The Study of the Ground State Properties of Heavy Famion System Using an Extended Kondo-Anderson Model in One Dimension

Okunzuwa I. Samuel¹ and C. Okaro Augustine¹

¹Department of Physics, University of Benin, Benin City, Nigeria.

Authors’ contributions

This work was carried out in collaboration between both authors. Author OIS designed the study, performed the analysis and wrote the discussion of result and conclusion. Author COA carried out the calculations and wrote the introduction. Both authors read and approved the final manuscript.

Article Information

DOI: 10.9734/PSIJ/2020/v24i1130226

Editor(s):
(1) Dr. Lei Zhang, Winston-Salem State University, USA.
(2) Dr. Roberto Oscar Aquilano, National University of Rosario (UNR), Argentina.

Reviewers:
(1) Abderrahim Achouri, University of Ouargla, Algeria.
(2) Abeer Majeed Jasim, College of Science, Iraq.

Complete Peer review History: http://www.sdiarticle4.com/review-history/65022

Received 25 October 2020
Accepted 30 December 2020
Published 31 December 2020

Original Research Article

ABSTRACT

The Kondo interaction coupling, Heisenberg exchange coupling, and Coulomb interactions within d-sites, were introduced in a one dimensional Periodic Anderson Model Hamiltonian (PAMH) to further investigate the effects of interaction parameters on the ground state energy of systems with heavy fermions (HF) behavior. Periodic Anderson model PAM being one of the most successful model for studying the heavy fermions System (HFS) was used in an extended version (mixed Kondo-Anderson representation) on a system of three-electrons interacting on three-sites cluster. Exact Diagonalization technique (EDT) normally used to solve conventional PAM calculation was considered in this work for a very small cluster. Hamiltonian used to describe this model contains the usual term describing the kinetic energy of the system, on-site coulomb repulsion and a hopping integral. The Hamiltonian is acted on the different Hilbert states of the lattice system and results of the interactions were obtained in terms of hopping integral, coulomb repulsions, exchange couplings and the hybridization term. Graphs of ground state energy $E_o$ plotted against these interaction parameters were presented in a clear format. As these parameters were varied numerically through a finite range of values, the individual effects of these parameters on the system’s ground state energy were observed and discussed. Hence, the results obtained from this

*Corresponding author: E-mail: ikponmwosa.okunzuwa@uniben.edu, ikponmwosa.okunzuwa@uniben.edu;
work shows theoretically how the tuning of the Coulombic interaction within the conduction band \(U_c\) and \(J_c\) couplings provides information that sheds light on the underlying physics of the heavy fermions systems models. Results obtained from this work further demonstrate the reliability of the model Hamiltonians that we have harnessed and the importance of considering electron-lattice interactions as well as interactions that account for magnetic impurities for the proper description of heavy fermions material.

**Keywords:** Periodic Anderson model; Heavy fermion system; Hilbert states; exact diagonalization technique; Kondo lattice model.

1. **INTRODUCTION**

Proper understanding of the electron’s motion as well as its interaction with the neighboring electrons in metals, semiconductors and other materials of technological importance is an important task in condensed matter physics. Strong electron correlations observed in rare-earth or actinide compounds have attracted considerable attention, where exotic low-temperature properties have also been observed such as heavy fermion behavior [1,2], valence fluctuations and quantum critical behavior [3]. It has been understood that these interesting properties are attributed to the itinerancy of \(f\) electrons to hybridize unto conduction bands and strong electron correlations. The intriguing phenomena have been observed in the Au-Al-Yb alloy [4]. Electron-electron interaction in solids enhances interaction between the electron and lattice system, thus, tends to localize electrons [5–9]. This problem of electronic states in a solid is a many-body problem of a macroscopic number of particles since the electrons interact with each other through Coulomb repulsion [10]. Materials such as rare-earth metals and their composites exhibit many remarkable phenomena like heavy-fermion behavior, valence fluctuations [11], and unconventional superconductivity. The simple models that can account for these phenomena are the periodic Anderson model (PAM) and Kondo Lattice model (KLM) where mobile conduction electrons in a wide band can hybridize with localized \(f\)-electrons sitting at the lattice sites [12].

The extensions of the mixed Kondo-Anderson model would be introduced to discuss systems with heavy-fermions behavior and mixed-valence fluctuations. We talk about mixed-valence behavior when the \(f\)-level is near the Fermi level and here the number of electron that occupy the \(f\)-level is not an integer. In the case of heavy-fermions system, the \(f\)-level is deep below the Fermi level but its occupancy is almost integer and the ions have magnetic moments. In this case according to the low temperature measurements of the specific heat of electrons, the Sommerfeld coefficient is larger than the value of the usual materials. The main reason is that the narrow \(f\)-level of rare-earth elements may lie close to the wide conduction band consisting of the \(d\) and \(s\)-electrons. Because of the mixing of delocalized electrons, we cannot make difference between core electron and electron belonging to the band that allows a simple description of the solid state [13]. Electron correlations in flat-band lattices represent an attractive field that continues to expand its horizon. In flat-band systems the Coulomb interaction between electrons is dominant over the kinetic energy, and as a consequence it can be minimized without any cost in the kinetic energy [14].

Generally, in heavy fermion materials, the 4f or 5f electrons are localized under the Fermi surface, while the valence electrons on the \(s\), \(p\) or sometimes \(d\)-orbital are free to move about. Heavy-fermion metal can develop electron masses 1000 times that of copper; it can also develop unconventional superconductivity, transform into new forms of quantum order and exhibit quantum criticality. In the periodic table, the most strongly interacting electrons reside in orbitals that are well localized. In order of increasing localization, partially filled orbitals are ordered as follows [15]: 5d < 4d < 3d < 5f < 4f. From the tight-binding point of view, the heavy fermion materials form a periodic Anderson model, where the electrons on the \(s\), \(p\) and \(d\) orbitals are treated as the conduction electrons and electrons on the \(f\)-orbital are treated as localized electrons. The valence electrons can hop to the orbital of ions and vice versa, which is called the hybridization. At weak hybridization, the model can be described by the Fermi-liquid theory and the properties are closer to the free electrons. But at strong hybridization, the screening between localized \(f\)-electrons and the conduction electrons will enhance the mass of the later by more than 100 times. As a consequence, the specific heat, the conductivity...
and the magnetic susceptibility of heavy fermion material will be changed drastically. Because of hybridization, f-electrons of neighboring sites can interact with each other, which may lead to the long range magnetic ordering. Then the model will experience a phase transition from a paramagnetic state to a magnetically ordered state (ferromagnetic or antiferromagnetic state) forming a Kondo lattice.

According to Hal Tasaki’s work [16], for a very general class of models, including the Hubbard, the periodic Anderson, and the Emery models with certain hopping matrices and large on-site Coulomb interaction on d sites, it was shown that the exact ground state is indeed for a certain number of electrons. This uniqueness guarantees that one can discuss the physics of various strongly interacting electron systems by analyzing the exact ground states of the system.

1.1 Mixed Kondo-Anderson Lattice Model

The periodic Anderson and Kondo lattice models describe the physics of conduction electrons in extended orbitals interacting with strongly correlated electrons in localized orbitals. These models are relevant for the so-called heavy-fermion and related systems such as the Kondo insulators.

For the first time a model Hamiltonian of the kind used in this work was used to study the ground state properties of a HFS. The extended Gutzwiller-type approach to the periodic Anderson model (PAM) in presence of magnetic impurities and in the strong-correlation limit has been applied by [17]. The finite U corrections are included systematically by transforming the PAM into the form with the Kondo-type interactions plus the residual hybridization, both appearing at the same time in the model hamiltonian. The effective Hamiltonian in (2) represents the essence of our Anderson-Kondo lattice model. It may be necessary to notice the subtle difference between the formulation used in this work and the original Anderson- or Kondo-lattice models which was induced by the introduction of on-site Coulomb interactions within the conduction site. In the usual description of HFS by Anderson Hamiltonian, the Coulomb interaction is taken into account explicitly only between the f-electrons. All other parts of the Coulomb interaction, in particular the coulomb interaction between d-electron is to be considered on the average in the parameters of the Hamiltonian. However, in conventional treatments of the Kondo lattice model, the Kondo interaction is decoupled in favour of a hybridization of conduction and localized f electrons. However, such an approximation breaks the local gauge symmetry and implicates that the local f-occupation is no longer conserved [18]. To avoid these problems, we use in this work a mixed model Hamiltonian containing various interaction parameters that account for electronic movement in both sites. One has to note that in the standard Kondo-lattice Hamiltonian which takes the general form as in (1), the numbers of f- and d-particles are conserved separately as the case may be.

\[
H = -t \sum_{\mu, \sigma} (c_{\mu \sigma}^+ c_{\mu+1 \sigma} + H. C) + J_k \sum_{i \mu} S_i^\mu \sigma_i^\mu + J_{i \mu} \sum_{i \mu} S_i^\mu \sigma_i^{\sigma_i} \tag{1}
\]

The localized spins \( S_i^\mu \) interact with the conduction electron spin density \( \sigma_i^{\sigma_i} \) via a local Kondo coupling \( J_K \). Here attention is restricted to the case that all J coupling constants are positive (ferromagnetic) and external field terms are not included in the Hamiltonian in order to reduce the ambiguity that may be involved in the calculation. We find from the study of [19], that Anderson's Hamiltonian can be transformed to a form similar to that in the s-d exchange model used by Kondo, with an energy-dependent antiferromagnetic exchange interaction \( J_K \).

2. METHODOLOGY

The exact diagonalization technique shows how to calculate a few eigenstates of the full Hamiltonian matrix of an interacting quantum system. This implies that the Hilbert space of the problem has to be truncated, either by considering finite systems or by imposing suitable cut-offs, or both. All of the presented methods are iterative, i.e., the Hamiltonian matrix is applied repeatedly to a set of vectors from the Hilbert space. As it is here, most quantum many-particle problems lead to a sparse matrix representation of the Hamiltonian, where only a very small fraction of the matrix elements is non zero.

We study the ground state of 3 electrons interacting on 3 lattice sites with periodic boundary condition in an extended periodic Anderson model EPAM [20], which is described by the following Hamiltonian in one dimension;
3.1 The Following are the Summary of Interactions Obtained after Acting the Hamiltonian on Each of the 20 Basic States Listed above

\[
H = -t \sum_{i,\sigma} \left( C_{i\sigma}^\dagger C_{i+\sigma} + H.C \right) + J_K \sum_{i,\mu} S_i^\mu \sigma_i^\mu + J_H \sum_{i,\mu} S_i^\mu \sigma_i^\mu + U_c \sum_i \left( C_i^+ C_i - \frac{1}{2} \right) \left( C_i^+ C_i - \frac{1}{2} \right)
\]

\[
+ U_f \sum_i \left( n_i^f n_i^f \right) + V \sum_{i,j} \left( C_i^+ f_{i\sigma} + f_{i\sigma}^+ C_i + H.C \right)
\]

Where, \( S_i^\mu \) is the localized spins
\( \sigma \) is conduction electron spin density (which could be spin-up or spin down)
\( C_{i\sigma} \) (\( f_{i\sigma} \)) is an annihilation operator of a conduction electron (f electron) with spin.
\( C_{i\sigma}^\dagger \) (\( f_{i\sigma}^\dagger \)) is a creation operator of a conduction electron (f electron) with spin.
H.C is the Hermitian conjugation of \( C_{i\sigma} C_{i+\sigma} \)
\( J_H \) is the Heisenberg exchange interaction coupling parameter
\( J_K \) is the Kondo interaction coupling parameter
\( U_c \) is the columbic interaction within the conduction band
\( U_f \) is the strength of the on-site coulomb repulsion between localized f-electrons
\( V \) is the hopping integral which is the overlap of energy band e.g. in the conduction band and f-orbital.

Although the hopping matrix of the conducting electrons is far from the realistic case (electronshop between the nearest neighbouring sites in the tight-binding picture).

Where; \( n_i^f \equiv f_{i1}^+ f_{11} \) and \( n_i^f \equiv f_{i1}^+ f_{11} \)

3. CALCULATIONS

The number of possible electronic states of asystem of 3 electron on 3 lattices using 1-DPeriodic Anderson Model (PAM) is calculated using a combination relation:

\[
S = \frac{(2N)!}{n!(2N-n)!}
\]

where; \( N \) = Number of sites, \( n \) = Number of electrons

For three electrons on three lattice sites, \( S = 20 \) basic states

The 20 possible basic states of the lattice system are listed as follows;

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>2</td>
<td>( \uparrow )</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>3</td>
<td>( \uparrow )</td>
<td>( \uparrow )</td>
<td>( \uparrow )</td>
</tr>
<tr>
<td>4</td>
<td>( \uparrow )</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>5</td>
<td>( \uparrow )</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>6</td>
<td>( \uparrow )</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>7</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>8</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
<td>( \uparrow )</td>
</tr>
<tr>
<td>9</td>
<td>( \uparrow )</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>10</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>11</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>12</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>13</td>
<td>( \downarrow )</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>14</td>
<td>( \downarrow )</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>15</td>
<td>( \downarrow )</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>16</td>
<td>( \downarrow )</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>17</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>18</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>19</td>
<td>( \uparrow )</td>
<td>( \downarrow )</td>
<td>( \downarrow )</td>
</tr>
<tr>
<td>20</td>
<td>( \downarrow )</td>
<td>( \downarrow )</td>
<td>( \downarrow )</td>
</tr>
</tbody>
</table>

3.1 The Following are the Summary of Interactions Obtained after Acting the Hamiltonian on Each of the 20 Basic States Listed above

\[
H \mid 1 \rangle = t \langle 5 \mid - t \langle 3 \mid + \frac{J_K}{4} \langle 1 \mid + \frac{1}{4} U_c \langle 1 \mid + 2 U_f \langle 1 \mid + 6 V \langle 1 \mid
\]

\[
H \mid 2 \rangle = t \langle 6 \mid - t \langle 4 \mid + \frac{J_K}{4} \langle 2 \mid + \frac{1}{4} U_c \langle 2 \mid + 2 U_f \langle 2 \mid + 6 V \langle 2 \mid
\]

\[
H \mid 3 \rangle = t \langle 19 \mid - t \langle 17 \mid + \frac{J_K}{4} \langle 3 \mid + \frac{1}{4} U_c \langle 3 \mid + 2 U_f \langle 3 \mid + 6 V \langle 3 \mid
\]
The least Eigen values which implies the Ground state Energy $E_o$ of the system is given by (4);

$$E_o = \frac{1}{2} \left( -2J + J - u + 2U - \sqrt{4J^2 - 4JJ + J^2 + 2t^2 + 4Ju + 2ju + 8JU - 4fU + 4uU + 4U^2 + 8v} \right)$$

(4) is the numerical ground state energy obtained for three electron on three sites system using a mixed Kondo-Anderson model, basically calculated when $t = J_k = J_H = U_c = U_F = V = 1$.  

$E_o = 2.0 \ldots (4)$
3.2 Various Plots of Interacting Parameters versus $E_0$.

Table 1. Result of the increase of the Columbic interaction within the conduction band "$U_c$" and the resultant ground state energy $E_0$ at constant $t, J, J_H, U_c, U_F$ and $V$

<table>
<thead>
<tr>
<th>$t$</th>
<th>$J_H$</th>
<th>$J_k$</th>
<th>$U_c$</th>
<th>$U_F$</th>
<th>$V$</th>
<th>$j$</th>
<th>$J$</th>
<th>$E_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>2</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>1.171573</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>0.298438</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>4</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>-0.60555</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>5</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>-1.53113</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>6</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>-2.47214</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>7</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>-3.42443</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>8</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>-4.38516</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>9</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>-5.35235</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>10</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>-6.32456</td>
</tr>
</tbody>
</table>

Fig. 1. The plot of $E_0$ against $U_c$

Table 2. The increase of the Kondo interaction coupling parameter "$J_k$" and the resultant ground state energy $E_0$ at constant $t, J_H, U_c, U_F$ and $V$

<table>
<thead>
<tr>
<th>$t$</th>
<th>$J_H$</th>
<th>$J_k$</th>
<th>$U_c$</th>
<th>$U_F$</th>
<th>$V$</th>
<th>$j$</th>
<th>$J$</th>
<th>$E_0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>2</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>1</td>
<td>2.391505</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>1.5</td>
<td>2.763932</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>4</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>2</td>
<td>3.113999</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>5</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>2.5</td>
<td>3.438447</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>6</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>3</td>
<td>3.734436</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>7</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>3.5</td>
<td>4</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>8</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>4</td>
<td>4.234436</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>9</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>4.5</td>
<td>4.438447</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>10</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>5</td>
<td>4.613999</td>
</tr>
</tbody>
</table>
Fig. 2. The plot of $E_0$ against $J_k$

Fig. 3. The plot of $E_0$ against $J_H$
Table 3. The increase of the Heisenberg interaction coupling parameter \(J_H\) and the resultant ground state energy \(E_0\) at constant \(t, J_K, U_c, U_F, V\) and \(V\)

<table>
<thead>
<tr>
<th>(t)</th>
<th>(J_H)</th>
<th>(J_K)</th>
<th>(U_c)</th>
<th>(U_F)</th>
<th>(V)</th>
<th>(j)</th>
<th>(J)</th>
<th>(E_0)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.25</td>
<td>0.5</td>
<td>2</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.5</td>
<td>0.5</td>
<td>1.592464</td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.75</td>
<td>0.5</td>
<td>1.171573</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0.5</td>
<td>0.739601</td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1.25</td>
<td>0.5</td>
<td>0.739601</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1.5</td>
<td>0.5</td>
<td>0.298438</td>
</tr>
<tr>
<td>1</td>
<td>7</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1.75</td>
<td>0.5</td>
<td>0.05037</td>
</tr>
<tr>
<td>1</td>
<td>8</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>0.5</td>
<td>-0.15037</td>
</tr>
<tr>
<td>1</td>
<td>9</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2.25</td>
<td>0.5</td>
<td>-0.60555</td>
</tr>
<tr>
<td>1</td>
<td>10</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>2.5</td>
<td>0.5</td>
<td>-2.05113</td>
</tr>
</tbody>
</table>

4. RESULTS AND DISCUSSION

In this chapter, we shall be discussing the result and findings gotten from the simulations based on the lattice system of three electrons on three sites system and the effects of variation of the interaction parameters on the ground state energy of the system.

4.1 The Effect of Variation of "\(U_c\)" on the Ground State Energy

When \(t, J_K, U_F\) and \(V\) constant and the Columbic interaction within the conduction band are "\(U_c\)" is being varied gradually from 1 through 10. The ground state Energy \(E_0\) is noticed to be decreased systematically from \(E_0= 2\) down to \(E_0= -6.32456\) as shown Table 1, Fig. 1. Results has shown that the inclusion of this new interaction parameter which was initially not included in the conventional model Hamiltonian greatly lowers the ground state as \(U_c\rightarrow \infty\).

4.2 The Effect of Variation of "\(J_K\)" on the Ground State Energy

The gradual increase of Kondo interaction coupling parameter "\(J_K\)" from 1 through 10 at constant \(t, J_H, U_c, U_F\) and \(V\), the ground state Energy \(E_0\) is noticed to increase from 2 to 4.613999 as shown in Table 2, Fig. 2. We observe from here some uniqueness on the effect of \(J_K\) and \(V\) on the ground state Energy \(E_0\) of this system. A systematic increase in ground state energy as \(V\) is being varied was also observed. Hence, for a unit increase in \(V\), the value of the ground state Energy \(E_0\) is noticed to increase by 4 units. Thus, we say that energy-dependent Kondo exchange interaction \(J_K\) varies directly as the energy of the system.

4.3 The Effect of Variation of "\(J_H\)" on the Ground State Energy

The gradual increase of Heisenberg interaction coupling parameter "\(J_H\)" from 1 through 10 at constant \(t, J_K, U_c, U_F\) and \(V\). The ground state Energy \(E_0\) is noticed to decrease from \(E_0= 2\) up to \(E_0= -2\) as shown in Table 3, Fig. 3 from these we show that in ferromagnetic phases the ground state energy of \(n\) interacting particles in HFS are strongly affected by the spin alignment through Heisenberg exchange couplings and columbic interaction at d-sites. Unlike \(J_K, J_H\) varies inversely as \(E_0\). The interaction of electronic charges in motion gives rise to minute magnetic field which has to be accounted for by J-coupling parameters.

5. CONCLUSIONS

The exact diagonalization technique has been employed in a system of 3 electrons interacting on 3 lattice sites study and the periodic boundary condition was considered using an extended Kondo-Anderson Hamiltonian in one dimension to further investigate the contributions of d-electron interactions and exchange couplings on the ground state energy of heavy fermion systems. Based on the result obtained, it was observed that the ground state energy \(E_0\) of this system decreased as the parameters \(U_c\) and \(J_H\) were increased while keeping other coupling parameters constant. The increase in the parameter \(J_H\) causes the ground state energy \(E_0\) of the system to increase at a stable rate as long as the rest coupling parameters are kept constant. We can say that for the Kondo lattice model, the exchange coupling is the source of interesting many-body effects.
In summary, the overall results demonstrate the importance of taking the electron-lattice interactions as well as their magnetic nature into consideration in materials simulation and modelling. Irrespective of the fact that magnetic impurities due to spin alignment might be considered to have a small effect on heavy-fermions properties, in this work we have shown the importance of taking them into account as the tuning of Heisenberg and Kondo interaction coupling affects the ground state of an extended PAM. Thus, the accuracy of any semi-classical model Hamiltonian in the description of any system also depends on how well the interaction of the electronic and lattice degrees of freedom is reflected through its interaction parameters. It was thus observed from the overall result that the contributions of coulomb interactions and exchange coupling parameters in this model strongly influence the ground state properties of HFS.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES


7. Electron-electron interactions the electronic structure theory of metals, developed in the. 1930;0–52.


