Research Article

A Canonical Transformation for the Anderson Lattice Hamiltonian with f–f Electron Coupling

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In this work, a new canonical transformation for the Anderson lattice Hamiltonian with f–f electron coupling was developed, which was further used to identify a new Kondo lattice Hamiltonian. Different from the single impurity Kondo effect, the resulted new Kondo lattice Hamiltonian only includes the spin-flip scattering processes between conduction electrons and f-electrons, while the normal process of non-spin-flip scattering is absent in this Hamiltonian, under the second order approximation. The new Kondo lattice Hamiltonian may be used to study some anomalous physical properties in some Kondo lattice intermetallic compounds.

1. Introduction

The single impurity Kondo effect is the consequence of magnetic atoms diluted in a nonmagnetic metal (e.g., 0.1% of iron in copper). The interaction mechanism of the single impurity Kondo effect is well-studied [1–4]. In 1961, Anderson [5] examined the localized magnetic moment problem of a single magnetic atom in a nonmagnetic metal and used the Hamiltonian such as the following:

\[
H = \sum_{k,\sigma} \epsilon_k C_{k\sigma}^+ C_{k\sigma} + \sum_{\sigma} \epsilon_d C_{d\sigma}^+ C_{d\sigma} + U C_{d\uparrow}^+ C_{d\downarrow}^+ C_{d\downarrow}^+ C_{d\uparrow},
\]

where \( C_{k\sigma}^+ \) (\( C_{k\sigma} \)) is the creation (destruction) operator of conduction electrons with momentum \( k \) and spin \( \sigma \); \( C_{d\sigma}^+ \) or \( C_{d\sigma} \) is the creation or destruction operator of the localized \( d \)-electrons of the transition metal magnetic atom; \( U \) is the on-site Coulomb repulsive energy of localized \( d \)-electrons; \( V_{dk} \) is the coupling constant between \( d \)-electrons and conduction electrons. As Schrieffer–Wolff demonstrated by using a canonical transformation [6, 7], such single impurity Anderson Hamiltonian can be transformed to a single Kondo impurity Hamiltonian as the following:

\[
\tilde{H} = \sum_{k,\sigma} \epsilon_k C_{k\sigma}^+ C_{k\sigma} - \frac{J}{2N} \sum_{k, k' \sigma} \left\{ \left( C_{k\uparrow}^+ C_{k'\downarrow} - C_{k\downarrow}^+ C_{k'\uparrow} \right) S_z + C_{k\uparrow}^+ C_{k'\downarrow} S_+ + C_{k\downarrow}^+ C_{k'\uparrow} S_- \right\},
\]

in which

\[
S_z = \frac{\sigma_z}{2},
\]

\[
S_\pm = \frac{\sigma_x \pm i\sigma_y}{2},
\]

where \( \sigma_x, \sigma_y, \) and \( \sigma_z \) are the Pauli spin matrices.

When rare-earth or actinide atoms constitute a sublattice in a compound, the system may be called Kondo lattice compound. The examples may include CeAl_3 [8–10], CeCu_2Si_2 [11–13], UBe_13 [14–16], CeB_6 [17, 18], CeCu_6 [19–21], CePtSi [22], CePdIn_8 [23], CeGe [24], (Ce,La)_4Cu_2Ge_2 [25], Yb_2Ru_4Al_12 [26], UAuB_2 [27], Ce(Cu, Al, Si)_2 [28], CeCu_2Mg [29], CeRh_3Sn_5 [30], CeRhIn_5 [31], CeCu_4In_2 [32], and
others. Doniach [33] studied a one-dimensional Kondo lattice model for Kondo lattice compound and suggested that a second-order transition from an antiferromagnetic state to a Kondo spin compensated ground state could occur as the exchange coupling constant $J$ increased to a critical value $J_c$; for systems in which $J > J_c$, a very weak sublattice magnetization may occur as a result of nearly complete spin-compensation. Lacroix and Cyrot [34] studied the phase diagram of the Kondo-lattice model at zero temperature and discussed that the Kondo state is stable when the exchange interaction is larger than a critical value and the state is insulating when the conduction band is half filled. Lopes et al. [35] studied the properties of the Anderson lattice Hamiltonian without f-f electron coupling by using the Schrieffer–Wolff transformation. However, the f-f electron coupling in some of the rare-earth and actinide compounds may not be negligible, especially for some of those compounds with partially filled f-electron shells/bands. Lawrence et al. [36] studied the valence-band photoemission spectra for CeAl$_3$, CeCu$_2$Si$_2$, and other Ce compounds. They obtained the 4f valence band width of about 0.9 eV for CeAl$_3$ and about 1.1 eV for CeCu$_2$Si$_2$. Wuilloud et al. [37] studied the X-ray photoemission spectroscopies of the occupied and unoccupied states of UBe$_{13}$, and they found a surprisingly broad 5 f band tail (up to 5 eV) of some extended states. The f-f electron coupling may mainly be attributed to the indirect interaction of the weak hybridization of f-electron wavefunction with the wavefunction tails of the nearest neighbor atoms [38–41]. Howczak and Spalek [42] studied Anderson–Kondo lattice model and found that for large values of hybridization strength, the system enters the so-called locked heavy fermion state; under strong magnetic field, the system transforms from the locked state to the fully spin-polarized phase.

This paper will present the results of a canonical transformation (which is also a unitary transformation) for the Anderson lattice Hamiltonian with f-f electron coupling, which is an extension of the Schrieffer–Wolff transformation. The properties of a unitary canonical transformation may include the following: the transformation preserves the canonical commutation relations of the Hamiltonian with other physical quantities; the eigenvalues of the Hamiltonian remain the same after the unitary canonical transformation; and the Hermitian operator remains as Hermitian after the transformation.

2. A Canonical Transformation for the Anderson Lattice Hamiltonian with f-f Electron Coupling

The Anderson lattice Hamiltonian with f-f electron coupling can be written as follows:

$$H_{AL} = \sum_{k,\sigma} \epsilon_k C_{k\sigma}^+ C_{k\sigma}^- + \sum_{\sigma} \epsilon_0 f_{\sigma 0}^+ f_{\sigma 0}^- + \sum_{i \neq j} T(\vec{R}_i - \vec{R}_j) f_{i\sigma 0}^+ f_{j\sigma 0}^- + \sum_j U f_{j\uparrow}^+ f_{j\uparrow}^- f_{j\uparrow} + \sum_{k,\sigma} \left( h_{kj} C_{k\sigma}^+ f_{\sigma 0} + h.c. \right),$$

where $C_{k\sigma}^+$ or $C_{k\sigma}^-$ is the operator for conduction electrons with a momentum $\vec{k}$ and spin $\sigma$; $f_{\sigma 0}^+$ or $f_{\sigma 0}^-$ is the operator for f-electrons at site $\vec{R}_i$ with a spin $\sigma$; $T(\vec{R}_i - \vec{R}_j)$ in the coupling term for f-electrons between sites $\vec{R}_i$ and $\vec{R}_j$; $U$ is the on-site Coulomb repulsive energy of localized f-electrons; $h_{kj}$ is the mixing interaction between f-electrons and conduction electrons and the h.c. means the Hermitian conjugate of the first part in the expression. $C_{k\sigma}^+$ and $f_{\sigma 0}$ satisfy the following anticommutation relations:

$$\left[ C_{k\sigma}^+, C_{q\tau}^+ \right] = C_{k\sigma}^+ C_{q\tau}^+ + C_{q\tau}^+ C_{k\sigma}^- = \delta_{kq} \delta_{\sigma\tau},$$

$$\left[ f_{\sigma \alpha}^+, f_{\sigma \beta}^+ \right] = f_{\sigma \alpha}^+ f_{\sigma \beta}^+ + f_{\sigma \beta}^+ f_{\sigma \alpha}^- = \delta_{\alpha\beta} \delta_{\sigma\tau}.$$  

For a model calculation, $h_{kj}$ and $T(\vec{R}_i - \vec{R}_j)$ may be approximated as follows:

$$h_{kj} = h_{k\sigma} e^{-ik\vec{R}_j} = \frac{h}{\sqrt{N}} e^{-ik\vec{R}_j},$$

$$T(\vec{R}_i - \vec{R}_j) = T_0 e^{i(\vec{R}_i - \vec{R}_j)}.$$  

The Anderson lattice Hamiltonian can be rewritten as follows:

$$H_{AL} = H_0 + H_1,$$

where

$$H_1 = \sum_{k,\sigma} \left( h_{kj} C_{k\sigma}^+ f_{\sigma 0} + h.c. \right).$$

So,

$$H_0 = H_{AL} - H_1 = \sum_{k,\sigma} e_k C_{k\sigma}^+ C_{k\sigma}^- + \sum_{\sigma} e_0 f_{\sigma 0}^+ f_{\sigma 0}^- + \sum_{i \neq j} T(\vec{R}_i - \vec{R}_j) f_{i\sigma 0}^+ f_{j\sigma 0}^- + \sum_j U f_{j\uparrow}^+ f_{j\uparrow}^- f_{j\uparrow}.$$  

We can perform the canonical transformation for the Anderson lattice Hamiltonian as follows:

$$\mathcal{T} = e^{\epsilon H_{AL} e^{-\epsilon}},$$

where $\mathcal{T}$ is the transformed Hamiltonian. We expand the above equation as a series as given below:
\[ H = H_{\text{AL}} + \{s, H_{\text{AL}}\} + \frac{1}{2} \{s, \{s, H_{\text{AL}}\}\} + \ldots \]
\[ = H_0 + H_1 - [H_0, s] + [s, H_1] + \frac{1}{2} \{s, \{s, H_{\text{AL}}\}\} + \ldots \] (15)

The generator \( s \) of the canonical transformation is given below:
\[ s = s^{(1)} - \text{h.c.}, \] (16)

\[ [H_0, s^{(1)}] = \frac{\hbar}{\sqrt{N}} \sum_{k, \sigma} e^{-ik \cdot \vec{R}_j} \left[ \left( \varepsilon_k - \varepsilon_0 - U f_j^{+} f_{j-\sigma} - T(\vec{k}) \right) \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) \right) \right] \left[ C^+_{k \sigma} f_n \right] \]
\[ + \frac{\hbar}{\sqrt{N}} \sum_{k, \sigma} e^{-ik \cdot \vec{R}_j} U \left[ \left( \varepsilon_k - \varepsilon_0 - U f_j^{+} f_{j-\sigma} - T(\vec{k}) \right) \left( n_{\sigma} - f_j^{+} f_{j-\sigma} \right) \right] \left[ C^+_{k \sigma} f_n \right], \] (19)
in which
\[ n_{\sigma} = \frac{1}{N} \sum_{j} f_j^{+} f_{j-\sigma}. \] (20)

\[ [H_0, s^{(1)}] = \frac{\hbar}{\sqrt{N}} \sum_{k, \sigma} e^{-ik \cdot \vec{R}_j} \left[ C^+_{k \sigma} f_n \right] + \frac{\hbar}{\sqrt{N}} \sum_{k, \sigma} e^{-ik \cdot \vec{R}_j} U \left[ \left( \varepsilon_k - \varepsilon_0 - U f_j^{+} f_{j-\sigma} - T(\vec{k}) \right) \left( n_{\sigma} - f_j^{+} f_{j-\sigma} \right) \right] \left[ C^+_{k \sigma} f_n \right]. \] (21)

We introduce the notation \( H^{\text{fluc}} \) as follows:
\[ H^{\text{fluc}} = H_1 - [H_0, s] = \frac{\hbar}{\sqrt{N}} \sum_{k, \sigma} U \left[ \left( \varepsilon_k - \varepsilon_0 - U f_j^{+} f_{j-\sigma} - T(\vec{k}) \right) \left( n_{\sigma} - f_j^{+} f_{j-\sigma} \right) \right] \left[ C^+_{k \sigma} f_n \right] + \frac{\hbar}{\sqrt{N}} \sum_{k, \sigma} e^{-ik \cdot \vec{R}_j} U \left[ \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) \right) \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) \right) \right] \left[ C^+_{k \sigma} f_n \right] \] (22)

Here, \( H^{\text{fluc}} \) results from the fluctuation of f-electron density. In most of the Kondo lattice compounds, the energies/ bands of occupied f-electron states are much below the Fermi energy, and the fluctuation of the f-electron density is quite small. In addition, the energy difference between the conduction electron and f-electron bands states is quite large in most of such systems. We are now only interested in such case that
\[ \left| \frac{\hbar}{\varepsilon_k - \varepsilon_0 - T(\vec{k})} \right| \ll 1, \quad \left| \frac{\hbar}{\varepsilon_k - \varepsilon_0} \right| \ll 1. \] (23)

So, the expansion of the series in Equation (15) converges quite rapidly. Retaining to the second order in the expansion in Equation (15), the transformed Hamiltonian \( \tilde{H} \) can be approximated as follows:
\[ \mathcal{H} = H_0 + \frac{1}{2} [s, H_1] + H_{\text{fluc}} + \frac{1}{2} [s, H_{\text{fluc}}], \]  

(24)

where \( H_1, H_0, \) and \( H_{\text{fluc}} \) are given by Equations (12), (13), and (22), respectively.

### 3. Discussion of the Properties of the Transformed Hamiltonian

Using the expressions of \( H_1, H_0, \) and \( H_{\text{fluc}} \), the second term of Equation (24) can be rewritten as follows:

\[ \frac{1}{2} [s, H_1] = H_{\text{ex}} + H_0' + H_{\text{ch}}, \]

(25)

in which,

\[ H_{\text{ex}} = -\frac{1}{2} \sum_{kq} J_{kq} C_{\sigma}^+ C_{\bar{\sigma}}^+ f_{q,\bar{\sigma}}^+ f_{q,\sigma}^-, \]

(26)

\[ H_0' = \frac{h^2}{2N} \sum_{kq} \left[ \frac{1}{\epsilon_k - \epsilon_+ (\mathbf{k})} - \frac{1}{\epsilon_k - \epsilon_- (\mathbf{k})} \right] \left[ C_{\sigma}^+ C_{\bar{\sigma}} - f_{q,\bar{\sigma}}^+ f_{q,\sigma}^- \right], \]

(27)

\[ H_{\text{ch}} = \frac{h^2}{2N} \sum_{kq} \left\{ \left[ \frac{1}{\epsilon_k - \epsilon_+ (\mathbf{k})} - \frac{1}{\epsilon_k - \epsilon_- (\mathbf{k})} \right] \left[ C_{\sigma}^+ C_{\bar{\sigma}}^+ + \text{h.c.} \right] \right\}, \]

(28)

where

\[ \epsilon_+ (\mathbf{k}) = \epsilon_0 + T(\mathbf{k}) + U, \]

(29)

\[ \epsilon_- (\mathbf{k}) = \epsilon_0 + T(\mathbf{k}), \]

(30)

\[ J_{kq} = \frac{1}{\sqrt{N}} \sum_j e^{-i\mathbf{k} \cdot \mathbf{r}_j} f_{\sigma}, \]

(31)

\[ J_{kq} = \hbar^2 \left[ \frac{1}{\epsilon_k - \epsilon_+ (\mathbf{k})} - \frac{1}{\epsilon_k - \epsilon_- (\mathbf{k})} \right] + \left[ \frac{1}{\epsilon_q - \epsilon_+ (\mathbf{q})} - \frac{1}{\epsilon_q - \epsilon_- (\mathbf{q})} \right]. \]

(32)

We introduce the notations as follows:

\[ \Phi^+_{q} = \left( f_{q,1}^+ \ f_{q,1}^- \right), \]

(34)

Hence, \( H_{\text{ex}} \) can be rewritten as follows:

\[ H_{\text{ex}} = -\sum_{kq} \mathbf{S}_{k\bar{\sigma}} \mathbf{S}_{k\sigma} \left( \Phi^+_{k} \Phi^+_{k} + \Phi^-_{k} \Phi^-_{k} \right). \]

(35)

where \( S_{\sigma} \) and \( S_{\bar{\sigma}} \) are the spin matrices for conduction electrons, and \( T_x \) and \( T_y \) are the spin matrices for f-electrons, respectively.

\( H_{\text{ex}} \) is the exchange interaction between conduction electrons and f-electrons for the Kondo lattice compounds. It is different from the results of single impurity Kondo problem. There only exists the spin-flip scattering terms in Equation (35), while the normal process of non-spin-flip scattering is absent, that is different from the single impurity Kondo model. \( H'' \) is the change of the band energies resulting from the mixing interaction between conduction electrons and f-electrons. \( H' \) changes the occupancies of f-orbitals and conduction bands by two electrons. Similar to the consideration in the single impurity problem as discussed by Schrieffer and Wolff [6], \( H_{\text{ch}} \) can be neglected. The transformed Hamiltonian \( \mathcal{H} \) can be rewritten as follows:

\[ \mathcal{H} = H_0 + H_0' + H_{\text{ex}} + H_{\text{fluc}} + \frac{1}{2} [s, H_{\text{fluc}}]. \]

(36)

The details of the last term of Equation (36), \( \frac{1}{2} [s, H_{\text{fluc}}] \), will be given in the appendix. It is noticed that the scattering of f-electron density fluctuation to conduction electrons contributes to both the spin-flip and non-spin-flip processes. If the fluctuation of f-electron density in some cases is very small and can be neglected, then the transformed Hamiltonian \( \mathcal{H} \) can be written as a new Kondo lattice Hamiltonian \( H_{KL} \) as below:

\[ H_{KL} = H_0 + H_0' + H_{\text{ex}}, \]

(37)

where \( H_{KL} \) is the new Kondo lattice Hamiltonian \( H_{KL} \) only includes the spin-flip scattering processes between conduction electrons and f-electrons; and, however, the normal process of non-spin-flip scattering is absent in Equation (37). In the case of single impurity Kondo effect, conduction electrons can be scattered by both of the non-spin-flip and spin-flip processes. When those “impurity” magnetic atoms form a periodic sublattice in the conductive compounds, conduction electrons may not be scattered by the non-spin-flip normal scattering process, because of the periodic nature of those magnetic sublattice atoms. Nevertheless, the spin-flip scattering process still exists in such Kondo lattice Hamiltonian.
4. Conclusion

A canonical transformation for the Anderson lattice Hamiltonian with \( f-f \) electron coupling was developed, which was used to identify a new Kondo lattice Hamiltonian. The new Kondo lattice Hamiltonian \( H_{\text{Kl}} \) only includes the spin-flip scattering processes between conduction electrons and f-electrons; and however, the normal process of non-spin-flip scattering is absent in such Kondo lattice Hamiltonian, under the second order approximation. The new Kondo lattice Hamiltonian had been used to study the anomalous temperature dependence of the electrical resistivity in the Kondo lattice intermetallic compound such as CeCu6, by using the Green’s function method and numerical computations, and the obtained numerical result was consistent with the experimental data of CeCu6 [43]. The new Kondo lattice Hamiltonian may also be used to study some anomalous physical properties in other Kondo lattice intermetallic systems [44–48], e.g., Kondo spin compensated state, or the state with local magnetic moments quenched at low temperature.

\[ [S, H_{\text{bac}}] = -\frac{\hbar^2}{N} \sum_{k,iq,j} e^{i\vec{k} \cdot \vec{R}_j} e^{-i\vec{q} \cdot \vec{R}_i} \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) \right)^2 \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) - U \right) \left[ C_{\sigma \sigma}^{-\text{f} \rightarrow \text{f}} n_{-\sigma} \left( C_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} n_{-\sigma} + f_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} \right) \right] \]

\[ + \frac{\hbar^2}{N} \sum_{k,iq,j} e^{i\vec{k} \cdot \vec{R}_j} e^{-i\vec{q} \cdot \vec{R}_i} \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) \right)^2 \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) - U \right) \left[ f_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} C_{\sigma \sigma}^{-\text{f} \rightarrow \text{f}} n_{-\sigma} \left( C_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} n_{-\sigma} + f_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} \right) \right] \]

\[ -\frac{\hbar^2}{N} \sum_{k,iq,j} e^{i\vec{k} \cdot \vec{R}_j} e^{-i\vec{q} \cdot \vec{R}_i} \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) \right)^2 \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) - U \right) \left[ n_{-\sigma} f_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} C_{\sigma \sigma}^{-\text{f} \rightarrow \text{f}} n_{-\sigma} \left( C_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} n_{-\sigma} + f_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} \right) \right] \]

\[ -\frac{\hbar^2}{N} \sum_{k,iq,j} e^{i\vec{k} \cdot \vec{R}_j} e^{-i\vec{q} \cdot \vec{R}_i} \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) \right)^2 \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) - U \right) n_{-\sigma} \left( -\delta_{\sigma \sigma} f_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} + C_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} \right) + \text{h.c.} \]

\[ -\frac{\hbar^2}{N} \sum_{k,iq,j} e^{i\vec{k} \cdot \vec{R}_j} e^{-i\vec{q} \cdot \vec{R}_i} \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) \right)^2 \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) - U \right) n_{-\sigma} \left( -\delta_{\sigma \sigma} f_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} + C_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} \right) + \text{h.c.} \]

\[ -\frac{\hbar^2}{N} \sum_{k,iq,j} e^{i\vec{k} \cdot \vec{R}_j} e^{-i\vec{q} \cdot \vec{R}_i} \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) \right)^2 \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) - U \right) n_{-\sigma} n_{-\sigma} C_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} C_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} + \text{h.c.} \]

Data Availability

There is no additional data for this paper.

Disclosure

Preprint source of the manuscript file is submitted in the following link https://papers.ssrn.com/sol3/papers.cfm?abstract_id=4485170.

Appendix

The appendix will list the detail calculations of the term \( s, H_{\text{bac}} \) in Equation (36). In order to simplify the calculations, we do not consider the degeneracy of the f-electron orbital. Equation (22) can be rewritten as follows:

\[ H_{\text{bac}} = H_{\text{i}} - [H_{\text{o}}, s] = -\frac{\hbar}{\sqrt{N}} \sum_{k,iq,j} \left[ \right] \]

\[ U \left[ \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) - U \right) \left( \varepsilon_k - \varepsilon_0 - T(\vec{k}) - U \right) \right] \]

\[ e^{i\vec{q} \cdot \vec{R}_i} f_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} C_{\sigma \sigma}^{\text{f} \rightarrow \text{f}} \]

(A.1)

Using Equations (16)–(18), we have:

Conflicts of Interest

The author declares that he has no conflicts of interest.

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