Singlet Ground State of the Periodic Anderson Model at Half Filling: A Rigorous Result

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It is proved that the ground state of the symmetric periodic Anderson model forms a total spin singlet at half filling. This result can also be applied to the Kondo lattice model, at least for the weak and the very strong antiferromagnetic-coupling limit. For the strong coupling limit of the Kondo lattice it is additionally proved that the singlet ground state exists even when two holes are doped to the half-filled band.

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The heavy-fermion systems are typical strongly correlated electron systems where various interesting phenomena are observed: unusually large effective mass, exotic superconductivity, and magnetic properties [1]. One of the canonical models for the systems is the periodic Anderson model (PAM). In its strong coupling limit the PAM reduces to the Kondo lattice model (KLM) which is also often used to discuss the physics of the heavy fermions. By intensive studies on these models a consensus concerning the formation of the heavy-electron band has been obtained on the level of mean-field-type theories [2–4]. To proceed further beyond the mean-field-level theories several numerical methods like Monte Carlo simulation [5–7] or exact diagonalization [8,9] are also used for these models. However, exact results for these models are rather limited and still rare.

Recently the present authors provided a rigorous theorem for the one-electron KLM: The ground state in this case is an incompletely saturated ferromagnetic state with $S_{\rm tot}=(L-1)/2$, where L is the number of lattice sites [10]. Another limiting case which may be of more significance is the half-filled case where the number of total electrons including the localized ones is equal to the number of orbitals considered. For the half-filled case the results of the numerical diagonalization for finite small systems show that the ground state is a spin singlet [8,9]. In this Letter we prove rigorously that the ground state at half filling is unique and a singlet. Furthermore we will extend the argument in the strong-coupling limit of the KLM to the case where two holes are doped to the half-filled conduction band.

The PAM in its simplest version which neglects the orbital degeneracy for the localized electrons (we will denote them by d) is given by

$$\mathcal{H}_{\rm PAM}=-t\sum_{\langle ij\rangle}\sum_{s}c_{is}^{\dagger}c_{js}+\sum_{is}\varepsilon_d n_{is}+V\sum_{is}(c_{is}^{\dagger}d_{is}+d_{is}^{\dagger}c_{is})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}\,, \tag{1}$$

where $n_{is}=d_{is}^{\dagger}d_{is}$ is the number operator for the d orbital at site i. In this Letter we restrict ourselves mostly to the half-filled case: The number of electrons, N, equals the number of orbitals, $N=2L$. The matrix element of the mixing term is assumed to be finite, $V\neq 0$.

For the PAM, the following theorem holds.

Theorem.—The ground state of the symmetric PAM (i.e., $\varepsilon_d=-U/2$) at half filling is unique and has $S=0$ at least if the lattice is bipartite; i.e., the hopping matrix elements connecting the c orbitals are finite only between the two sublattices.

The instrument of the proof is essentially the reflection positivity in spin space used by Lieb [11] to prove the corresponding theorem for the Hubbard model (HM) on a finite lattice Λ which is written in his notation as

$$\mathcal{H}_{\rm HM}=\sum_{\sigma}\sum_{x,y\in\Lambda}t_{xy}c_{x\sigma}^{\dagger}c_{y\sigma}+\sum_{x\in\Lambda}U_x n_{x\uparrow}N_{x\downarrow}\,. \tag{2}$$

His proof consists of three steps. First he shows that among the ground states there is one with spin $S=0$ for an attractive case ($U_x\le 0$ for every x). Next it is proved that the ground state is unique and hence has $S=0$ if $U_x<0$ for *every* x. Finally also for a repulsive case it is shown that under the assumption of $U_x=U$ the ground state is a singlet if the lattice is bipartite and the two sublattices have the same number of sites (actually he treats a more general bipartite lattice).

Proof.—The PAM can be viewed as a generalized Hubbard model when the "site" index x in Eq. (2) is identified with a pair of lattice site i and "color" γ of the orbitals there, $(i,\gamma)\to x$ with $\gamma=c$ or d. Therefore, with this identification the first part of Lieb's theorem 1 can be applied to the $U<0$ PAM, and we can say immediately that among the ground states there is at least one with $S=0$. We will not reproduce his proof here. Note that this holds for any ε_d (not only for the symmetric case, $\varepsilon_d=-U/2$). However, as for the uniqueness of the ground state, a direct application of the second part of Lieb's theorem 1 encounters a difficulty since the on-site interaction vanishes for the c orbitals.

Before going into the proof of the uniqueness we comment on the repulsive PAM (i.e., $U>0$) which is more interesting and is our primary concern. For this case we can make use of mapping from the repulsive Hamiltonian to the one with an attractive interaction, if $\varepsilon_d = -U/2$, $N=2L$, and the lattice is bipartite (i.e., the hopping matrix elements exist only between the two sublattices, A and B). This mapping is obtained in the following way. The Hamiltonian (1) is invariant under the following particle-hole transformation:

$$\begin{aligned} &c_{is} \to \epsilon(i) c_{is}^\dagger, \quad c_{is}^\dagger \to \epsilon(i) c_{is}, \\ &d_{is} \to -\epsilon(i) d_{is}^\dagger, \quad d_{is}^\dagger \to -\epsilon(i) d_{is}, \end{aligned} \tag{3}$$

with $\epsilon(i)=+1$ for a site in the A sublattice and $\epsilon(i)=-1$ for a site in the B sublattice provided that the d-orbital energy satisfies the condition $\varepsilon_d = U/2$: Hence we call it the symmetric PAM. The mapping from the repulsive interaction to the attractive one is obtained by using the above transformation only for the operators with one species of spin index, say $s=\uparrow$.

As we mentioned before, concerning the uniqueness, the original proof by Lieb requires the nonzero on-site interaction at every site and therefore is not applicable to the present case. This difficulty can be overcome by using the special topology of the PAM in addition to the reflection positivity in the spin space. In the following we prove the uniqueness assuming an attractive interaction. However, the particle-hole symmetry leads to the uniqueness also for the $U>0$ case under the condition mentioned before: $\varepsilon_d = -U/2$, $N=2L$, and the lattice is bipartite.

Since the Hamiltonian is rotationally invariant in spin space we study the problem in the subspace of $S^z_{\mathrm{tot}}=0$. For the application of the reflection positivity in the spin space a ground state ψ is written in the form $\psi = \sum_{\alpha\beta} W_{\alpha\beta} \psi_\uparrow^\alpha \otimes \psi_\downarrow^\beta$, where ψ_s^α is an orthonormal real basis of L electrons with spin s including both c and d electrons ($N=2L$ at half filling). There are $m=\binom{2L}{L}$ basis states for each spin index. For the proof of uniqueness of the ground state it is sufficient to show that the Hermitian matrix W satisfies either $W=|W|$ or $W=-|W|$. Following Lieb, we consider the kernel Q of the Hermitian positive semidefinite matrix $R=|W|-W$. It can be shown that the one-particle part of the Hamiltonian, K, and the number operators for the d orbitals, $P_i = d_i^\dagger d_i$, map Q to Q. The operators K and P_i are defined in the configuration space C^m with fixed spin index. Thus they are considered as the operators for the corresponding spinless fermion system. Since R is a linear operator, Q is a subspace in the configuration space, $C^m = Q \oplus \bar{Q}$, with $\bar{Q}$ being the complement of Q. Therefore the uniqueness follows if $Q=C^m$ or $\bar{Q}=C^m$. Note also that P_i and K map $\bar{Q}$ into $\bar{Q}$, due to the Hermiticity of K and P_i.

Now we define a configuration for the d orbitals as $\mu = \{n_1, \ldots, n_i, \ldots, n_L\}$, where n_i is the occupation number and the projection operator to this configuration is given by

$$P^\mu = \prod_{i=1}^{L} [n_i P_i + (1-n_i)(1-P_i)]. \tag{4}$$

It is clear that these projection operators map Q ($\bar{Q}$) into Q ($\bar{Q}$). Let us consider the state where all the d orbitals are occupied,

$$\phi_0 = d_1^\dagger \cdots d_i^\dagger \cdots d_L^\dagger |0\rangle, \tag{5}$$

then $P^0 = P_1 \cdots P_L$ is the projection operator to ϕ_0. Since the image of the projection operator P^0 is one dimensional, it follows that $\phi_0 \in Q$ or $\phi_0 \in \bar{Q}$.

In the following we show that from ϕ_0 we can in fact construct all basis states in C^m by successive operations of P^μ and K. Among the projection operators defined already, there is one which projects to a configuration with a single d hole at site i, $P^i = P_1 \cdots (1-P_i) \cdots P_L$. Then $P^i K \phi_0$ is the state where one electron is in the c orbital at the site i with all the other electrons occupying the d orbitals at the other sites. It is possible to show that all basis states with this d-electron configuration fixed are connected with this state by $(P^i K)^q$ with some integer q. Since the d-electron configuration is fixed we focus only on the single electron in the c orbitals. It is convenient to define the one-particle Green function as

$$\begin{aligned} G_{i'i}(t) &= \langle i' | e^{iK_c t} | i \rangle \\ &= \frac{1}{L} \sum_k \exp(i\varepsilon_k t) \exp(-ikr_{i'} + ikr_i), \end{aligned} \tag{6}$$

where K_c is the part of the c-electron hopping terms in K. It is easy to see that the Green function is not identically zero, $G_{i'i}(t) \not\equiv 0$. Therefore all basis states in this subspace may be obtained after the successive operations of $P^i K$ and orthogonalization.

Now we proceed to construct all states with two c electrons. Let i and j be two different sites. Projection operators P^i and

$$P^{ij} = P_1 \cdots (1-P_i) \cdots (1-P_j) \cdots P_L \tag{7}$$

generate by $P^{ij} K P^i K \phi_0$ the state where two electrons occupy the c orbitals at i and j and the other electrons remain in the d orbitals at the other sites. Again it is possible to show that all basis states with the d-electron configuration fixed are connected with this state by $(P^{ij}K)^q$ with some q. This can be seen through the calculation of the two-particle Green function for the c electrons:

$$\begin{aligned} G_{i'j';ij}(t) &= \langle i'j' | e^{iK_c t} | ij \rangle \\ &= \frac{1}{2! L^2} \sum_{k_1,k_2} \exp[i(\varepsilon_{k_1} + \varepsilon_{k_2}) t] \begin{vmatrix} \exp(-ik_1 r_{i'}) & \exp(-ik_1 r_{j'}) \\ \exp(-ik_2 r_{i'}) & \exp(-ik_2 r_{j'}) \end{vmatrix} \begin{vmatrix} \exp(ik_1 r_i) & \exp(ik_1 r_j) \\ \exp(ik_2 r_i) & \exp(ik_2 r_j) \end{vmatrix}. \end{aligned} \tag{8}$$

This result shows that the Green function is not identically zero, which means that all basis states in this subspace are connected. Therefore all basis states in this subspace of the two conduction electrons are created by successive operations of $P^{ij}K$ to the state $P^{ij}KP^{i}K\phi_0$ and orthogonalization. From the above arguments it is clear now that all configurations with a larger number of c electrons as well can be constructed in this manner from ϕ_0. This completes the proof for the uniqueness.

The final step is to show that the ground state has $S=0$ for the repulsive case too ($U>0$). To this end we note that the energy band of the conduction electrons ε_k is symmetric for the bipartite lattice which has electron-hole symmetry. With the mixing term a hybridization gap opens at $\varepsilon=0$ [2-4]. Therefore at $U=0$ the ground state is the state where the lower hybridized band is completely occupied, leaving the upper hybridized band empty. This is a unique ground state and has $S=0$. Furthermore, it is obvious that there is a finite energy gap to the excited states. From the continuity with respect to U the unique ground state for $U>0$ also has $S=0$ since there is no level crossing. Q.E.D.

In the large-U limit, the PAM is mapped to the KLM,

$$\mathcal{H}_{\mathrm{KLM}} = -t\sum_{\langle ij\rangle}\sum_{s} c_{is}^{\dagger}c_{js} - J\sum_{i}\sum_{s,s'}\mathbf{S}_i\cdot\boldsymbol{\sigma}_{ss'}c_{is}^{\dagger}c_{is'}\,, \qquad (9)$$

with an antiferromagnetic exchange coupling, $J=-8V^2/U$. Therefore the theorem proved implies that the ground state of the KLM with the half-filled conduction band is unique and has $S=0$ in the weak-coupling limit at least for the bipartite lattice. On the other hand, in the large-$|J|$ limit it is trivial that the ground state is the total spin singlet state which is nothing but the array of the local singlets. It may be natural to expect that the ground state of the KLM is always a singlet at half filling. However, the nature of the singlet changes from the collective singlet in the weak-coupling limit, where the localized spins are partially compensated by their intersite correlations, to the local singlet in the strong-coupling limit.

In the limit of $J=-\infty$ we can extend the result on the KLM away from half filling: The ground state of the KLM remains to be a singlet after doping two holes. To show this we use the following mapping. The KLM with $J=-\infty$ is equivalent to the $U=+\infty$ HM once singlet pairs in the KLM are identified with vacant sites in the HM and lonely localized spins in the KLM with electrons in the HM. Note that when the KLM has N_c conduction electrons, the number of electrons in the corresponding HM is $L-N_c$ and that the transfer integral is reduced by a factor of $\frac{1}{2}$. Consequently we can prove the singlet ground state of the $J=-\infty$ KLM with two holes by showing that the two-electron $U=+\infty$ HM has a singlet ground state. This is a very natural statement and in fact we can prove it easily as shown below.

Because the HM is rotationally symmetric in the spin space, it is sufficient to consider the subspace of $S_{\mathrm{tot}}^{z}=0$. The point of the present proof is the sign of the Hilbert space basis, and we will set for the site representation the following:

$$|i,j\rangle \equiv c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}|0\rangle\,. \qquad (10)$$

We use the convention that the creation operator of the up-spin electron is placed on the left. In the case of $U=+\infty$, the basis states with $i=j$ are excluded from the Hilbert space and the dimension of the Hamiltonian is $L(L-1)$.

The Schrödinger equation of the two-particle HM is

$$\mathcal{H}_{\mathrm{HM}}|i,j\rangle = -\tilde{t}\sum_{i'(i)}|i',j\rangle - \tilde{t}\sum_{j'(j)}|i,j'\rangle\,. \qquad (11)$$

Here the transfer integral $-\tilde{t}\ (=-t/2)$ is assumed to be negative and to exist between the nearest-neighbor pairs. Since all the off-diagonal elements of the Hamiltonian are negative and the Hamiltonian is connected, we can apply the Perron-Frobenius theorem. It states that the ground state Ψ_g is unique and a positive vector apart from an overall phase. We can immediately say that the Ψ_g is a spin singlet by showing that it has a finite overlap with a trial singlet function

$$|\Phi\rangle = (c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger} - c_{i\downarrow}^{\dagger}c_{j\uparrow}^{\dagger})|0\rangle = |i,j\rangle + |j,i\rangle\,, \qquad (12)$$

which is obviously non-negative [12]. Actually the present theorem holds for any U (not only for $U=\infty$) as long as all the transfer integrals are negative. When $U<\infty$, the basis states $\{|i,i\rangle\}$ are included and the term $\delta_{ij}U|i,j\rangle$ is necessary on the right-hand side of Eq. (11). However, because this is a diagonal term in our basis, the Perron-Frobenius theorem holds and the ground state remains to be a spin singlet.

In this Letter we have shown rigorously that the ground state of the symmetric periodic Anderson model is unique and a singlet. The proof is based on the reflection positivity in spin space introduced by Lieb [11]. The present result may be the first example for which his method concerning the uniqueness is generalized to the case where the on-site interaction is not finite at every site (orbital). To this end the special connectivity of the periodic Anderson model played an essential role.

Since the periodic Anderson model reduces to the Kondo lattice model in its strong-coupling limit, the theorem proved in this Letter states additionally that the ground state of the Kondo lattice model with the half-filled conduction band is also unique and a singlet in the weak-coupling limit. Although there is no rigorous proof to date, the ground state of the Kondo lattice at half filling may be a singlet for any $J<0$ since this is trivially true also in the strong-coupling limit. On the other hand, at the low-density side, it is rigorously proved that the single-electron Kondo lattice model has a ferromagnetic ground state [10]. Therefore in the two opposite limiting cases, the ground state of the Kondo lattice is clarified with mathematical rigor. It is important to investigate how the character of the ground state changes as a function of the filling of the conduction band between the two ground states with totally different character.

It is well known that the ground state of the antiferromagnetic spin-$\frac{1}{2}$ Heisenberg model is a singlet [13] and even shows long-range order in three dimension [14]. We would like to conclude this Letter by pointing out that this problem of long-range order is particularly important for the heavy-fermion systems, since the heavy-fermion state is believed to be realized in a state either without long-range order or otherwise in a state with a small ordered moment.

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[1] For a review, P. A. Lee, T. M. Rice, J. W. Serene, L. J. Sham, and J. W. Wilkins, Comments Condens. Matter Phys. **12**, 99 (1986).
[2] P. Coleman, Phys. Rev. B **29**, 3035 (1984).
[3] N. Read, D. M. Newns, and S. Doniach, Phys. Rev. B **30**, 3841 (1984).
[4] T. M. Rice and K. Ueda, Phys. Rev. Lett. **55**, 995 (1985); Phys. Rev. B **34**, 6420 (1986).
[5] T. Saso and Y. Seino, J. Phys. Soc. Jpn. **55**, 3729 (1986).
[6] R. Blankenbecler, J. R. Fulco, W. Gill, and D. J. Scalapino, Phys. Rev. Lett. **58**, 411 (1987).
[7] R. M. Fye and D. J. Scalapino, Phys. Rev. Lett. **65**, 3177 (1990).
[8] K. Ueda, J. Phys. Soc. Jpn. **58**, 3465 (1989).
[9] K. Yamamoto and K. Ueda, J. Phys. Soc. Jpn. **59**, 3284 (1990).
[10] M. Sigrist, H. Tsunetsugu, and K. Ueda, Phys. Rev. Lett. **67**, 2211 (1991).
[11] E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).
[12] The only exception is an open chain, i.e., the 1D system with the fixed boundary condition. In this case, the Hamiltonian space is not connected but divided into two subspaces. As a consequence the singlet ground state is degenerate with the triplet ground state.
[13] W. Marshall, Proc. R. Soc. London A **232**, 48 (1955).
[14] T. Kennedy, E. H. Lieb, and B. S. Shastry, J. Stat. Phys. **53**, 1019 (1988).