized, where \( E_k \) (the approximate energy) is given by

\[ E_k = \langle \xi, s, s, k | H | \xi, s, s, k \rangle, \]

and \( |\xi, s, s, k\rangle \) satisfies the normalization condition

\[ \langle \xi, s, s, k | \xi, s, s, k \rangle = 1. \]

In this article, we will consider only the lowest \((n = 1)\) approximation. From Eqs. (59)–(61) it is clear that this approximation gives the exact result in the atomic limit and it should, therefore, yield precise results around this limit. It also describes exactly the bare electrons when \( J = 0 \) and it is thus expected to express accurately how these excitations are modified when a small interaction is introduced. Away from these situations, this approximation is expected to describe the spectrum only qualitatively.

The determination of the states \(|\xi, 1/2, 1/2, k\rangle\) and \(|\xi, 3/2, 3/2, k\rangle\) in the lowest approximation is straightforward, the result being

\[ |[\alpha, \beta], \frac{1}{2}, \frac{1}{2}, k\rangle = \left[ \alpha_k c_{k, \uparrow}^\dagger + N^{-1/2} \beta_k (q) (c_{q, s_0, k-q, \uparrow}^\dagger s_{0, k-q} + \sqrt{2} c_{q, s_1, k-q, \uparrow}^\dagger s_{1, k-q}^\dagger) \right] |\Phi\rangle, \]

\[ |[\gamma], \frac{3}{2}, \frac{3}{2}, k\rangle = N^{-1/2} \gamma_k (q) c_{q, \uparrow}^\dagger s_{1, k-q} |\Phi\rangle, \]

where sum over \( q \) is implicitly understood. It is also assumed that \( k - q \) is in the first Brillouin zone, which occasionally requires the addition of a reciprocal lattice vector. \( \alpha, \beta, \) and \( \gamma \) are the variational parameters whose optimal values should be determined by the conditions (59)–(61). The mathematical development of these conditions is a lengthy technical task which is outlined in the Appendix.

Since we will be considering the system in all the situations between the atomic and \( J = 0 \) limits, it is important to write the Hamiltonian in terms of parameters that scale in a convenient way. Since the number of conduction electrons is a constant, we can shift the bare dispersion relation \( \varepsilon_k \) so that \( \varepsilon_k = \Delta \eta_k \), where \( \Delta \) is the band width and \( \eta_k \) is a normalized band of unit width centered at \( \varepsilon = 0 \) \((-1/2 \leq \eta_k \leq 1/2)\).
Instead of working with $J$, $\Delta$, and $\eta_k$, we will use the more convenient parameters $\lambda$, $\Lambda$, and $\eta_k$ given by

\begin{align}
\lambda &\equiv \frac{J}{(\Delta + |J|)}, \\
\Lambda &\equiv \Delta + |J|.
\end{align}

$|\lambda|$ is a dimensionless parameter describing the strength of the interaction and it varies from zero (no interaction) to one (atomic limit). Positive and negative values of $\lambda$ correspond, respectively, to antiferromagnetic and ferromagnetic couplings. $\Lambda$ is just a measure of the global energy scale of the system which factorizes in $H$, and can thus be set equal to one without loss of generality. The Hamiltonian, therefore, depends essentially on the parameters $\lambda$ and $\eta_k$ and is given by

\begin{align}
H = \varepsilon_k c_k^\dagger c_k + \lambda S_{ei} S_{fi},
\end{align}

where $\varepsilon_k = (1 - |\lambda|)\eta_k$, $-1/2 \leq \eta_k \leq 1/2$, and $-1 \leq \lambda \leq 1$.

As we said before, the development of the conditions (59)–(61) that determine the optimal parameters of the approximate eigenstates (62) and (63) is carried out in the Appendix. We next summarize the results obtained for the doublet and quadruplet bands:

1. Doublet bands: The optimal parameters $\alpha$ and $\beta$ in Eq. (62) and the approximate energy $E$ are given by

\begin{align}
\alpha_k &= \text{Re} [4a_k A_k], \\
\beta_k(q) &= \frac{\lambda a_k}{\varepsilon_q - \varepsilon_k + w_k} + \frac{\lambda a^*_k}{\varepsilon_q - \varepsilon_k + w^*_k}, \\
E_k &= \varepsilon_k - \text{Re}[w_k],
\end{align}

where

\begin{align}
a^2 &= -\frac{w^2 A^*}{w A} \frac{\text{Im}[w^* w]}{\text{Im}[w^* A^*[8 A w^* w - (4 A + 3 B/A)w^*(w^* - w) - 6 \lambda w]]}, \\
A_k &= \lambda \int_{-1/2}^{1/2} \frac{D(\eta) d\eta}{(1 - |\lambda|)\eta - \varepsilon_k + w_k} - 2, \\
B_k &= \lambda^2 \int_{-1/2}^{1/2} \frac{D(\eta) d\eta}{[(1 - |\lambda|)\eta - \varepsilon_k + w_k]^2},
\end{align}

\text{(70)} \quad \text{(71)} \quad \text{(72)}
and \( w_k \) is the solution of the following pair of equations

\[
\text{Im} \left[ w^*(8w^*w + 3\lambda(1 + 2/A)w^* - 3\lambda^2/2) \right] = 0, \tag{73}
\]

\[
\text{Im} \left[ w'^2 A^* \left[ (4A + 3B/A)(w^* - w)^2 + 3\lambda(A + 2)(w^* - 3w) + 6\lambda(1 - A/A^*)w \right] \right] = 0. \tag{74}
\]

\( D(\eta) \) in Eqs. (71) and (72) represents the density of states of the normalized band \( \eta_k \). The subscripts \( k \) in Eqs. (70), (73), and (74) have been omitted to simplify the notation.

2. Quadruplet band: The optimal \( \gamma \) in Eq. (63) and the approximate energy \( E \) are given by

\[
\gamma(q) = \frac{a}{\varepsilon_q - z} + \frac{a^*}{\varepsilon_q - z^*}, \quad E = \text{Re}[z], \tag{75}
\]

where

\[
a^2 = \frac{\lambda C^* \text{Im}[z]}{2C \text{Im} \left[ C^*(1 + Dz/C) \right]}, \tag{76}
\]

\[
C = \lambda \int_{-1/2}^{1/2} \frac{D(\eta) \, d\eta}{(1 - |\lambda|\eta - z)} + 4, \tag{77}
\]

\[
D = \lambda \int_{-1/2}^{1/2} \frac{D(\eta) \, d\eta}{|(1 - |\lambda|\eta - z)|^2}, \tag{78}
\]

and \( z \) is the simultaneous solution of

\[
\text{Im} \left[ C^2 D^* \right] = 0, \quad \text{Im} \left[ C(zC^* - 3\lambda) \right] = 0. \tag{79}
\]

It is clear from these equations that the energy \( E_k \) of the doublet bands depends on \( \lambda \), \( \varepsilon_k \), and \( D(\eta) \). In the case of the quadruplet, however, \( E_k \) depends exclusively on \( \lambda \) and \( D(\eta) \), which implies that this band is flat in this approximation.

In order to carry out explicit calculations, we must specify \( D(\eta) \). A realistic density of states should behave like \( \sqrt{1/2 \pm \eta} \) at the extreme points \( \eta = \mp 1/2 \) and must be normalized. We shall take the simplest function satisfying these conditions, namely,
\[
D(\eta) = \frac{8}{\pi} \sqrt{\frac{1}{4} - \eta^2}, \tag{80}
\]

which leads to simple expressions for A, B, C, and D [see Eqs. (A34) and (A35)].

At this point, we can already determine the lowest approximation to the spectrum of the system by numerically solving Eqs. (73), (74) and (79).

The solutions for the energies satisfy \( E(-\lambda, -\varepsilon) = -E(\lambda, \varepsilon) \) for the doublet bands, and \( E(-\lambda) = -E(\lambda) \) for the quadruplet. Since we can relate, with these equations, the spectra for positive and negative values of \( \lambda \), we will restrict our study to the antiferromagnetic case (\( \lambda > 0 \)).

The numerical results obtained are displayed in Fig. 1. In order to make the physical interpretation of the results easier, we have parameterized the values of the bare band \( \varepsilon \) in a band-like manner, namely, with the function \( \varepsilon(\theta) = -1/2(1 - \lambda) \cos \theta \) (\( \theta \in [0, \pi] \)), which is represented by the dashed curve. The solid curves correspond to the solutions obtained for the two doublets \( E(\lambda, \varepsilon(\theta)) \) and the quadruplet \( E(\lambda) \).

Fig. 1(a) represents the atomic limit, with completely localized bands at \( E = 1/4 \) (quadruplet and upper doublet) and \( E = -3/4 \) (lower doublet). In Fig. 1(b), the degeneracy of the upper bands in the atomic limit is broken; as we already mentioned, the quadruplet band remains flat for all values of \( \lambda \) in this approximation. The transition from Fig. 1(c) to Fig. 1(d) is very revealing: There is a clear tendency to form, with the states of the superior and inferior parts of the upper and lower doublets respectively, a band that closely follows the bare conduction band, while the rest of the states tend to form a practically flat band. We shall call these bands the \textit{continuous} (because it is essentially a continuation of the bare band) and the \textit{heavy-fermion} band respectively. Fig. 1(d) can actually be interpreted as a hybridization of these two bands with the characteristic pseudogap structure.

To get a deeper insight into the nature of these bands, we will study the parameter \( \alpha \). It is clear from Eq. (72), that \( \alpha_k^2 \) represents the probability for the mode \( |[\alpha, \beta], 1/2, 1/2, \mathbf{k} \rangle \) to be in the bare state \( c^+_{\mathbf{k} \uparrow} |\Phi \rangle \). If the subscripts \( U \) and \( L \) denote the upper and lower doublets respectively, we get, for \( \lambda = 0.26 \),
\[ \alpha_L^2(\theta = 0) = 0.77, \alpha_U^2(\theta = \pi) = 0.93, \]  
\[ \alpha_U^2(\theta = 0) = 0.22, \alpha_L^2(\theta = \pi) = 0.018. \]  

The points in rows (81) and (82) correspond to the continuous and heavy-fermion bands respectively. The interpretation is clear: While the continuous band consists essentially in a small modification of the bare electronic states, in the heavy-fermion modes, the conduction electron strongly combines with spin fluctuations forming a complex, collective state as in the Kondo problem. It should be noted that the \( s = 3/2 \) quadruplet states are also collective modes in the most strict sense since, due to spin conservation, they have no probability to be in the bare states.

Calculations for very small values of \( \lambda \) show that the continuous band actually coincides with the bare band as \( \lambda \to 0 \). Since, as we already argued, these calculations are very reliable, we can assert that there is no hybridization of the continuous and heavy-fermion bands for very small couplings. Figs. 1(f), 1(e), and 1(d), describe the process of hybridization of these bands around \( \lambda = 0.24 \). We find that beyond the points A, B, C, and D in Figs. 1(e) and 1(f), the system of Eqs. (73) and (74) no longer has a solution. We have interpreted this fact as a mathematical expression of the inadequacy of the lowest order approximation around these points: one should physically expect that the precise description of the collective states will require considering more than just a single spin fluctuation combining with the bare conduction electron.

V. SUMMARY AND CONCLUSIONS

With the introduction of a new representation of the algebra of the local moments, we have established a new framework for the study of the Kondo lattice which enables a very clear mathematical description of heavy fermions as collective states of conduction electrons and spin fluctuations of the lattice of local moments.
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APPENDIX: LOWEST ORDER EQUATIONS FOR THE DOUBLET BANDS

We shall briefly develop here the conditions (59)–(61) for determining the optimal parameters $\alpha$ and $\beta$ that characterize the doublet bands of the one-electron Kondo lattice in the lowest approximation. The development of the corresponding equations for the quadruplet band is completely analogous and will be omitted.

Let us summarize the problem: We have to determine the parameters $\alpha$ and $\beta$ of the vector $|\alpha,\beta,1/2,1/2,k\rangle$ in Eq. (62) that minimize the function

$$\Psi_k([\alpha,\beta]) = \langle[\alpha,\beta],1/2,1/2,k|H^2|[\alpha,\beta],1/2,1/2,k\rangle - E_k^2,$$

where

$$E_k = \langle[\alpha,\beta],1/2,1/2,k|H|[\alpha,\beta],1/2,1/2,k\rangle,$$

while satisfying the normalization condition

$$\langle[\alpha,\beta],1/2,1/2,k|\alpha,\beta,1/2,1/2,k\rangle = 1.$$

In order to handle this normalization condition, it is very convenient to introduce a Lagrange multiplier $\tau$. Thus, the objective will be to find the parameters $\alpha$ and $\beta$ that minimize

$$\Omega_k([\alpha,\beta],\tau) = \Psi_k([\alpha,\beta]) + \tau\langle[\alpha,\beta],1/2,1/2,k|\alpha,\beta,1/2,1/2,k\rangle,$$

for an arbitrary $\tau$, and then select the value of $\tau$ for which the normalization condition (A3) is satisfied.
To simplify the notation, we will often omit the subindexes \( k \) in the forthcoming equations. If \( m_1, m_2, n_1, \) and \( n_2 \) are defined by

\[
m_1 = \frac{1}{\Gamma} \int \beta(q) \, dq, \quad m_2 = \frac{1}{\Gamma} \int \beta^*(q)\beta(q) \, dq,
\]

\[
n_1 = \frac{1}{\Gamma} \int \varepsilon_q \beta(q) \, dq, \quad n_2 = \frac{1}{\Gamma} \int \varepsilon_q \beta^*(q)\beta(q) \, dq,
\]

where the integrals are extended over the first Brillouin zone and \( \Gamma \) is the volume of this zone, a lengthy calculation yields

\[
\langle [\alpha, \beta], \frac{1}{2}, \frac{1}{2}, k | [\alpha, \beta], \frac{1}{2}, \frac{1}{2}, k \rangle = \alpha^* \alpha + 3m_2,
\]

(A6)

\[
E = \alpha^* \alpha \varepsilon + \frac{3\lambda}{4} (\alpha m_1^* + \alpha^* m_1) - \frac{3\lambda}{2} m_1^* m_1 + 3n_2,
\]

(A7)

\[
\langle [\alpha, \beta], \frac{1}{2}, \frac{1}{2}, k | H^2 | [\alpha, \beta], \frac{1}{2}, \frac{1}{2}, k \rangle = \frac{3}{\Gamma} \int \varepsilon_q^2 \beta^*(q)\beta(q) \, dq + \frac{3\lambda n_1^*}{2} (\alpha/2 - m_1) + \frac{3\lambda n_1}{2} (\alpha^*/2 - m_1^*) + \frac{9}{16} \lambda^2 m_2 + \frac{3}{4} \lambda^2 m_1^* m_1 + \frac{3}{4} \lambda (\varepsilon - \lambda/2) (\alpha m_1^* + \alpha^* m_1) + (\varepsilon^2 + 3\lambda^2/16) \alpha^* \alpha.
\]

(A8)

Substituting these equations in (A4), we can determine \( \Omega_k ([\alpha, \beta], \tau) \) and calculate its variations with respect to \( \beta(q) \) and \( \alpha \). The equations that express the vanishing of these variations are, respectively,

\[
0 = \beta(q) \left[ \varepsilon_q^2 - 2E\varepsilon_q + \frac{3\lambda^2}{16} + \tau \right] + \frac{\lambda}{2} (\alpha/2 - m_1) \varepsilon_q + \frac{\lambda^2 m_1}{4} + \frac{\lambda \alpha}{4} (\varepsilon - \lambda/2) - \frac{\lambda n_1}{2} - \lambda E (\alpha/2 - m_1) \forall q,
\]

(A9)

\[
0 = \alpha (\varepsilon^2 + 3\lambda^2/16 + \tau - 2E \varepsilon) + \frac{3\lambda}{4} [m_1 + m_1 (\varepsilon - \lambda/2 - 2E)].
\]

(A10)

We see from Eq. (A9), that the function \( \beta(q) \) has the structure

\[
\beta(q) = \frac{\lambda a}{\varepsilon_q - z} + \frac{\lambda b}{\varepsilon_q - z^*},
\]

(A11)

where the complex parameters \( a, b, \) and \( z \) satisfy
\[ a + b = -\frac{\alpha}{4} + \frac{m_1}{2}, \quad (A12) \]
\[-zb - z^*a = \frac{n_1}{2} - \frac{m_1}{2}(z + z^* + \lambda/2) + \frac{\alpha}{4}(z + z^* + \lambda/2 - \varepsilon), \quad (A13)\]
\[ z + z^* = 2E = 2\alpha \alpha^* \varepsilon + \frac{3\lambda}{2}(\alpha m_1^* + \alpha^* m_1) - 3\lambda m_1^* m_1 + 6n_2, \quad (A14)\]
\[ z^*z = \frac{3\lambda^2}{16} + \tau. \quad (A15)\]

A complete set of equations is formed by Eqs. (A12)–(A15) plus Eq. (A10), which can be written as
\[ \alpha(\varepsilon - z)(\varepsilon - z^*) + \frac{3\lambda}{4}[n_1 - (z + z^* + \lambda/2 - \varepsilon)] = 0, \quad (A16)\]

plus the normalization condition
\[ \alpha^* \alpha + 3m_2 = 1. \quad (A17)\]

Manipulating these equations and reparameterizing them with \( w \equiv \varepsilon - z \), we get the following equivalent set of equations:
\[ 0 = a(2w - \lambda) + b(2w^* - \lambda) - m_1\varepsilon + n_1, \quad (A18)\]
\[ 0 = \frac{3\lambda}{2}[a(w - \lambda/2) + b(w^* - \lambda/2)] + 4w^*w(a + b - m_1/2) - \frac{3\lambda}{4}(w + w^* - \lambda/2)m_1, \quad (A19)\]
\[ 0 = w^* + w - 6(\varepsilon m_2 - n_2) - 3\lambda[2(\alpha^* + b^*)m_1 + 2m_1^*(a + b) - m_1^* m_1], \quad (A20)\]
\[ 0 = \frac{1}{4} - 4(\alpha^* + b^*)(a + b) - \frac{3m_2}{4} - m_1^* m_1 + 2[(\alpha^* + b^*)m_1 + m_1^*(a + b)], \quad (A21)\]
\[ \alpha = 2m_1 - 4(a + b), \quad (A22)\]
\[ \tau = (\varepsilon - w^*)(\varepsilon - w) - \frac{3\lambda^2}{16}. \quad (A23)\]

The first four equations of this set should determine the parameters \( a, b, \) and \( w \), while the last two equations simply give us the values of \( \alpha \) and \( \tau \) in terms of these parameters. To get closed relations between \( a, b, \) and \( w \), we have to substitute in Eqs. (A18)–(A21) the explicit expressions of \( m_1, m_2, n_1, \) and \( n_2 \) in terms of \( a, b, \) and \( w \), namely,
\[ m_1 = aM + bM^*, \quad (A24)\]
\[ n_1 = a[\lambda + (\varepsilon - w)M] + b[\lambda + (\varepsilon - w^*)M^*], \quad (A25)\]
\[ m_2 = a^* b B^* + b^* a B + \lambda \frac{a^* a + b^* b}{w^* - w} (M - M^*), \]  
\[ n_2 = a b^* [\lambda M + (\varepsilon - w) B] + a^* b [\lambda M^* + (\varepsilon - w^*) B^*] + \lambda \frac{a^* a + b^* b}{w^* - w} [(\varepsilon - w) M - (\varepsilon - w^*) M^*], \]  
where \( M \) and \( B \) are given by
\[ M = \frac{\lambda}{\Gamma} \int \frac{d\eta}{\varepsilon - \varepsilon + w}, \quad B = \frac{\lambda^2}{\Gamma} \int \frac{d\eta}{(\varepsilon - \varepsilon + w)^2}. \]  
The result of this substitution is, after some manipulations,
\[ 0 = \text{Im} \left[ w^* (8w^* w + 3\lambda(1 + 2/A) w^* - 3\lambda^2/2) \right], \]  
\[ 0 = \text{Im} \left[ w^*^2 A^* [(4A + 3B/A)(w^* - w)^2 + 3\lambda(A + 2)(w^* - 3w) + 6\lambda(1 - A/A^*)w] \right], \]  
\[ a^* a = \frac{\text{Im}[w^*^2 w]}{\text{Im}[w^* w]} \]  
\[ b = -\frac{w A}{w^* A^* a}, \]  
where \( A \equiv M - 2. \)

It should be noted that Eqs. (A29)–(A32) determine everything except the phase of \( a. \) This is understandable since a change of this phase leads to the multiplication of the state by a global phase factor. Thus, we can fix the phase of \( a \) by demanding, for example, that \( b = a^* \). This selection yields a real wave function and gives rise to the final equations listed in Section IV.

\( A \) and \( B \) are given, in terms of the density of states \( D(\eta) \) of the normalized band \( \eta_k, \) by
\[ A = \lambda \int_{-1/2}^{1/2} \frac{D(\eta) d\eta}{(1 - |\lambda|) \eta - \varepsilon + w} - 2, \quad B = \lambda^2 \int_{-1/2}^{1/2} \frac{D(\eta) d\eta}{[(1 - |\lambda|) \eta - \varepsilon + w]^2}. \]

For the model density selected in Section IV \( (D(\eta) = \frac{8}{\pi} \sqrt{1/4 - \eta^2}) \), these expressions can be integrated analytically. We get, for \( \text{Im}[w] < 0, \)
\[ A = \frac{8\lambda}{(1 - |\lambda|)^2} \left[ w - \varepsilon + i \sqrt{(1 - |\lambda|)^2/4 - (\varepsilon - w)^2} \right] - 2, \]  
\[ B = \frac{-8\lambda^2}{(1 - |\lambda|)^2} \left[ 1 + \frac{i(\varepsilon - w)}{\sqrt{(1 - |\lambda|)^2/4 - (\varepsilon - w)^2}} \right]. \]
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FIGURES

FIG. 1. Zero-temperature spectrum of the antiferromagnetic Kondo lattice with one conduction electron, in the lowest approximation, for decreasing values of $\lambda$. The dashed curve parameterizes the values of the bare conduction band and the solid curves correspond to the quadruplet (horizontal line) and the two doublets. For low values of $\lambda$, the doublets give rise to a band that closely follows the bare conduction states and a practically flat, heavy-fermion band.
