Exact results for the one dimensional periodic Anderson model at
finite $U$

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Abstract

We present exact results for the periodic Anderson model for finite Hubbard
interaction $0 \leq U < \infty$ on certain restricted domains of the model’s phase
diagram, in $d = 1$ dimension. Decomposing the Hamiltonian into positive
semidefinite terms we find two quantum states to be ground state, an insu-
lating and a metallic one. The ground state energy and several ground state
expectation values are calculated.

I. INTRODUCTION

Since the last decades compounds with lanthanide or actinide elements as heavy-fermion
systems have attracted great interest because of their interesting experimental behavior.
Numerous strange phases are thought to be possible as the ground state of such a system,
ordered and disordered phases as well. As a theoretical background the periodic Anderson
model (PAM) is one of the most important applicants to explain the physics in these systems.
However, despite its relatively simple structure up to now the complete exact solution of the
model is not known even in one dimension and there are mostly approximative results. In
1993, using a method proposed by Brandt and Giesekeus, Strack found the exact ground
state in $d = 1$ for the strong coupling $U = \infty$ case. His results were generalized for
\[ d = 2, 3 \text{ dimensions by Orlik and Gulácsi}\] also in \( U = \infty \). This strong coupling limit is however an extremal case and is important to look for results in the physical domain where \( U < \infty \). Here we present for the first time exact results for PAM at finite \( U < \infty \), in \( d = 1 \) dimension. Two different solutions are reported, one insulating and a metallic one, both at 3/4 filling. The paper is organized as follows: The following Section is devoted to introduce the model and to show the positive decomposed form of the Hamiltonian used in the remaining part of the paper. Section III. contains the results of the calculations, and finally Section IV. concludes the results and closes the paper.

II. THE HAMILTONIAN

To start our study we use the Hamiltonian \((H)\) of PAM as presented below:

\[
H = \hat{T}_f + \hat{T}_c + \hat{V}_0 + \hat{V}_1 + E_f \sum_{i,\sigma} n_f^i, + U \hat{U},
\]

where \(\hat{T}_d = \sum_{i,\sigma} [t d_{i+1,\sigma} d_i, + h.c.]\) with \(d = c, f\) are hoppings for \(c\) and \(f\) electrons, \(\hat{V}_0 = \sum_{i,\sigma} [V_0 c_i, c_i, + h.c.]\) is the on-site and \(\hat{V}_1 = \sum_{i,\sigma} [V_1 (c_{i,} f_{i+1,\sigma} + f_{i,} c_{i,}) + h.c.]\) is the first-neighbor hybridization term, \(\hat{U} = \sum_i n_{i,\uparrow}^f n_{i,\downarrow}^f\) is the Hubbard on-site interaction, and \(n_{i,\sigma}^d = d_{i,\sigma}^+ d_{i,\sigma}\) are the particle-number operators.

To have a form of \(H\) appropriate for our goal let us transform Eq.(1) to the following form:

\[
H = -\sum_{i,\sigma} (|x|^2 + |y|^2 + |z|^2 + |v|^2) + \sum_{i,\sigma} a_{i,\sigma} a_{i,\sigma}^+ + (|x|^2 + |y|^2) \sum_{i,\sigma} n_{i,\sigma}^c + (|z|^2 + |v|^2 + E_f) \sum_{i,\sigma} n_{i,\sigma}^f + U \sum_{i,\sigma} n_{i,\uparrow}^f n_{i,\downarrow}^f
\]

where \(a_{i,\sigma} = x c_{i,\sigma}^+ + y c_{i+1,\sigma}^+ + z f_{i,\sigma}^+ + v f_{i+1,\sigma}^+\) and \(x, y, z\) and \(v\) are given by the following equations:

\[
x y^* = -t_c, \quad z v^* = -t_f, \quad x z^* + y v^* = -V_0, \quad x v^* = z y^* = -V_1.
\]

In order to solve Eqs.(3) let us introduce \(m = \frac{t_f}{t_c}\). Using \(m\), from Eqs.(3) we have \(z = m x, v = m^* y\) and the square of \(x\) is determined by \(|x|^2 = -\frac{V_0}{2m} \pm \sqrt{\frac{V_0^2}{4m^2} - t_c^2 \frac{m}{m^*}}\). During the calculation we used the conditions

\[2\]
\[ t_f t_c = V_1^2, \quad \frac{V_0^2}{4m^*} + t^2_c \geq 0, \quad -\frac{V_0}{2m^*} \pm \sqrt{\frac{V_0^2}{4m^*} - t^2_c \frac{m}{m^*}} \geq 0. \]  

(4)

Going on with transforming \( H \) we get from Eq.(2)

\[
H = P + P' + (|x|^2 + |y|^2) \sum_{i,\sigma} n_{i,\sigma}^c + (|z|^2 + |v|^2 + E_f + U) \sum_{i,\sigma} n_{i,\sigma}^f
\]

\[ + K - U L, \]  

(5)

where \( L \) is the lattice size, \( P = \sum_{i,\sigma} a_{i,\sigma} a_{i,\sigma}^+ \), \( P' = U \sum_i (1 - n_{i,\uparrow}^f - n_{i,\downarrow}^f + n_{i,\uparrow}^f n_{i,\downarrow}^f) \) and \( K = - \sum_{i,\sigma} (|x|^2 + |y|^2) (|m|^2 + 1) \). After this step, from Eq.(3) in the case of \( E_f = (1 - |m|^2)(|x|^2 + |y|^2) - U \), the final form of \( H \) is given by

\[
H = P + P' + (|x|^2 + |y|^2) \sum_{i,\sigma} (n_{i,\sigma}^c + n_{i,\sigma}^f) + K - U L.
\]  

(6)

This form of \( H \) consists of constants \( K \) and \( UL \), positive semidefinite operators \( P \) and \( P' \), and \( \sum_{i,\sigma}(n_{i,\sigma}^c + n_{i,\sigma}^f) \) which is related to the particle number as \( \langle n \rangle = 1/L \sum_{i,\sigma}(n_{i,\sigma}^c + n_{i,\sigma}^f) \). Because \( P \) and \( P' \) are positive semidefinite, omitting them the ground state of the operator built up of the remaining terms must be a lower bound to the ground-state energy:

\[
E_l = (|x|^2 + |y|^2) \langle n \rangle L + K - U L.
\]  

(7)

An upper limit \( E_u \) for the ground state energy \( E_0 \) can be derived from the variational principle, assuming some wave function \( |\psi\rangle \) to be the ground state. If there is any domain in the space of the model parameters with \( E_l = E_u = E_0 \) then on that domain the exact ground state is \( |\psi\rangle \) and the exact ground state energy is \( E_0 \). This procedure will be followed in the next Section.

**III. THE OBTAINED SOLUTIONS**

In this Section we describe two different and exact ground-state solutions for PAM at finite \( U \) related to an insulating and a metallic phase. We start the presentation with the insulating case.
A. The insulating state

Consider that all the coupling constants are real. We have in this case from Eqs.(3)

\[
x = (-\frac{V_0 V_1}{2 t_f}) \pm \sqrt{\frac{V_0^2 V_1^2}{4 t_f^2} - t_c^2} e^{i \phi_x},
\]

(8)

\[
y = -t_c (-\frac{V_0 V_1}{2 t_f}) \pm \sqrt{\frac{V_0^2 V_1^2}{4 t_f^2} - t_c^2} e^{-i \phi_x},
\]

\[
z = \frac{V_1}{t_c} (-\frac{V_0 V_1}{2 t_f}) \pm \sqrt{\frac{V_0^2 V_1^2}{4 t_f^2} - t_c^2} e^{i \phi_x},
\]

\[
v = -V_1 (-\frac{V_0 V_1}{2 t_f}) \pm \sqrt{\frac{V_0^2 V_1^2}{4 t_f^2} - t_c^2} e^{-i \phi_x},
\]

where \( \phi_x \) is an arbitrary phase. Inserting \( x \) and \( y \) into the expression of \( E_f \) given above we have \( E_f = - \left( 1 - \frac{t_f^2}{V_1^2} \right) \frac{V_0 V_1}{t_f} - U \). We also need the conditions \( t_f t_c = V_1^2, \frac{V_0^2}{V_1^2} \geq 4, \)
\( -\frac{V_0 V_1}{2 t_f} \geq 0 \), that are counterparts of those given in Eq.(4) but for the case of real coupling constants. In these conditions we have a lower limit for the ground state energy from Eq.(7)

\[
E_{l,1} = \left[ -\frac{V_0 V_1}{t_f} \left( 1 - \frac{2 t_f^2}{V_1^2} \right) - U \right] L.
\]

(9)

To get also an upper bound we call the variational principle. Let the trial wave function be

\[
| \psi_1 \rangle = \prod_i \left( c_{i,\uparrow}^+ + m f_{i,\uparrow}^+ \right) \left( c_{i,\downarrow}^+ + m f_{i,\downarrow}^+ \right) \left( \alpha_i c_{i,\uparrow}^+ + \beta_i c_{i,\downarrow}^+ + \gamma_i f_{i,\uparrow}^+ + \delta_i f_{i,\downarrow}^+ \right) | 0 \rangle
\]

(10)

\[
= \prod_i \left( \epsilon_i \left( c_{i,\uparrow}^+ c_{i,\downarrow}^+ f_{i,\uparrow}^+ - m f_{i,\uparrow}^+ f_{i,\downarrow}^+ c_{i,\downarrow}^+ \right) + \nu_i \left( c_{i,\uparrow}^+ c_{i,\downarrow}^+ f_{i,\uparrow}^+ - m f_{i,\uparrow}^+ f_{i,\downarrow}^+ c_{i,\downarrow}^+ \right) \right) | 0 \rangle
\]

where \( \epsilon_i \) and \( \nu_i \) are related to the quantities \( \alpha_i, \beta_i, \gamma_i, \delta_i \). Since \( | \psi_1 \rangle \) sets three electrons on any lattice site it belongs to band filling \( \langle n \rangle = 3 \). Using Eq.(10) we have an upper limit for the ground state energy: \( E_{u,1} = \langle \psi_1 | H | \psi_1 \rangle / \langle \psi_1 | \psi_1 \rangle \). Since \( P | \psi_1 \rangle = P' | \psi_1 \rangle = 0 \), it follows that \( E_{u,1} = E_{l,1} = E_0 \), where \( E_0 \) is the ground state energy. Collecting all the conditions we used: \( U \geq 0, t_f t_c = V_1^2, \frac{V_0^2}{V_1^2} \geq 4, -\frac{V_0 V_1}{2 t_f} \geq 0, \)
\( E_f = - \left( 1 - \frac{t_f^2}{V_1^2} \right) \frac{V_0 V_1}{t_f} - U, \langle n \rangle = 3 \),
the ground state is given by Eq.(10) and the ground state energy is of the form of Eq.(9).

To get a deeper insight into the nature of the state represented by \( | \psi_1 \rangle \) we show some
expectation values calculated with it. Since \( | \psi_1 \rangle \) sets three electrons on each site it is obvious that any way of moving an electron from a certain site \( i \) to an other \( j (\neq i) \) results an orthogonal state to it so we have

\[
\langle T_c \rangle = \langle T_f \rangle = \langle V_1 \rangle = 0.
\]  

(11)

Expectation values of other terms after normalization are given as

\[
\langle n^I_{i,\uparrow} \rangle = \frac{m^2}{1 + m^2} + \frac{\epsilon_i^2}{(\epsilon_i^2 + \nu_i^2)(1 + m^2)},
\]

\[
\langle n^I_{i,\downarrow} \rangle = \frac{m^2}{1 + m^2} + \frac{\nu_i^2}{(\epsilon_i^2 + \nu_i^2)(1 + m^2)},
\]

\[
\langle n^E_{i,\uparrow} \rangle = \frac{1}{1 + m^2} + \frac{\epsilon_i^2 m^2}{(\epsilon_i^2 + \nu_i^2)(1 + m^2)},
\]

\[
\langle n^E_{i,\downarrow} \rangle = \frac{1}{1 + m^2} + \frac{\nu_i^2 m^2}{(\epsilon_i^2 + \nu_i^2)(1 + m^2)},
\]

\[
\langle n^I_{i,\uparrow} - n^I_{i,\downarrow} \rangle = \frac{\epsilon_i^2 - \nu_i^2}{(\epsilon_i^2 + \nu_i^2)(1 + m^2)},
\]

\[
\langle n^E_{i,\uparrow} - n^E_{i,\downarrow} \rangle = \frac{m^2 (\epsilon_i^2 - \nu_i^2)}{(\epsilon_i^2 + \nu_i^2)(1 + m^2)},
\]

\[
\langle U \rangle = U \frac{m^2}{1 + m^2} L, \quad \langle V_0 \rangle = V_0 \frac{2m}{1 + m^2} L.
\]

It is known that in the case of large \( U \) the periodic Anderson model goes to the Kondo lattice model which has an interesting insulating ground state at half-filling called the Kondo-insulator. As can be seen, PAM in strong coupling limit is able to give an insulating phase not only at half-filling, but also at 3/4 filling as presented here. From Eq.(12) we see that \( | \psi_1 \rangle \) contains all the possible spin directions (i.e. is degenerate in spin) and thus describes an insulating paramagnetic state with zero net magnetic moment. Figure 1. and 2. present the emergence domains of \( | \psi_1 \rangle \) in the parameter space.

**B. The metallic state**

Let consider the parameters \( t_c \) and \( t_f \) real, \( V_0 \) and \( V_1 \) imaginary, the Hamiltonian remaining of course Hermitian. We have from Eq.(3)
where \( \phi_x \) is arbitrary. Similarly to the previous case, from \( x \) and \( y \) given here we have 
\[
E_f = -2 \left( 1 - \frac{t_f^2}{|V_1|^2} \right) \sqrt{\frac{V_0^2 V_1^2}{4 t_f^2}} + t_c^2 - U.
\]
The only condition coming from Eq.(4) is \( t_f t_c = V_1^2 \) because the others are automatically valid. In the case of \( \langle n \rangle = 3 \) from Eq.(4) and Eq.(12) we find a lower limit for the ground state energy as
\[
E_{l,2} = 2 \sqrt{\frac{V_0^2}{4m^2}} + t_c^2 \left( 1 - 2 \frac{t_f^2}{|V_1|^2} \right) - U \] L
(13)

The upper limit to \( E_0 \) is derived with the trial function
\[
| \psi_2 \rangle = \prod_i x_{i,\uparrow}^+ x_{i,\downarrow}^+ \left( \alpha_i f_{i,\uparrow}^+ + \beta_i f_{i,\downarrow}^+ \right) | 0 \rangle
\]
where \( \alpha_i, \beta_i \) arbitrary, \( x_{i,\sigma}^+ = d_{i,\sigma}^+ \) or \( e_{i,\sigma}^+ \) \( \forall \ i \) and
\[
d_{i,\sigma}^+ = x \left( c_{i,\sigma}^+ + m f_{i,\sigma}^+ \right), \quad e_{i,\sigma}^+ = y \left( c_{i+1,\sigma}^+ + m f_{i+1,\sigma}^+ \right)
\]
and \( x, y \) are given in Eqs.(12). It can be verified that \( | \psi_2 \rangle \) belongs to \( \langle n \rangle = 3 \). The upper limit to the ground state energy is \( E_{u,2} = \langle \psi_2 | H | \psi_2 \rangle / \langle \psi_2 | \psi_2 \rangle \). Since \( P | \psi_2 \rangle = P' | \psi_2 \rangle = 0 \), it follows that \( E_{u,2} = E_{l,2} = E_0 \) is the ground state energy. Collecting all conditions: \( U \geq 0, \ t_f t_c = V_1^2, \ E_f = -2 \left( 1 - \frac{t_f^2}{|V_1|^2} \right) \sqrt{\frac{V_0^2 V_1^2}{4 t_f^2}} + t_c^2 - U, \ \langle n \rangle = 3 \) we find that the ground state is given in Eq.(14) and the ground state energy is as shown in Eq.(13). In order to understand the physical behavior of this state let us examine expectation values calculated with it. Imposing the constraint in Eq.(14) \( \alpha = \alpha_i, \ \beta = \beta_i \ \forall \ i \) we can express \( | \psi_2 \rangle \) in the momentum space:
\[
| \psi_2 \rangle = \prod_j \left[ x \left( c_{j,\uparrow}^+ + m f_{j,\uparrow}^+ \right) + y \left( c_{j+1,\uparrow}^+ + m^* f_{j+1,\uparrow}^+ \right) \right] \times
\]
\[ \times \left[ x \left( e_{j,k}^+ + m f_{j,k}^+ \right) + y \left( c_{j+1,k}^+ + m^* f_{j+1,k}^+ \right) \right] = \prod \left[ \sum_{j} d_{k_1,j}^+ e^{-ik_1j} \right] \| \sum_{k_2} d_{k_2,j}^+ e^{-ik_2j} \| \sum_{k_3} \left( \alpha f_{k_3,j}^+ + \beta f_{k_3,j}^+ \right) e^{-ik_3j} \| \] \\
with \( d_{k_1,\sigma} = (x + y e^{-ik_1}) c_{k_1,\sigma}^+ + (x m + y m^* e^{-ik_1}) f_{k_1,\sigma}^+ \) \( k = 1, \ldots, N \).
From Eqs. (17) it is seen that \( |\psi_2}\) describes an insulating state. This state is also paramagnetic because \( |\psi_2}\) is degenerate in spin. This degeneration is given by the arbitrary quantities \( \alpha \) and \( \beta \). Furthermore, because \( \langle n_k \rangle = \langle n_{c,\uparrow}(k) + n_{c,\downarrow}(k) + n_{f,\uparrow}(k) + n_{f,\downarrow}(k) \rangle = 3 \) is \( k \) independent, in \( \langle n_k \rangle \) there is no any change present at the Fermi-momentum \( k_F \). Fig 3. presents the \( |\psi_2\rangle \) phase in the parameter space while Fig 4. shows the relative situation of the phases \( |\psi_1\rangle \) and \( |\psi_2\rangle \).

C. Comparison of the two states

Let us compare the wave functions \( |\psi_1\rangle \) and \( |\psi_2\rangle \). The mathematical relationship between Eq. (13) and Eq. (14) can be seen in more transparent form after an orthogonalisation procedure. For this reason we decompose Eq. (13) as follows

\[
|\psi_2\rangle = |\psi_2\rangle - 2 \prod_i d_{i,\uparrow}^+ d_{i,\downarrow}^+ (\alpha_i f_{i,\uparrow}^+ + \beta_i f_{i,\downarrow}^+) |0\rangle
\]

\[
= |\psi_2\rangle - 2 \prod_i e_{i,\uparrow}^+ e_{i,\downarrow}^+ (\alpha_i f_{i,\uparrow}^+ + \beta_i f_{i,\downarrow}^+) |0\rangle \quad (18)
\]

The wave-vector \( |\psi_2'\rangle \) is zero if \( m \) is a real number. This is seen from the fact that \( |\psi_2'\rangle \) contains at least one term of the form

\[
e_{j,\sigma}^+ d_{j+1,\sigma}^+ = x y (c_{j+1,\sigma}^+ + m^* f_{j+1,\sigma}^+) (c_{j+1,\sigma}^+ + m f_{j+1,\sigma}^+)
\]

which, due to the fermionic anticommutation rules, is zero if \( m \) is real. It is also seen that in the case of infinite lattice \( \prod_i d_{i,\uparrow}^+ d_{i,\downarrow}^+ (\alpha_i f_{i,\uparrow}^+ + \beta_i f_{i,\downarrow}^+) |0\rangle = \prod_i e_{i,\uparrow}^+ e_{i,\downarrow}^+ (\alpha_i f_{i,\uparrow}^+ + \beta_i f_{i,\downarrow}^+) |0\rangle = |\psi_1\rangle.\)
The state $|\psi_1\rangle$ sets rigorously 3 electrons on each site, while $|\psi_2'\rangle$ contains at least one site with 4 electron an one with 2 electrons. As a consequence, $|\psi_1\rangle$ and $|\psi_2'\rangle$ are orthogonal. If $m$ is a real number then the ground-state is $|\psi_1\rangle$, and, if $m$ is imaginary then the ground-state is $|\psi_2\rangle = |\psi_2'\rangle + 2|\psi_1\rangle$. The fact that $\langle \psi_1 | T_c | \psi_1 \rangle = 0$ but $\langle \psi_2 | T_c | \psi_2 \rangle \neq 0$ is attributed to the effect of $|\psi_2'\rangle$ in the ground state.

IV. CONCLUSION

Using a positive semidefinite decomposition of the Hamiltonian we have found exact results for the periodic Anderson model at finite $U$ in $d = 1$ dimension and $3/4$ band filling. The result detailed in first is for the case when all the coupling parameters have real value. In this case we found that the ground state is Eq.(10) and the ground state energy is of the form of Eq.(9). The ground state Eq.(10) describes a paramagnetic insulating state that interestingly is present also in the strong coupling limit (i.e. Kondo lattice case) at three-quarters band filling.

The second solution presented is for the case when the hopping amplitudes are real and the hybridization amplitudes are imaginary (the Hamiltonian remaining Hermitian). We found a ground state presented in Eq.(14) and a ground state energy as given in Eq.(13). This state has nonzero expectation values for the $c$ and $f$ hoppings so it is a metallic state. We have found that the state has no discontinuities in $n_k$ at $k_F$.

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FIGURE CAPTIONS

Fig.1.: The $|\psi_1\rangle$ insulating state in the phase diagram. Notations are $X = \frac{V_1}{t_f}$, $Y = \frac{V_0}{t_f}$, $Z = \frac{U}{t_f}$, $\alpha = \frac{E_f}{t_f}$. Setting for example $\alpha = -0.5$ the quantum state $|\psi_1\rangle$ is ground state when $Z = -\left(1 - \frac{1}{X^2}\right)XY - \alpha$, with the constraints $XY > 0$, $\frac{Y^2}{X^2} \geq 4$.

Fig.2.: A part of the $|\psi_1\rangle$ phase surface. Notations are the same as in Fig.1.

Fig.3.: The $|\psi_2\rangle$ metallic state in the phase diagram. For this Figure the notations are $X = \frac{V_2}{t_f}$, $Y = \frac{V_2}{t_f}$, $Z = \frac{U}{t_f}$, $\alpha = \frac{E_f}{t_f}$. Coosing $\alpha = -0.5$ quantum state $|\psi_2\rangle$ is found to be ground state when $Z = -\left(1 - \frac{1}{X}\right)\sqrt{X^2 + \frac{1}{4}XY} - \alpha$.

Fig.4.: The phases $|\psi_1\rangle$ and $|\psi_2\rangle$ in the phase diagram presented together.
