Exact Unitary Transformation of the One-Dimensional Periodic Anderson Model

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(Dated: January 14, 2022)

An effective hamiltonian is derived exactly for the one-dimensional periodic Anderson model via a canonical transformation. The canonical transformation has been calculated up to infinite order, thus an exact transformation was performed in the strict mathematical sense. We also discuss briefly the impact of the obtained result on understanding the magnetic properties of several Kondo lattice compounds.

PACS numbers: 05.30.Fk, 67.40.Db, 71.10.-w, 71.10.Fd, 71.27.+a

The periodic Anderson model (PAM) is believed to contain the essential physics to describe the low temperature magnetic, superconducting or semiconducting properties of the heavy fermion materials and yet the understanding of it is still very limited. The model is exactly solvable via Bethe Ansatz only in the single impurity case[1] and even in one-dimension (1D) it’s Kondo lattice limit only allows an exact solution via bosonization[2].

To begin understanding the role that PAM plays in determining the properties of heavy fermion systems we must gain a better understanding of the effective interactions and local correlation present in the model. We achieved this by applying a canonical transformation to PAM, similar to that used by Schrieffer and Wolff[3].

The Schrieffer-Wolff transformation[3] was performed only up to first order, which restricts the validity of the transformation to a very limited range of the original parameters. In this Letter we focus on the 1D case, where we developed a method that allows us to derive recursive equations for arbitrary order of the canonical transformation, and enabled us to sum up the transformation to infinite order. Thus the canonical transformation is exact, and it is not suppose to eliminate any irrelevant degrees of freedom. After the transformation is carried out a new Hamiltonian is derived and the exact microscopic expressions for the effective interaction constants obtained.

From these coupling constants, we will analyse in more detail the value of the effective magnetic coupling between the impurities (the so-called Kondo coupling) to gain a deeper insight into the magnetic property of the 1D PAM. This problem has generated considerable interest since Möller and Wölfle[4] have shown, using a slave boson approximation, that both ferro- and antiferromagnetism may exists in the 1D PAM. Recent numerical calculations[7] have also shown the existence of ferromagnetic phase in the PAM for a wide range of doping ratios between quarter-filling and half-filling. On the contrary, the ground state of the symmetric 1D PAM is antiferro-magnetic in the half-filled case[7] and favours antiferro-magnetic interaction in the vicinity of quarter filling[5]. In addition to this, there are many cerium mixed valence materials[8], which exhibit ferromagnetic nature in the presence of strong Kondo-like behavior.

The exact Kondo coupling, as calculated hereafter, will shed light on this complex magnetic behavior of 1D PAM.

1. Canonical Transformation.

We write the standard PAM Hamiltonian in 1D as \( H_0 = H_0 + H_V \), with

\[
H_0 = -t \sum_{i,\sigma} (c_{i+1,\sigma}^\dagger c_{i,\sigma} + \text{h.c.}) + \mu \sum_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma}
+ \epsilon_f \sum_{i,\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} + U \sum_i n_{i,\sigma}^f n_{i,-\sigma}^f \; , 
\]

and \( H_V = V \sum_{i,\sigma} (f_{i,\sigma}^\dagger c_{i,\sigma} + \text{h.c.}) \). Here \( c_{i,\sigma}^\dagger \) (\( c_{i,\sigma} \)) create (annihilate) conduction electrons with spin \( \sigma \) at lattice site \( i \). \( f_{i,\sigma}^\dagger \) (\( f_{i,\sigma} \)) create (annihilate) \( f \)-orbital impurity electrons \( (n_{i,\sigma}^f = f_{i,\sigma}^\dagger f_{i,\sigma}) \), and \( \mu \) (\( \epsilon_f \)) are the energies of the conduction (\( f \)-orbital electrons, respectively. \( t \) is the nearest-neighbour hopping matrix element, \( U \) the on-site Coulomb repulsion of the \( f \)-electrons, and \( V \) is the strength of the on-site hybridization matrix element between electrons in the \( f \)-orbitals and the conduction band.

Its unitary transform is simply written as:

\[
\hat{H} = e^S (H_0 + H_V) e^{-S} 
= H_0 + [S, H_V]/2 + [S, [S, H_V]]/3 + \ldots ,
\]

where \( S \) is determined by the condition \( H_V + [S, H_0] = 0 \). One can easily verify that

\[
S = \sum_{i,\sigma} V (A + Z f_{i,-\sigma}^\dagger f_{i,\sigma}) (f_{i,\sigma}^\dagger c_{i,\sigma} - c_{i,\sigma}^\dagger f_{i,\sigma}) ,
\]

with \( A = 1/(2t - \mu + \epsilon_f) \) and \( Z = 1/(2t - \mu + \epsilon_f + U) - A \) satisfies this condition. In \( H_0 \) of Eq. (1) a continuum representation (similar to the field theoretical bosonization scheme[4]) for the kinetic energy has been used.
Having found \( S \), it is straightforward to determine the first \((n = 1)\), third \((n = 3)\) and fifth \((n = 5)\) order terms of the transformed Hamiltonian which depend on the following commutation,

\[
[[S, H_V]]_n = \sum_{\sigma} \left[j_n(c_{i,\sigma}^\dagger c_{i,-\sigma}\hat{f}_{i,-\sigma}^\dagger \hat{f}_{i,\sigma} - n_{i,\sigma}^c n_{i,-\sigma}^c) + P_n(c_{i,\sigma}^\dagger c_{i,-\sigma}\hat{f}_{i,-\sigma}^\dagger \hat{f}_{i,\sigma} + f_{i,\sigma}^\dagger f_{i,-\sigma}^\dagger c_{i,\sigma} c_{i,-\sigma}) + G_n(n_{i,\sigma}^\dagger n_{i,-\sigma}) + I_n n_{i,\sigma}^c n_{i,-\sigma} + M_n n_{i,\sigma}^c n_{i,-\sigma} - n_{i,\sigma}^c + K_n n_{i,-\sigma}^c n_{i,-\sigma}^c \right],
\]

The values of the coefficients \( J, P, G \) and \( I, K, M \) for the first three odd \( n \) are summarized in Table I. Besides the terms which renormalize the starting Hamiltonian, we obtained three new effective interactions: \( J \), the well-known Kondo coupling; \( P \), a Josephson type two particle intersite tunnelling; \( K \), an effective on-site Coulomb repulsion for the conduction electrons; and a higher order term, \( M \). From these, \( K \) and \( M \) are absent in the first order Schrieffer-Wolff result, as they depict a higher order coupling between the impurity and conduction electrons. This coupling becomes stronger as \( U \) increases, but only to a certain extent before the coupling decreases.

It is not by incident that the first three odd order commutation Eq. (4) is given by a close form Eq. (5). In fact, we will prove in the following using induction that the form of the \( n \) odd order commutation Eq. (5) is given by Eq. (6) in general.

Other than the form of the commutation, one can also find a pattern in the coefficients of the common terms among the first, third and fifth orders, from Table I. This pattern has been verified true up to eleventh order and can be proven valid for any order by the same induction.

2. Proof by Induction. The \( n = 1 \) case is the well known Schrieffer and Wolf result which represents the first rows of Table I. By visual inspection, it can be observed that there is a pattern in the coefficients of the common terms among the first, third and fifth orders. This pattern can be proven to exist for any order by induction, if the same pattern remains after commuting Eq. (5) with \( S \) twice.

To do this, two different indices are introduced to differentiate the order of the commutation \( n \) from the recurrence of the coefficients \( J_m, P_m, \ldots \) over odd orders. The mapping of the two sequences can be written as \( n = 2m + 1 \) for odd order \( n \). Assuming that Eq. (5) is true for any \( m \), we calculate its commutation with \( S \) for \([S, H_V]]_n+1\), which yields:

\[
\sum_{i,\sigma} \left[ -2V J_m (A + Z n_{i,\sigma}^l - n_{i,-\sigma}^c) (n_{i,-\sigma}^l - n_{i,-\sigma}^c) - 2V P_m (A + Z n_{i,-\sigma}^c) (n_{i,\sigma}^l - n_{i,-\sigma}^c) - 2V G_m (A + Z n_{i,-\sigma}^l) - 2V M_m (A + Z n_{i,-\sigma}^c) - 2V I_m (A + Z n_{i,-\sigma}^l) n_{i,-\sigma}^c - 2V K_m (A + Z n_{i,-\sigma}^c) n_{i,-\sigma}^c \right] \left[ c_{i,\sigma}^\dagger \hat{f}_{i,\sigma} + f_{i,\sigma}^\dagger c_{i,\sigma} \right].
\]

In the next step of the proof, calculating the commutator of Eq. (6) with \( S \) again reveals that the obtained \([S, H_V]]_n+2\) has exactly the same form as \([S, H_V]]_n\), with coefficients:

\[
J_{m+1} = -J_m 4V^2(2AZ + Z^2) - P_m 8V^2(A^2 + AZ) - G_m 4V^2(2AZ + Z^2) - I_m 4V^2(A + Z)^2 - K_m 4V^2A^2,
\]

\[
P_{m+1} = -J_m 4V^2(A^2 + AZ) - P_m 4V^2((A + Z)^2 + A^2) - (I_m + K_m) 2V^2(A + Z) A,
\]

\[
I_{m+1} = -J_m 4V^2(A + Z)^2 - P_m 4V^2(A^2 + AZ)
\]
\[-G_m 4V^2(2AZ + Z^2) - I_m 4V^2(A + Z)^2,\]
\[K_{m+1} = -J_m 4V^2 A^2 - P_m 4V^2(A^2 + AZ) - K_m 4V^2 A^2,\]
\[M_{m+1} = +K_m 4V^2(2AZ + Z^2) - M_m 4V^2(A + Z)^2\]
\[+J_m 4V^2(2AZ + Z^2),\]
\[G_{m+1} = -G_m 4V^2 A^2.\]  
(7)

This proves that Eq. \([5]\) is true for any \(m\). Thus, using mathematical induction, we conclude that the form of the \(n\)th commutation of \(HV\) with \(S\) is closed and is always given by Eq. \([5]\).

4. Evaluating the Coefficients. The recursive equations \([7]\) can be solved simultaneously to give the odd order coefficients of the transformed Hamiltonian, \(J_m, P_m, I_m, K_m\) and \(M_m\).

These recursive equations can be summarized into an matrix form in which
\[
\begin{pmatrix}
J_{m+1} \\
2P_{m+1} \\
I_{m+1} \\
K_{m+1}
\end{pmatrix} = -4V^2 M \begin{pmatrix} J_m \\ P_m \\ I_m \\ K_m \end{pmatrix} - 4V^2 \begin{pmatrix} \alpha^2 - \beta^2 \\ 2\alpha\beta \\ \alpha^2 \\ 2\beta \end{pmatrix} G_m ,
\]  
where \(\alpha = A + Z\) and \(\beta = A\). \(M\) is a matrix given by:
\[
M = \begin{pmatrix}
\alpha^2 + \beta^2 \\
2\alpha\beta \\
\alpha^2 \\
\beta^2
\end{pmatrix} = \begin{pmatrix}
\alpha^2 - \beta^2 \\
2\alpha\beta \\
\alpha^2 \\
\beta^2
\end{pmatrix} \begin{pmatrix} 0 \\ \alpha^2 - \beta^2 \end{pmatrix} G_m ,
\]  
(8)

These forms are a set of simultaneous recursive equations with the first order, i.e., the Schrieffer and Wolff \([8]\) result as the initial condition, and their solution is:
\[
J_m = (-2V^2\alpha^2 + \beta^2)m^2(\alpha + \beta)V^2 ,
\]
\[
P_m = (-2V^2\alpha^2 + \beta^2)m^{-1}[2m^1\alpha\beta - (\alpha + \beta)]V^2 ,
\]
\[
G_m = (-2V^2m(2\beta^2)^m2\beta V^2 ,
\]
\[
K_m = \{(-2V^2\alpha^2 + \beta^2)m^{-1}[4m^2(\alpha - \beta) - \alpha(\alpha + \beta)] + (-2V^2m(2\beta^2)^m2\beta V^2 ,
\]
\[
I_m = (-2V^2\alpha^2 + \beta^2)m^{-1}(2\alpha^2 - \beta^2)V^2 + (-2V^2\alpha^2 + \beta^2)m^{-1}2\alpha\beta(\alpha + \beta)V^2 - (-2V^2m(2\beta^2)^m2\beta V^2 ,
\]
\[
M_m = (-2V^2\alpha^2 + \beta^2)m^{-1}(2\alpha^2 - \beta^2)V^2 + (-2V^2\alpha^2 + \beta^2)m^{-1}2\alpha\beta(\alpha + \beta)V^2 + (-4\alpha^2 + \beta^2)m^{2}\alpha V^2 + (-4\alpha^2 + \beta^2)m^{2}\beta V^2 .
\]

The even order coefficients can then be deduced from the odd order coefficients, by applying another commutation. These coefficients also have a form, as one would expect, but the pattern is quite different to that of odd order. The \((n+1)^{th}\) commutation result can be summarized in the form:
\[
[[S, HV]]_{n+1} = \sum_{i, \sigma} (R_m + S_m n_{i,-\sigma}^f + T_m n_{i,\sigma}^c) (c_{\lambda i,\sigma}^\dagger f_{i,-\sigma}^f + f_{i,\sigma}^c c_{\lambda i,\sigma}^\dagger) ,
\]  
(10)

where
\[
R_m = -(4V^2\beta^2)^m(2\beta V^2 ,
\]
\[
S_m = [-2V^2(\alpha^2 + \beta^2)^m2\beta(\alpha + \beta)V^2 + (-4V^2\beta^2)^m4\beta V^2 ,
\]
\[
T_m = [-2V^2(\alpha^2 + \beta^2)^m8\beta(\alpha + \beta)V^3 + [-2V^2(\alpha^2 + \beta^2)^m2\alpha(\alpha + \beta)V^3 + (-4V^2\beta^2)^m4\beta V^3 ,
\]
\[
Q_m = [-2V^2(\alpha^2 + \beta^2)^m8(\alpha - \beta)^2V^3 + [(-2V^2(\alpha^2 + \beta^2)^m2\alpha(\alpha + \beta)V^3 + (-4V^2\beta^2)^m4\beta V^3 .
\]

Accordingly, we have obtained the result of the commutation of \(HV\) with \(S\) to any order, and hence have all the information needed to re-build the Hamiltonian after the transformation.

4. The Transformed Hamiltonian. Using the general expression for the \(n\)th and the \((n+1)^{th}\) commutation of \(S\) with \(HV\), the infinite order transformation can be calculated. The transformed Hamiltonian comprises \(H_0\), the sum of the odd order commutations of \(S\) with \(HV\) and the sum of the even order commutations: \(H_0 + H_{odd} + H_{even}\), where \(H_{odd} = \sum_{m=0}^{\infty}[1/(2m+1)!-1/(2m+2)++){[[S, HV]]_{2m+1}}\) is:
\[
H_{odd} = \sum_{i, \sigma} J(c_{\lambda i,\sigma}^\dagger f_{i,-\sigma}^f + n_{i,\sigma}^c n_{i,-\sigma}^f)
\]
\[
+P(c_{\lambda i,\sigma}^\dagger f_{i,-\sigma}^f + f_{i,\sigma}^c c_{\lambda i,\sigma}^\dagger c_{\lambda i,\sigma}^\dagger n_{i,-\sigma}^f)
\]
\[
+G(n_{i,\sigma}^f - n_{i,\sigma}^c) + M n_{i,-\sigma}^c n_{i,-\sigma}^f(n_{i,\sigma}^f - n_{i,\sigma}^c)
\]
\[
+I n_{i,-\sigma}^f n_{i,\sigma}^c + K n_{i,\sigma}^c n_{i,-\sigma}^f .
\]  
(11)

\(J, P, G, I, K\) and \(M\) are the summation of the corresponding \(J_m, P_m, G_m, I_m, K_m\) and \(M_m\) over infinite number of \(m\). If we define \(\alpha = A + Z, \beta = A, \theta = \sqrt{2V^2(\alpha^2 + \beta^2)}, \theta_{\beta} = 2\beta V, \theta_{\alpha} = 2\alpha V\) and \(F(x) = \sin x/x + (\cos x - 1)/x^2\) then the exact values of the coupling constants from Eq. \([11]\) are:
\[
J = 2(\alpha - \beta) V^2 F(2\theta) ,
\]
\[
P = 2\alpha\beta(\alpha - \beta) V^2 F(2\theta) - (\alpha - \beta)V^2(\alpha + \beta)^2 F(\theta) ,
\]
\[
G = 2\beta V^2 F(\theta) ,
\]
\[
K = 2\beta V^2(\alpha - \beta)\alpha^2 + \beta^2 F(2\theta) - 2\alpha\beta V^2(\alpha + \beta)\alpha^2 + \beta^2 F(\theta) + G ,
\]
\[
I = 2\alpha V^2(\alpha - \beta)\alpha^2 + \beta^2 F(2\theta) + 2\alpha\beta V^2(\alpha + \beta)\alpha^2 + \beta^2 F(\theta) - G ,
\]
\[
M = -2(\alpha - \beta)\alpha^2 + \beta^2 V^2 F(2\theta) - 4\alpha\beta\alpha^2 + \beta^2 V^2 F(\theta)
\]
\[
+2\alpha V^2 F(\theta_{\alpha}) + 2\beta V^2 F(\theta_{\beta}) .
\]
Similarly, the even order Hamiltonian $H_{\text{even}} = \sum_{m=0}^{\infty} [1/(2m+2)! - 1/(2m+3)!][S, H_{V}]_{2m+2}$ can be evaluated by substitution,

$$H_{\text{even}} = \sum_{i,\sigma} (R + Sn_{i,-\sigma}^f + Tn_{i,-\sigma}^c + Qn_{i,-\sigma}^f n_{i,-\sigma}^c)$$

$$\times (c_{i,\sigma}^f f_{i,\sigma}^f + f_{i,\sigma}^c c_{i,\sigma}) ,$$ (12)

where $R$, $S$, $T$ and $Q$ are the summation of the corresponding $R_m$, $S_m$, $Q_m$ and $T_m$ over infinite number of $m$. Using the same notations for $\alpha$, $\beta$, $\theta$, $\theta_R$, $\theta_\alpha$ as above, and $F'(x) = \sin x/x^3 - \cos x/x^2$, we obtain:

$$R = \theta R = -4\beta^2 V^3 F'(\theta),$$

$$S = -8(\alpha - \beta)\alpha V^3 F'(2\theta) - 2(\alpha + \beta)\beta V^3 F'/(\theta) - R ,$$

$$T = 8\beta(\alpha - \beta)\alpha V^3 F'(2\theta) - 2\alpha(\alpha + \beta)\beta V^3 F'/(\theta) - R ,$$

$$Q = 8(\alpha - \beta)^2 V^3 F'(2\theta) + 2(\alpha + \beta)^3 V^3 F'(\theta)$$

$$-4\beta V^3 F'(\theta_R) - 3\beta V^3 F'(\theta_\alpha) .$$

In the symmetric case ($\epsilon_f = -U/2$), one gets $Z = -2A$, $\theta = \theta_R = -\theta_\alpha = 2AV$, $\alpha = -A$ and $\beta = A$, both the odd and even order Hamiltonian coefficients simplify considerably.

5. Discussions. We have shown that an unitary transformation of the 1D PAM can be calculated to infinite order. The obtained series for every coefficient generated by the transformation are convergent. Even though the transformed Hamiltonian appears to be more complicated than the original one, it gives the exact expression of the effective interactions which are valid for any $U$ and $V$. These represent a vital source of information due to the lack of similar, exactly soluble theories of PAM.

The Kondo coupling $J$ from our exact result has a behaviour different to that of the well known Schrieffer-Wolff result. This difference is attributed to the higher order terms of the coupling coefficient $J$ in the transformation. As depicted in Fig. 1 these higher order terms seem to have an effect of suppressing the antiferromagnetic coupling between the localized electrons for large values of $V/U$. As $V/U$ increases, $J$ can change sign, indicating a possible change of the magnetic coupling state which has been observed in numerical approaches [2, 3]. The value of $J$ is also crucial to determine the Kondo ($\propto \exp[-[1/|\rho|])$ and Néel ($\propto |\rho|^2$) temperatures, where $\rho$ is the density of states for the conduction band at the Fermi level. In the Kondo regime, see Fig. 1, $J$ passes through a maximum, as a function of $U$ and $V$. Accordingly, the Kondo and Néel temperatures will show a similar behavior. Such behavior has been observed experimentally with increasing pressure (i.e., $V$) in several cerium Kondo compounds [6]. Hence, this exact result will also shed new light in understanding the competition between the Kondo effect and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction in 1D and revisit the Doniach diagram [10].

Finally, one may notice that the hybridization term is still present in the final result of the transformation, see Eq. [12]. However, the strength of the hybridization is substantially reduced to the third order of $V$ as $-V((\sin 2VA)/2VA - \cos 2VA) \approx -\frac{1}{2}V^2A^2V^3$ for small $V$. It is in fact possible to remove this hybridization term completely, but the transformation involved will be slightly different [11].

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