Strong coupling Kondo lattice model as a Fermi gas

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The strong coupling half-filled Kondo lattice model is an important example of a strongly interacting dense Fermi system for which conventional Fermi gas analysis has thus far failed. We remedy this by deriving an exact transformation that maps the model to a dilute gas of weakly interacting electron and hole quasiparticles that can then be analyzed by conventional dilute Fermi gas methods. The quasiparticle vacuum is a singlet Mott insulator for which the quasiparticle dynamics are simple. Since the transformation is exact, the electron spectral weight sum rules are obeyed exactly. Subtleties in the behavior of electrons in the singlet Mott insulator can be reduced to a complicated but precise relation between quasiparticles and bare electrons. The theory of free quasiparticles can also be interpreted as an exactly solvable model for a singlet Mott insulator, providing an exact model in which to explore the strong coupling regime of a singlet Kondo insulator.

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 $: 71.10 - w, 71.27 + a$

INTRODUCTION

A Fermi liquid is described by starting with an ideal noninteracting Fermi gas. We then adiabatically "switch on" the interactions between particles. States of the interacting system are then identified with those of the noninteracting system. Fermi quasiparticles have the same relation to Fermi liquid ground state as the electron operators do to the vacuum; if $|\Psi_G\rangle$ is the Fermi liquid ground state, there should exist a quasiparticle creation operator c^{\dagger}_{β} so that $0 = c_{\beta} |\Psi_G\rangle$, $\{c_{\alpha}, c_{\beta}^{\dagger}\} = \delta_{\alpha\beta}$, and $Hc_{\alpha}^{\dagger} |\Psi_G\rangle = e_{\alpha} c_{\alpha}^{\dagger} |\Psi_G\rangle$. The spectral weight sum rule follows directly from this.

Previous work usually introduces new quantum mechanical degrees of freedom which are then reduced by constraints which are ultimately treated approximately.¹ The present work demonstrates an exact transformation that can be utilized to map the dense strongly interacting singlet Mott insulator to a weak coupling dilute Fermi gas. This allows conventional Fermi gas techniques to be used in the new basis allowing us to derive both precise ground state properties and exact spectral spectral weight sum rules.

We begin by considering a lattice of sites each consisting of conduction band *c* electrons that can hop between neighboring sites and core *f* electrons that are confined. At half filling a total of two electrons tend to be located on the site. An on site potential favors single occupancy of the *f* electron, forcing the second electron into the conduction band. The extended model consists of a lattice of such sites with only the *c* electrons hopping between neighbors.

There are four states with one *c* and one *f* electron present. The resulting triplet-singlet degeneracy is lifted by a spin exchange term that gives the singlet lowest energy.² This behavior is most easily encoded in the Kondo lattice Hamiltonian³

$$
H_{\text{KLM}} = t \sum_{rr'} (c_{c,\sigma}^{\dagger}(r)c_{c,\sigma}(r') + CC) + \sum_{r} \{JS_{c}(r) \cdot S_{f}(r) + U_{f}[n_{f}(r) - 1]^{2} \}.
$$
 (1)

The atomic ground state is given by $|\Psi_G\rangle$

 $=\frac{1}{\sqrt{2}}(c_{c,\uparrow}^{\dagger}c_{f,\downarrow}^{\dagger}-c_{c,\downarrow}^{\dagger}c_{f,\uparrow}^{\dagger})|\text{Vac}\rangle$. For *t*=0 the full ground state is a product of such two-electron singlets at each site and is nondegenerate with finite gap to the excited states. The gap will persist for small values of the hopping *t* and the local conduction electron will then simply make virtual excursions to the neighboring sites. The system will remain a singlet Mott insulator.

Before describing quasiparticles for nonzero *t* we begin with the limit of zero hopping. For each site, there are four charged spin half excitations consisting of each of the four states with three electrons.³ We first attempt to define a quasiparticle operator simply by $c_{c,\sigma}^{\dagger}$ which one might hope adds an extra conduction electron to the singlet.

This ansatz immediately leads to problems. First we find $c_{c,\uparrow}^{\dagger} | \Psi_G \rangle = -\frac{1}{2} c_{c,\uparrow}^{\dagger} c_{c,\downarrow}^{\dagger} c_{f,\uparrow}^{\dagger} | \text{Vac} \rangle$. Although the operator indeed creates a state with an extra charge, this state is not normalized.

A second problem is the following inequality: $c_{c,\uparrow}|\Psi_G\rangle = \frac{1}{2}c_{f,\downarrow}^{\uparrow}|\text{Vac}\rangle \neq 0$ which shows that our attempted quasiparticle annihilation operator does not annihilate the atomic ground state. Finally, we note that $c_{c,1} c_{c,1}^{\dagger} |\Psi_G\rangle$ $=-\frac{1}{\sqrt{2}}c_{c,\downarrow}^{\dagger}c_{f,\uparrow}^{\dagger}|\text{Vac}\rangle \neq |\Psi_G\rangle$ so that this simple annihilation operator does not reconstruct the original singlet ground state. We conclude that none of the conditions we require of a proper quasiparticle operator is fulfilled with this ansatz. This simple analysis reveals the source of the difficulty; the ground state is "entangled" in the sense that it cannot be created from the true vacuum by a simple product of bare electron operators.

CONSTRUCTING CORRECT LOCAL QUASIPARTICLES

We now discuss how to define proper local quasiparticle operators. The local Hilbert space consists of 16 states which we label from 1 to 16. First we list the eightstates 1–8 with even particle number ordered first by increasing particle number. Degeneracies are split by total spin, and remaining degeneracies are split by *s_z*. States with odd particle number are similarly assigned labels 9–16.

This "canonical" ordering is shown on an energy versus particle number diagram for the Hamiltonian *h*_{canonical}

FIG. 1. In (a), the energy $E = n_{\text{tot}} - \frac{2}{3}(n_f - n_c)$ is plotted vs particle number and labeled with the state that has the smallest value of *S*² and S_z . A dotted arrow indicates a *c*-type creation operator is used to create the state at the tip of the arrow from the state at the base. A solid arrow indicates an *f*-type creation operator is used. A soliddotted combination indicates a singlet combination is used. In (b) a similar construction is used in an interacting model. The dotted arrow here indicates a hole operator.

 $=n_{\text{tot}} - \frac{2}{3}(n_f - n_c)$ in Fig. [1](#page-1-0)(a). On the horizontal axis is plotted n_{tot} . On the vertical axis is the energy eigenstate labeled with the state of minimum *z* component of spin for each degenerate multiplet. In Fig. $1(b)$ $1(b)$ is a hypothetical diagram with an interacting Hamiltonian h_{atomic} favoring the Kondo singlet ground state. To avoid cluttering the figure, triplet states are not included.

We denote $|n\rangle_a = |n\rangle_{\text{atomic}}$ states in Fig. [1](#page-1-0)(b) and $|n\rangle_c$ \equiv $|n\rangle$ _{canonical} states states in Fig. [1](#page-1-0)(a). A precise description of these states is needed to continue.

The singlets are given by $|1\rangle_c = 1|\text{Vac}\rangle$, $|2\rangle_c = c_{f,\uparrow}^{\dagger} c_{f,\downarrow}^{\dagger}|\text{Vac}\rangle$, $|3\rangle_c = \frac{1}{\sqrt{2}} (c_{c,\uparrow}^{\dagger} c_{f,\downarrow}^{\dagger} - c_{c,\downarrow}^{\dagger} c_{f,\uparrow}^{\dagger}) | \text{Vac}\rangle, \qquad |4\rangle_c = c_{c,\uparrow}^{\dagger} c_{c,\downarrow}^{\dagger} | \text{Vac}\rangle, \qquad \text{and}$ $|5\rangle_c = c_{c,\uparrow}^\dagger c_{c,\downarrow}^\dagger c_{f,\uparrow}^\dagger c_{f,\downarrow}^\dagger |$ Vac). The triplets numbered $|6\rangle_c$, $|7\rangle_c$, and $|8\rangle_c$ are not shown in the diagram.

The four states of total spin $-\frac{1}{2}$ are given by $|9\rangle_c = c_{f,\downarrow}^{\dagger} | \text{Vac}\rangle$, $|10\rangle_c = c_{c,\downarrow}^{\dagger} | \text{Vac}\rangle$, $|11\rangle_c = c_{c,\downarrow}^{\dagger} c_{f,\uparrow}^{\dagger} c_{f,\downarrow}^{\dagger} | \text{Vac}\rangle$, and $|12\rangle_c = c_{c,\uparrow}^{\dagger} c_{c,\downarrow}^{\dagger} c_{f,\downarrow}^{\dagger} | \text{Vac} \rangle$. The states of total spin $\frac{1}{2}$ are $|13\rangle_c = c_{f,\uparrow}^{\dagger} | \text{Vac}\rangle$, $|14\rangle_c = c_{c,\uparrow}^{\dagger} | \text{Vac}\rangle$, $|15\rangle_c = c_{c,\uparrow}^{\dagger} c_{f,\uparrow}^{\dagger} c_{f,\downarrow}^{\dagger} | \text{Vac}\rangle$, and $|16\rangle_c = c_{c,\uparrow}^{\dagger} c_{c,\downarrow}^{\dagger} c_{f,\uparrow}^{\dagger} | \text{Vac} \rangle$. The states with $s_z = \frac{1}{2}$ are not labeled in the figure.

A local spin-symmetric Hamiltonian *H* is block diagonal in the blocks enclosed by parentheses: $([1],[2,3,4],[5])$, $([6])$, $(7]$), $(8]$) $(9,10][11,12]$) $(13,14][15,16]$). If particle number is also conserved, *H* is further block diagonal in the subblocks in square brackets.

We now draw in Fig. $1(b)$ $1(b)$ a similar diagram for a more complicated Kondo-lattice like Hamiltonian with identical but permuted eigenvalues. We assume it has the Kondo singlet ground state and lowest energy charge 2 ± 1 states consisting of zero or two *c* electrons together with a single *f* electron. Eigenstates in Fig. $1(b)$ $1(b)$ are labeled according to the same ordering scheme.

Our goal is to construct a unitary transformation *U* that maps the Kondo singlet ground state in Fig. $1(b)$ $1(b)$ $1(b)$ to the vacuum in Fig. $1(a)$ $1(a)$ and at the same time define quasiparticle operators that create the states of charge 2 ± 1 from the Kondo singlet. The arrows in Fig. $1(b)$ $1(b)$ illustrate the action of the quasiparticle operators. A dotted hole creation operator creates the singly charged states and or a solid electron operator creates the triply charged states. We thus map the ground state $|3\rangle_a$ to the vacuum $|1\rangle_c \equiv |\text{Vac}\rangle$, i.e., $U|3\rangle_a$ $=|1\rangle_c$. The low-energy state of one extra spin down electron $|12\rangle_a$ must map to $|9\rangle_c$; $U|12\rangle_a = |9\rangle_c$. Similarly we demand $U|9\rangle$ _a=|10}_c.

Symmetries can now be used to further specify *U*. We define *Q* to be the combined particle-hole spin flip transformation. This permutation is an inversion of the picture in Fig. [1](#page-1-0)(a) through the state $|3\rangle_c$. It can be verified that Q_{ij} =0 for all entries except

$$
1 = Q_{1,5} = -Q_{2,4} = Q_{3,3} = -Q_{4,2} = Q_{5,1} = Q_{6,6} = Q_{7,7} = Q_{8,8}
$$

= $Q_{9,12} = Q_{10,11} = -Q_{11,10} = -Q_{12,9} = Q_{13,16}$
= $Q_{14,15} = -Q_{15,14} = -Q_{16,13}$.

Signs are chosen to preserve spin.

We next define K to be the transformation that exchanges the two species of fermions. This corresponds to the permutation obtained by exchanging the high- and low-energy states for each value of n_{tot} in Fig. [1](#page-1-0)(a). Minus signs are inserted to make the transformation an element of group of continuous rotations. We find

$$
1 = K_{1,1} = K_{2,4} = -K_{3,3} = K_{4,2} = K_{5,5} = K_{6,6} = K_{7,7} = K_{8,8}
$$

= $- K_{9,10} = K_{10,9} = K_{11,12} = -K_{12,11} = -K_{13,14} = K_{14,13}$
= $K_{15,16} = -K_{16,15}$.

In order for *U* to preserve spin and also generate particle and hole operators from the original fermions, we demand *U* obeys the following: $[U, S] = 0$, $n_{tot}U = U(2 + n_e - n_h)$, and $UK=QU$. It can be verified that these constraints together with the demand that *U* be real and unitary is satisfied by

$$
1 = U_{1,4} = \sqrt{2}U_{2,3} = -\sqrt{2}U_{2,5} = U_{3,1} = \sqrt{2}U_{4,3} = \sqrt{2}U_{4,5} = U_{5,2}
$$

= $U_{6,6} = U_{7,7} = U_{8,8} = U_{9,10} = -U_{10,12} = U_{11,11} = U_{12,9}$
= $U_{13,14} = -U_{14,16} = U_{15,15} = U_{16,13}$.

This defines a new Hamiltonian $h'_{atomic} = U_r^{\dagger} h_{canonical} U_r$ which has the energy diagram shown in Fig. $1(b)$ $1(b)$. The demand that $U^{\dagger} n_{\text{tot}} U = 2 + n_e - n_h$ shows that *U* cannot be continued to the identity transformation.

From unitarity follows that $\hat{c}_{e,\sigma}^{\dagger}(r) \equiv U_r^{\dagger} c_{c,\sigma}^{\dagger}(r) U_r$ and $\hat{c}_{h,\sigma}^{\dagger}(r) \equiv U_r^{\dagger} c_{f,\sigma}^{\dagger}(r) U_r$ preserve the Fermi anticommutation relations. Inverting this formula and using the fact that $U_r |\Psi_G\rangle_a \equiv U_r |3\rangle_a = |1\rangle_c \equiv |\text{Vac}\rangle_c$ we find that $c_{cf,\sigma}(r) |\text{Vac}\rangle_c$ $=0$ is equivalent to $\hat{c}_{eh,\sigma}(r)|\Psi_G\rangle_a = 0$. We have therefore obtained a local unitary transformation that maps the original *c* and *f* bare electron operators to quasiparticle operators that annihilate the Kondo singlet. By construction the operators $\hat{c}_{eh}^{\dagger}(r)$ either add or remove exactly one charge in each of the states and $\hat{c}_{e,\sigma}^{\dagger}(r)$ is identified as an electron quasiparticle operator and $\hat{c}_{h,\sigma}^{\dagger}(r)$ as a hole.

Using the method in Ref. [4](#page-3-4) it is possible to explicitly write down the original operators c_{cf}^{\dagger} and c_{cf} as a polynomial of Fermion operators $\hat{c}_{eh,\sigma}^{\dagger}(r)$, $\hat{c}_{eh,\sigma}^{\dagger}(r)$. To lowest nonlinear order I find

$$
c_{c,\uparrow}^{\dagger} = \hat{c}_{h,\downarrow} \left(\tau_2 n_{e,\downarrow} + \frac{1}{2} \hat{c}_{h,\uparrow}^{\dagger} \hat{c}_{e,\downarrow}^{\dagger} - \tau_1 n_{e,\uparrow} - \frac{1}{\sqrt{2}} n_{h,\uparrow} \right) + \hat{c}_{e,\uparrow}^{\dagger} \left(\tau_1 n_{h,\downarrow} + \frac{-1}{2} \hat{c}_{h,\uparrow} \hat{c}_{e,\downarrow} + \frac{1}{\sqrt{2}} n_{e,\downarrow} - \tau_2 n_{h,\uparrow} \right) + \left(\frac{1}{\sqrt{2}} \hat{c}_{h,\downarrow} - \frac{1}{\sqrt{2}} \hat{c}_{e,\uparrow}^{\dagger} \right) + \cdots,
$$

where $\tau_2 = (1 - 1/\sqrt{2})$ and $\tau_1 = \frac{1}{2}(\sqrt{2} - 1)$. For the *f* electrons the result is

$$
c_{f,\uparrow}^{\dagger} = \hat{c}_{e,\uparrow}^{\dagger} \left(\frac{1}{2} n_{h,\downarrow} + n_{e,\downarrow} + \frac{-1}{2} \hat{c}_{h,\uparrow} \hat{c}_{e,\downarrow} + \frac{1}{\sqrt{2}} \hat{c}_{h,\uparrow}^{\dagger} \hat{c}_{e,\downarrow}^{\dagger} \right) + \hat{c}_{h,\downarrow} \left(\frac{-1}{2} n_{e,\uparrow} + \frac{1}{2} \hat{c}_{h,\uparrow}^{\dagger} \hat{c}_{e,\downarrow}^{\dagger} - \frac{1}{\sqrt{2}} \hat{c}_{h,\uparrow} \hat{c}_{e,\downarrow} - n_{h,\uparrow} \right) + \cdots.
$$

Similar formulas occur for the other spin component. We note that the *f* electron operators are constructed by third order electron and hole operators in contrast to the conduction electron operators that have a linear coupling to quasiparticles. Deriving or even verifying these formulas is formidable without the help of a computer.⁵

EFFECTIVE MODEL FOR QUASIPARTICLES

The transformation *U* is now used to define a global transformation by $U_{\text{global}} = \prod_r U_r$. Since U_r does not mix states of even and odd particle numbers we obtain $\{c_{i,\sigma}^{\dagger}(r), c_{j,\sigma}^{\dagger}(r')\}$ $= \delta_{i,j} \delta_{r,r'}$ verifying that *U* is indeed a global canonical transformation.

We now express the Kondo lattice model given by Eq. (1) (1) (1) in terms of electron and hole quasiparticle operators by replacing the Fermi operators $c_{cf,\sigma}(r)$ by their representation as polynomials in $\hat{c}^{\dagger}_{eh,\sigma}(r)$.

By construction, the Kondo singlet is the quasiparticle vacuum in the limit $t \rightarrow 0$. For small values of *t*, quasiparticles can hop between adjacent sites. The resultant lowenergy charged states that appear in the interacting ground state are therefore described by single quasiparticle operators and the unitary transformation guarantees these local states also have the correct energy.

For small *t* the states with local charge fluctuations will have a small amplitude in the interacting ground; the probability that a site is occupied by more than one quasiparticle will be accordingly less. The system should therefore be well approximated by a dilute Fermi gas.

We thus expand H_{KLM} in quasiparticle operators. Inserting the quasiparticle representation for the original Fermions, normal ordering, then truncating the Hamiltonian to second order we find⁶ $H_{\text{KLM}} = H_{\text{KLM}}^{\text{free}} + H_{\text{KLM}}^{\text{interacting}}$ with $H_{\text{KLM}}^{\text{free}}$ given by

$$
\frac{3}{4}J(n_c + n_f - 1) + \frac{1}{2}t\Sigma_s(-1)^{1/2+s}(\hat{c}_{e,s}^{\dagger}(r)\hat{c}_{h,-s}^{\dagger}(r')) \n- \hat{c}_{e,s}(r')\hat{c}_{h,-s}(r)) + \frac{1}{2}t\Sigma_s\hat{c}_{e,s}^{\dagger}(r)\hat{c}_{e,s}(r') - \hat{c}_{h,s}^{\dagger}(r)\hat{c}_{h,s}(r') \n+ \frac{1}{2}t\Sigma_s\hat{c}_{e,s}^{\dagger}(r')\hat{c}_{e,s}(r) - \hat{c}_{h,s}^{\dagger}(r')\hat{c}_{h,s}(r)
$$

$$
+\frac{1}{2}t\Sigma_{s}(-1)^{1/2+s}(\hat{c}_{h,s}(r')\hat{c}_{e,-s}(r)-\hat{c}_{h,s}^{\dagger}(r)\hat{c}_{e,-s}^{\dagger}(r')).
$$

 $H_{\text{KLM}}^{\text{free}}$ can then be treated exactly by transforming to momentum space and utilizing a conventional Bogoliubov transformation[.5](#page-3-5) With a chemical potential we compute the eigenvalues exactly. We let $e_k = \sum_i \cos(k \cdot \hat{i})$. The quasiparticle spectrum is then given by $E_k = \frac{3J}{4} \Delta_k \pm te_k \pm \mu$ where Δ_k $=\sqrt{1+(\frac{4te_k}{3J})^2}$.

It is reassuring that U_f does not appear to quadratic order. A value of J'' that is not small is what is crucial in creating the Kondo singlet and low-energy states; U_f only appears to higher order. For completeness, the entire onsite part of H_{KLM} is given by

$$
H_{\text{KLM}}^{\text{interacting}} = (n_e(n_e - 1)n_h + n_e n_h(n_h - 1)) \left(\frac{3}{16} J + \frac{-1}{4} U_f \right)
$$

+
$$
(n_e(n_e - 1) + n_h(n_h - 1)) \left(\frac{-3}{8} J + \frac{1}{2} U_f \right)
$$

+
$$
\left((S_e \cdot S_h) \left(\frac{1}{4} J - U_f \right) + n_e n_h \left(\frac{-9}{16} J + \frac{1}{4} U_f \right) \right).
$$

High order terms in the hopping become too lengthy to write out here. As we will see, however, they are unimportant for the small *t* physics since not only is the prefactor *t* small, but the fourth order fermion operators are also unimportant since the Fermi gas is dilute.

SPECTRAL WEIGHTS

Since the local electron operator is represented exactly in terms of quasiparticles the spectral weights can be computed for $H_{\text{KLM}}^{\text{free}}$ using Wick's theorem. In Fig. [2](#page-3-7) we plot the onedimensional spectral weight for the *c*-electron $A_c(k, \omega)$ as a function of ω several values of k from 0 to π . The quasiparticle coherent peak is a δ function which has been broadened only to make the plot easier to interpret. The very broad incoherent structure at higher energy is comprised of three quasiparticle contributions. Not shown are the five quasiparticle contributions that represent less than 1% of the total spectral weight and are outside the frequency domain plotted. We observe that $A_c(k+\pi,\omega) = A_c(k,-\omega)$ a consequence of the particle-hole symmetry of H_{KLM} .

NUMERICAL RESULTS

The quality of the wave function as an approximation to the Kondo Lattice ground state can be measured by the overlap of the ground state with the Hilbert space of H_{KLM} .

Let $\alpha = \frac{1}{2\lambda^2} \int \int \int T^d (1 - \Delta_k^{-1}) \left(\frac{dk}{2\pi} \right)^d \approx \frac{2d}{9} + O(\lambda^2)$ where $\lambda = t/J$ and *d* is the dimension. A measure of the deviation of the approximate ground state from the Hilbert space of the Kondo lattice model is measured by $\delta_p = \langle (1 - n_f)^2 \rangle$ which is exactly given by $\delta_p = \alpha^2 \lambda^4 (3 - 2\alpha \lambda^2)$ demonstrating convergence like $(t/J)^4$ for small *t*. We also find $\langle n_e + n_h \rangle = 4 \alpha \lambda^2$ which verifies that the number of quasiparticles remains sur-

FIG. 2. Square root of the spectral weight for *c*-electron $A_c(k, \omega)$ is plotted for $H_{\text{KLM}}^{\text{free}}$ for $t/J=0.4$ and $t=1$ in one dimension. To enable plotting the coherent and incoherent parts together, $A_c(k, \omega)$ has been smoothed by a Gaussian in ω before taking the square root. Plots are shown for $k=0$ to $k=\pi$.

prisingly small even as the Kondo lattice model approaches a phase transition.

A more challenging quantity to compute is the expectation value of the complete full Kondo lattice Hamiltonian in the ground state of $H_{\text{KLM}}^{\text{free}}$. This quantity is important since it is a rigorous upper bound to the *true* Kondo lattice ground state energy. We define $\beta = \int \int \int_{\gamma} d e_k^2 / \Delta_k \left(\frac{dk}{2\pi} \right)^d \approx \frac{d}{2} - \frac{d}{3} \lambda^2 + O(t^4)$ and find the exact answer⁵

$$
\langle H_{\text{KLM}}(U_f=0) \rangle_{\text{free}}
$$
\n
$$
= 1\left(\frac{-3}{4}\right) + \lambda^2 \left(3\alpha + \frac{-8}{3}\beta\right) + \lambda^4 \left(\alpha\beta(16 - 8\sqrt{2})\right)
$$
\n
$$
+ \beta^3 d^{-2} \left(\frac{-64}{9} + \frac{32}{9}\sqrt{2}\right) + \frac{-15}{4}\alpha^2\right) + \lambda^6 \left(\alpha^2\beta(-52 + 32\sqrt{2})\right)
$$
\n
$$
+ \beta^5 d^{-4} \left(\frac{-64}{27} + \frac{128}{81}\sqrt{2}\right) + \alpha\beta^3 d^{-2} \left(\frac{64}{3} + \frac{-128}{9}\sqrt{2}\right) + \frac{3}{2}\alpha^3\right)
$$
\n
$$
+ \lambda^8 \left(\alpha^2\beta^3 d^{-2} \left(\frac{-64}{3} + \frac{128}{9}\sqrt{2}\right) + \alpha^3\beta(72 - 48\sqrt{2})\right)
$$
\n
$$
+ \lambda^{10} \left(\alpha^4\beta(-36 + 24\sqrt{2})\right).
$$

This can be compared to high order series expansions.⁷ We find our result is at most about 3% above the series result, converging very rapidly for small values of λ . Errors are bounded by $0.61\lambda^4$ for $d=1$, $2.25\lambda^4$ for $d=2$, and $4.9\lambda^4$ for *d*=3 in the entire domain of convergence of the power series. See also Ref. [8.](#page-3-9)

CONCLUSIONS

An exact canonical transformation is derived that maps bare electron operators to quasiparticle electron and hole operators. This allows us to approximate the Kondo lattice model as a dilute Fermi gas for large values of the Kondo coupling. Properties of the Fermi gas can then be computed exactly. The overlap per site between the free Fermi gas ground state and the Hilbert space of the Kondo Lattice model is $(1 - O(t/J)^4)$ and ground state energies are also accurate to this order. Spectral weights can be computed that exactly obey the sum rules.

Together with the exact relation between quasiparticle operators, the free quasiparticle Hamiltonian represents an exactly solvable model of a singlet Mott insulator. The difficulty of understanding electrons in this Mott insulator is encoded in the complicated relation between electrons and quasiparticles rather than any subtlety in the quasiparticle dynamics.

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- 2We could have introduced a hopping instead of a spin exchange, leading to an effective spin exchange $J_{\text{eff}} = V^2 / U$; introducing more parameters makes the subsequent analysis more complicated but in principle it can still be carried out with the same rigor.
- 3We treat the Kondo spin as an extra fermion. In the exact KLM model the *U* term should not be present and the *f* electron should be strictly represented as a localized spin. Our treatment of particles and holes requires the *f* electron to represent a complete fermionic degree of freedom. This observation is consistent with others who have come to the same conclusion. See M. Oshikawa, Phys. Rev. Lett. 84, 3370 (2000); M. Oshikawa, M. Yamanaka, and I. Affleck, *ibid.* **78**, 1984 (1997); P. Coleman, I. Paul, and J. Rech, Phys. Rev. B 72, 094430 (2005).
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- 5Contrary to appearances, the formula for the energy expectation value is an exact answer and not a series expansion; the coefficients α and β are functions of λ given in the text. See EPAPS Document No. E-PRBMDO-76-079735 for more complete formulas as well as a guide to the computer algebra. For more information on EPAPS, see http://www.aip.org/pubservs/ epaps.html.
- 6This Hamiltonian is formally identical to that found in Ref. [1](#page-3-1) but in that work, the electron and hole operators represent constrained fermions yielding a number of difficulties that are circumvented in the present work.
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- 8Z. P. Shi, R. R. P. Singh, M. P. Gelfand, and Z. Wang, Phys. Rev. B 51, 15630 (1995); for $\lambda = 1/2$ and $d=1$, the most accurate estimate is *E*=−0.926. The present approximation gives *E*=−0.901.