

THEOREMS TO DEMONSTRATE THE PRESENCE OF ANTIFERROMAGNETISM IN THE PERIODIC ANDERSON MODEL.

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ABSTRACT

Anderson model is an important model in the theory of strongly correlated electron system. In this contribution, we introduce this model and the concept of electron correlation by bipartite lattice and prove rigorously theorems leading to the presence of spin singlet in the model. By using the results of Ueda et al (1992) and Tian (1994), we show theoretically that the ground state of the symmetric periodic Anderson model has a short – range order.

1.0. INTRODUCTION

The heavy fermion systems are well-known strongly correlated electron systems which exhibit unusual thermodynamic, magnetic, and transport properties.¹ microscopic investigations of these systems are generally based on the Periodic Anderson Model (PAM)

Take a finite lattice with N_{\square} lattice points. Neglecting the orbital degeneracy for the localized electrons, the Hamiltonian of the PAM can be written in the form

$$H_{\square} = -t \sum_{\sigma} \sum_{\langle i,j \rangle} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i \in \square} n_{i\uparrow} n_{i\downarrow} \quad (1)$$

Where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) is the creation (annihilation) of electrons, which creates (annihilates) an itinerant electron of spin σ at site i . Similarly, $d_{i\sigma}^{\dagger}$ and $d_{i\sigma}$ are the fermion operators for the localized electrons.

$n_{i\sigma} = d_{i\sigma}^\dagger d_{i\sigma}$ and $\langle i, j \rangle$ denotes a pair of lattice sites. ε_d is a local potential and $U > 0$ represent the on-site coulomb interaction for the localized electrons.

Since its introduction, the PAM and its variants constitute an important research topic in theoretical condensed matter physics, particularly in the context of strongly correlated electron system. Most of the many body techniques commonly used in condensed matter physics can be learnt in this context (Jafari, 2008). Also there are some theoretical tools and concepts which apply to this model only [Mahan, (2000); Enaroseha, (2012); Muhlbacher *et al*, (2011), Zhu and Zhu (2011)]. The aim of this paper is to provide a smooth introduction in the models and prove that the ground state of the symmetric PAM is a spin singlet.

2.0 METHODOLOGY AND MATHEMATICAL FORMULATION.

If we assume in particular that, when $E_d = E_f = -U/2$, the Hamiltonian of the PAM is called Symmetric. Lattice is called bipartite with respect to the Hamiltonian H_\square if it can be divided into two sublattices A and B , such that hopping of electrons does not occur between sites in the same sublattices. For a bipartite lattice, the signs of parameters t and V are not important for the mathematical analysis of this Hamiltonian. They can be changed by a unitary transformation. For definiteness, we shall choose $t > 0$ and $V > 0$ in the following.

To begin with, we first write the Hamiltonian H_\square of the symmetric PAM in a generalized Hubbard Hamiltonian. For simplicity, let us consider a specific bipartite lattice: the two-dimensional square lattice with $N = L^2$ lattice points (the lattice constant is taken to be unity). Take two identical copies of this square lattice, \square_1 and \square_2 . We make a doubly layered lattice $\tilde{\Lambda}$ by connecting the corresponding lattice points of \square_1 and \square_2 with bonds of

length 1. Now, each point of $\tilde{\Lambda}$ is labelled by $r = (i, m)$ where $m = 1$ or 2 . Obviously, $\tilde{\Lambda}$ has $2N_{\square}$ lattice points. Next, we introduce new fermion operators $f_{r\sigma}$ by

$$f_{r\sigma} = \begin{cases} C_{i\sigma} & \text{if } m=1 \\ 0 & \text{if } m=2 \end{cases} \quad (2) \quad \text{With}$$

the definitions of $\tilde{\Lambda}$ and $f_{r\sigma}$, the Hamiltonian H_{\square} of the symmetric PAM can be rewritten as the Hamiltonian of a generalized Hubbard model on $\tilde{\Lambda}$ by ignoring an uninteresting constant UH_{\square} .

$$H_{\square} = - \sum_{\sigma} \sum_{(rh)} t_{rh} c_{r\sigma}^{\dagger} c_{h\sigma} \quad (3)$$

where the new hopping constants t_{rh} are defined by

$$\mathbf{t}_{rh} = \begin{cases} t & \text{if } \mathbf{r} \text{ and } \mathbf{h} \text{ are nearest neighbors in } \square_1 \\ -V & \text{if } \mathbf{r} \text{ and } \mathbf{h} \text{ are in different layers and connected by a bond} \\ 0 & \text{otherwise.} \end{cases} \quad (4)$$

It is easy to see $\tilde{\Lambda}$ is still bipartite with respect to H_{\square} . Furthermore, we notice that the electrons in the second layer (the d -electron layer) do not hop and have an on-site Coulomb repulsion, while the electrons in the first layer are itinerant without interaction. That causes a little technical inconvenience. For this reason, we introduce an auxiliary interaction term

$$H_1 = \sum_{r \in \Lambda_1} \epsilon \left(n_{r\uparrow} - \frac{1}{2} \right) \left(n_{r\downarrow} - \frac{1}{2} \right) \quad (5)$$

to the Hamiltonian H_{\square} and study the ground state of the new Hamiltonian $\tilde{H}_{\square} = H_{\square} + H_1$. In the final step, we let $\epsilon \rightarrow 0$.

The purposes of the proofs are to show the existence of a short-range antiferromagnetic d -electron spin correlation in the ground state $\psi_0(\epsilon, U, \tilde{\Lambda})$ of the positive - (ϵ, U) symmetric PAM at half filling. However, reflection positivity in the spin space does not hold in this case. Fortunately, by the well-known unitary particle-hole transformation

$$\hat{U}_0 f_{r\uparrow} U_0^{-1} = f_{r\uparrow}, \hat{U}_0 f_{r\downarrow} U_0^{-1} = \epsilon(r) f_{r\downarrow} \quad (6)$$

Where $\varepsilon(r) = 1$ if $r \in A$ and $\varepsilon(r) = -1$ if $r \in B$, the Hamiltonian of the same form, which has reflection positivity in the spin space. Obviously, the transformed Hamiltonian has the same spectrum. In the following, we shall first study the ground state $\Psi_0(-\varepsilon, -U, \tilde{\Lambda})$ of the Hamiltonian $\tilde{H}_{\square}(-\varepsilon, -U)$ at half filling and then transform it back to the corresponding ground state $\Psi_0(\varepsilon, U, \tilde{\Lambda})$ of $H_{\square}(\varepsilon, U)$ by the inverse of the particle-hole transformation.

We notice that \tilde{H}_{\square} commutes with $N_{\uparrow} = \sum f_{r\uparrow} f_{r\uparrow}$ and $N_{\downarrow} = \sum f_{r\downarrow} f_{r\downarrow}$ respectively. Consequently, the Hilbert space of H_{\square} can be divided into numerous subspaces. Each of them is characterized by a pair of integers ($N_{\square} = n_1, N_{\square} = n_2$). For this Hamiltonian, following the formalism of Lieb (1989), we proved the following theorem.

Theorem. For any given even integer N , the ground state Ψ_0 of \tilde{H}_{\square} is unique and has quantum numbers $n_1 = n_2 = N/2$. Furthermore, Ψ_0 can be written as

$$\tilde{\Psi}_0 = \sum_{\alpha} W_{\alpha} \tilde{\psi}_{\alpha} \quad (7)$$

Where $\tilde{\psi}_{\alpha}$ is an orthogonal real basis for one species of $N/2$ spinless fermions. Take $W = (W_{\alpha\beta})$ as a $C_{2N_A}^{N/2} \times C_{2N_A}^{N/2}$ matrix; then W is a Hermitian and positive definite.

In Lieb (1989) proof, the uniqueness of $\tilde{\Psi}_0$ is the consequence of the positive definiteness of W , which was proved under the condition $\varepsilon \neq 0$. Ueda *et al* (1992) removed this condition by exploiting a special topology of the PAM in addition to the reflection positivity in the spin space. Consequently the ground state of \tilde{H}_{\square} is still non-degenerate even if $\varepsilon = 0$. With knowledge of this fact, we are able to make our proof simpler by introducing H_{\uparrow} and employing Lieb's theorem, whose proof is more direct. The theorem of Ueda *et al* (1992) guarantees that the ground state $\Psi_0(\varepsilon, U, \tilde{\Lambda}) \rightarrow \Psi_0(0, U, \tilde{\Lambda})$ as $\varepsilon \rightarrow 0$.

Theorem 1. Let $A_r \equiv f_{r\uparrow} f_{r\downarrow}$. Then, for any two distinct lattice points r and h , we have

$$\langle A_r A_h \rangle > 0 \quad (8)$$

Proof. By form (7) of $\Psi_0(N/2, N/2)$, we have

$$\langle \Psi_0 | A_r A_h | \Psi_0 \rangle = \langle \Psi_0 | f_{r\uparrow}^{\dagger} f_{r\downarrow} f_{h\downarrow}^{\dagger} f_{h\uparrow} | \Psi_0 \rangle$$

$$\begin{aligned}
& \sum_{\tau\delta} \sum_{\alpha\beta} \bar{W}_{\tau\delta} W_{\alpha\beta} \langle \Psi_{\tau}^{\dagger} \vee f_{r\uparrow}^{+\delta} f_{h\uparrow} \vee \Psi_{\tau}^{\alpha} \rangle \langle \Psi_{\tau}^{\delta} \vee f_{r\uparrow}^{+\delta} f_{h\uparrow} \vee \Psi_{\tau}^{\beta} \rangle \\
& \sum_{\tau\delta} \sum_{\alpha\beta} W_{\delta\tau}^{+\delta} W_{\alpha\beta} \langle \Psi_{\tau}^{\dagger} \vee f_r^{+\delta} f_h \vee \Psi_{\tau}^{\alpha} \rangle \overline{\langle \Psi_{\tau}^{\delta} \vee f_r^{+\delta} f_h \vee \Psi_{\tau}^{\beta} \rangle} \\
& \text{Tr}
\end{aligned}$$

Where $M \equiv f_r^{+\delta} f_h \langle \Psi_{\delta} \vee f_r^{+\delta} f_h \vee \Psi_{\delta} \rangle \overline{\langle \Psi_{\delta} \vee f_r^{+\delta} f_h \vee \Psi_{\delta} \rangle}$ and $W^{+\delta} = W$ (9)

$$\sum_{\tau\delta} \sum_{\alpha\beta} W_{\delta\tau} \langle \Psi_{\tau}^{\dagger} \vee f_r^{+\delta} f_h \vee \Psi_{\tau}^{\alpha} \rangle W_{\alpha\beta} \langle \Psi_{\tau}^{\beta} \vee f_r^{+\delta} f_h \vee \Psi_{\tau}^{\delta} \rangle$$

So we have,

$$\begin{aligned}
\langle \Psi_0 \vee A_r^{+\delta} f_h \vee \Psi_0 \rangle & \equiv \sum_{\tau\delta} \sum_{\alpha\beta} W_{\delta\tau} \langle \Psi_{\tau}^{\dagger} \vee M \vee \Psi_{\tau}^{\alpha} \rangle W_{\alpha\beta} \langle \Psi_{\tau}^{\beta} \vee M^{+\delta} \vee \Psi_{\tau}^{\delta} \rangle \\
& \text{Tr}
\end{aligned} \tag{10}$$

Since $\{\Psi_{\tau}\}$ is a real basis.

By Lieb's theorem, W is a positive definite matrix. Consequently, matrix $W^{1/2}$ is well defined. Therefore we have

$$\text{Tr} \tag{11}$$

Theorem 1 is proved. Q.E.D.

Remark 1. it is worthwhile to point out that theorem 1 has a physical implication. We noticed that

is, in fact, the reduced on-site two-particle density matrix of $\tilde{\Psi}_0$. If the largest eigenvalues λ_{\max} of this matrix satisfies the condition $\lambda_{\max} \geq \alpha H_{\square}$, where α is a positive constant independent of H_{\square} , then $\tilde{\Psi}_0$ has an off diagonal long-range order (ODLRO), which indicates that $\tilde{\Psi}_0$ is a superfluid. On the other hand, by theorem 1, we conclude that, if $\tilde{\Psi}_0$ is a superfluid, it must be a Bose – Einstein condensate, namely, a macroscopic on-site

pair of electrons is condensed at $\mathbf{p} = \mathbf{0}$ in $\tilde{\Psi}_0$. A detailed analysis on this point found in Tian (1992) article.

Since theorem 1 hold for any even integer N , in particular, it holds for the ground state $\Psi_0(-\varepsilon, -U, \tilde{\Lambda})$ of the negative (ε, U) symmetric PAM at half filling. Applying the inverse of the particle-hole transformation (6), we immediately obtain the following theorem.

Theorem 2: Let $\Psi_0(\varepsilon, U, \tilde{\Lambda})$ be the ground state of the positive- (ε, U) symmetric PAM Hamiltonian at half filling. Define the spin operators of the electron by

$$S_{i+\uparrow} = f_{i\uparrow}^\dagger f_{i\downarrow}, S_{i-\uparrow} = f_{i\downarrow}^\dagger f_{i\uparrow}, S_{iz} = \frac{1}{2} \quad (12)$$

$$i \quad \left. \begin{array}{l} \geq 0 \text{ if } r \text{ and } h \text{ are in the same sublattice} \\ \leq 0 \text{ if } r \text{ and } h \text{ are in the different sublattice} \end{array} \right\} \quad (13)$$

Proof. By the inverse of the unitary particle-hole transformation, we have

$$\Psi_0(-\varepsilon, U, \tilde{\square}) \rightarrow \Psi_0(\varepsilon, U, \tilde{\square})$$

$$f_{r\downarrow}^\dagger f_{r\uparrow}^{\dagger i - \varepsilon(r)} f_{r\downarrow}^{\dagger i}, f_{h\uparrow}^\dagger f_{h\downarrow}^{\dagger i - \varepsilon(h)} f_{h\uparrow}^{\dagger i} \quad (14)$$

Where $\varepsilon(r) = 1$ if $r \in A$, and $\varepsilon(r) = -1$ if $r \in B$

$$U_0 f_{r\uparrow} U_0^{-1} = f_{r\uparrow}, U_0 f_{r\downarrow} U_0^{-1} = \varepsilon(r) f_{r\downarrow}$$

Therefore by theorem 1,

$$0 \leq i$$

$$i i$$

$$i \varepsilon(r) \varepsilon(h) i \quad (15)$$

If \mathbf{r} and \mathbf{h} belong to the same sublattices, then $\varepsilon(\mathbf{r})\varepsilon(\mathbf{h}) = 1$ and hence

$$i$$

Otherwise, $\varepsilon(\mathbf{r})\varepsilon(\mathbf{h}) = -1$ and i

Theorem 2 is proved. Q.E.D.

Remark 2. Shen *et al* (1994) used the same technique to show the existence of ferrimagnetism in some positive-U Hubbard model.

Theorem 2 tells us that the short-range *transverse* spin correlation of d or f electrons in the ground state of the positive- (ε, U) symmetric PAM is antiferromagnetic. Since the Hamiltonian $\tilde{H}_{\tilde{\square}}$ has the SU(2) spin symmetry and its ground state $\Psi_0(\varepsilon, U, \tilde{\Lambda})$ at half filling is nondegenerate, one would expect that theorem 2 also holds for the *longitudinal* spin correlation functions. In fact, we have the following theorem.

Theorem 3. Let $\Psi_0(\varepsilon, U, \tilde{\Lambda})$ be the ground state of the positive- (ε, U) symmetric PAM Hamiltonian at half filling. Let

$$\lim_{\varepsilon \rightarrow 0} \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{rz} S_{hz} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{rz} S_{hz} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle \equiv C(r, h); \quad (16)$$

then the spin correlation function $C(\mathbf{r}, \mathbf{h})$ has satisfy inequality (13).

Proof. We first show that for any pair of distinct lattice points \mathbf{r} and \mathbf{h} ,

$$i2 \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{rz} S_{hz} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle \quad (17)$$

holds.

By definition, $S_{r+\hat{i}} = S_{rx} + iS_{ry}$, $S_{r-\hat{i}} = S_{rx} - iS_{ry}$, $S_{h-\hat{i}} = S_{hx} - iS_{hy}$.

Therefore we have

$$\begin{aligned} & i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | (S_{rx} + iS_{ry}) (S_{hx} - iS_{hy}) | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle \\ & \quad i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | (S_{rx} S_{hx} - iS_{rx} S_{hy} + iS_{ry} S_{hx} + S_{ry} S_{hy}) | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle \\ & \quad i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | (S_{rx} S_{hx} + S_{ry} S_{hy} + iS_{ry} S_{hx} - iS_{rx} S_{hy}) | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle \\ & \quad i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{rx} S_{hx} + S_{ry} S_{hy} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle + i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{ry} S_{hx} - S_{rx} S_{hy} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle \end{aligned} \quad (18)$$

We first simplify the last term on the right-hand side of (18). since \mathbf{r} and \mathbf{h} are distinct, $[S_{rz}, S_{hy}] = [S_{ry}, S_{hz}] = 0$. Therefore $S_{ry} S_{hx} - S_{rx} S_{hy}$ is a Hermitian operator. Consequently, its expectation value in any state is a real quantity. On the other hand, since $\tilde{H}_{\tilde{\square}}$ is a real matrix, its ground state $\Psi_0(\varepsilon, U, \tilde{\Lambda})$ must be chosen as state real vector. Therefore the expectation value F of $S_{ry} S_{hx} - S_{rx} S_{hy}$ in $\Psi_0(\varepsilon, U, \tilde{\Lambda})$ must be a pure imaginary matrix. Consequently $F \equiv 0$.

Next, we apply the unitary operator

$$U_2 = \exp\left[\left(\frac{i\pi}{2}\right) \sum_{i \in \tilde{\square}} S_{iz}\right]$$

Which rotates each spin about the S_z axis by an angle $\pi/2$, to the expectation value of $S_{ry} S_{hy}$ in $\Psi_0(\varepsilon, U, \tilde{\Lambda})$ and obtain

$$\langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{ry} S_{hy} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle + i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{rx} S_{hx} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle \quad (19)$$

Substituting (19) into (18), we obtain the identity (17).

That is:

i

$$i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{rx} S_{hx} + S_{ry} S_{hy} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle + i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{ry} S_{hx} - S_{rx} S_{hy} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle$$

So we have,

$$i i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{rx} S_{hx} + S_{ry} S_{hy} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle$$

$$i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{rx} S_{hx} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle + i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{ry} S_{hy} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle$$

$$i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{rx} S_{hx} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle + i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{rx} S_{hx} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle$$

$$i 2 \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{rx} S_{hx} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle$$

Equation (17) is proved.

Similarly, we can show that

$$\langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{rx} S_{hx} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle = i \langle \Psi_0(\varepsilon, U, \tilde{\square}) | S_{rz} S_{hz} | \Psi_0(\varepsilon, U, \tilde{\square}) \rangle \quad (20)$$

By applying the unitary operator

$$U_3 = \exp \left[\left(\frac{i\pi}{2} \right) \sum_{i \in \tilde{\square}} S_{iy} \right]$$

To the expectation value of $S_{rz} S_{hz}$ in $\Psi_0(\varepsilon, U, \tilde{\Lambda})$

Combining identities (17) and (20) and inequality (13), we see that the longitudinal spin correlation of $\Psi_0(\varepsilon, U, \tilde{\Lambda})$ is antiferromagnetic. Since this conclusion is true for any $\varepsilon > 0$, it must also hold for in the limit $\varepsilon \rightarrow 0$. Therefore the longitudinal spin correlation of the d or f electrons in the ground state of the positive- U symmetric PAM at half filling is antiferromagnetic.

Our proof is accomplished. Q.E D.

3.0 SUMMARY AND CONCLUSION

This work is an extension and detailed analysis of Tian (1994) article and Ueda (1992) articles in PAM and Hubbard model respectively. We proved the existence of the short – range antiferromagnetic order in the ground state of the symmetric PAM at half filling for arbitrary V and $U > 0$, we do not claim that the ground state has long – range antiferromagnetic order. In fact Moller and Wolfle (1993) show by using a mean field slave – boson theory that the half – filled ground state may be either antiferromagnetic or paramagnetic. The line separating their region of stability is given by the critical value of their exchange constant. In all the lattice systems studied recently show an antiferromagnetic ground state and the first excited state is always a spin singlet (Enaroseha, 2012).

In conclusion, in this paper, we showed rigorously that the spin correlation between (d, d) , (f, f) , (C, C) , (C, d) and (C, f) electrons are antiferromagnetic in the ground state of the PAM at half – fillings. The spin correlations of f electrons in the ground state $\Psi_0()$ which is

of fundamental importance was not discussed in this article, which hopefully will become possible in the near future.

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