

The Hopping Electron Effect On The Ground State Properties Of The Kondo Lattice Model

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Abstract

In recent years, the Kondo Lattice Model (KLM) has attracted a lot of interest from both the experimental and theoretical points of view. In an effort to gain better understanding and clarify the behaviour of this model, the nearest neighbour hopping parameter, t was considered. An increase in the hopping integral energy term, t , stabilizes the Paramagnetic (PM) phase, while a reduction in t destabilizes the PM phase. Hence, it is argued here that an increase in t favors the ground state of the conventional KLM but its activities are suppressed in the Kondo Lattice Model with coulombic interaction (KLMC). To the best of our knowledge, the role of t in the magnetic phase transition before now has not been investigated.

Keywords: : Paramagnetism, Ferromagnetism, Ground State energy, Transition Point.

1.0 Introduction

One of the great mysteries of solid state physics is how quantum magnetism emerges. The very existence of quantum magnetism implies that ferromagnetism can emerge from the competition between the kinetic and the interaction energy [1]. A number of well-known ground states occur in f – electron systems that result from the competition between electronic and magnetic correlations. The strongly correlated electronic ground states formed in rare – earth and actinide compounds have attracted much theoretical and experimental interest [2].

Interest in the kondo effect has therefore persisted because it provides clues to understanding the electronic properties of wide variety of materials where the interactions between electron are particularly strong, like the heavy-fermion material and high temperature super- conductors.

The Heavy Fermion (HF) materials which are typical examples of strongly correlated systems are materials in which the conduction electrons mix with the almost localized $4f$ or $5f$ electrons, and form the strongly renormalized quasiparticles, which have effective masses of 100 – 1000 times larger than the bare value. This strong renormalization is mainly due to the local-kondo-type process, which should be suppressed if an energy gap opens at the Fermi level [3].

One of the canonical models for the description of HF systems is the kondo lattice models [4].

The electrical resistance of a pure metal usually drops as its temperature is lowered because electrons can travel through a metallic crystal more easily when the vibrations of the atoms are small. However, the resistance saturates as the temperature is lowered below about 10K due to static defects in the material.

Some metals – for example lead, niobium and aluminum – can suddenly lose all their resistance to electrical current and become superconducting. Other metals like copper and gold, remain conducting and have a constant resistance even at the lowest accessible temperatures. The value of the low-temperature resistance depend on the number of defects in the material. Adding defects increases the values of this “saturation resistance” but the character of the temperature dependence remains the same.

However, this behavior changes dramatically when magnetic atoms, such as cobalt, are added. Rather than saturating, the electrical resistance increases as the temperature is lowered further.

This effect arises from the interactions between the single magnetic atoms (cobalt) and the many electrons in an otherwise non- magnetic metal. Such an impurity typically has an intrinsic angular momentum or “spin” that interacts with the electrons. As a result, the mathematical description of the system is a difficult many-body problem[5].

However, the kondo problem is well defined making it an attractive testing ground for the new numerical and analytical tools that have been developed to attack other challenging

many-body problems. Interest in the kondo effect has therefore persisted because it provides clues to understanding the electronic properties of wide variety of materials where the interactions between electron are particularly strong, like the heavy-fermion material and high temperature super conductors.

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Journal of the Nigerian Association of Mathematical Physics Volume 23 (March, 2013), 271 - 282

Although, this behavior involves a phase transition, the so-called Kondo temperature – roughly speaking the temperature at which the resistance starts to increase again completely determines the low-temperature electronic properties of the material [6].

One other common substitutional impurity is a Kondo hole. A kondo hole is a non magnetic impurity which has a conduction orbital but not f orbital. Experimentally, Kondo holes are made by replacing Ce ions with La ions in Ce₃Bi₄Pt₃ which is a Kondo insulator. Measurement on (Ce_{1-x}La_x)₃Bi₄Pt₃ indicate that introducing kondo holes reduces the charge and spin gaps [7].

In this paper, the work of Guerrero and Carruzo was considered. They studied the quasiparticle gap in order to determine whether the system is insulating or metallic when they considered the effect of t on the spin gap. This afforded us the opportunity to draw a correlation between the metallic-insulator ground state transition and the PM-FM ground state transition. Guerrero and Carruzo studied the effect of t on the KLMC [8]. They found out that for values of t>0, the quasiparticle gap does not vanish in the presence of dispersion in the f band. They also noticed that as the coulombic interaction, U, increases, the effect of t in the gap is smaller. This is not so surprising considering that as U increases, charge fluctuations are suppressed.

The suppression of the spin gap is associated with the enhancement of the antiferromagnetic correlations due to the hopping in the f band.

When the hopping is small, the electrons are localized and the strong coulomb repulsion suppresses states with doubly occupied orbitals.

Although the hopping matrix of the conducting electrons is far from the realistic case (electrons hop between the nearest neighbouring sites in the tight-binding picture), our model provides an example where its exact solution for the case of half filling and away from half filling explicitly demonstrate magnetic phase transition as the interaction between the local impurity moment and the conduction band is turned on[9].

The conventional KLM Hamiltonian, H, given by Tsunetsugu et al [10] is

$$H = -t \sum_{i\sigma} (C_{i\sigma}^+ C_{i+1\sigma} + H.C.) + J \sum_i S_{if} \cdot S_{ic} \tag{1}$$

where in eqn. (1) the hopping integral parameter, t (the t term of the Hamiltonian) describes the itinerancy tendency of electrons, H.C. is the Hermitian Conjugation of C_{iσ}⁺C_{i+1σ}.

and

$$S_{if} = \sum_{\alpha\beta} \frac{1}{2} f_{i\alpha}^+ \sigma_{\alpha\beta}^\mu f_{i\beta}$$

$$S_{ic} = \sum_{\alpha\beta} \frac{1}{2} c_{i\alpha}^+ \sigma_{\alpha\beta}^\mu c_{i\beta}$$

Despite the enormous effort put in by several researchers to describe the ground state of the KLM, only little have been achieved [5]. For example, the ferromagnetic ground state of the KLM has not been fully understood. This phenomenon has to do with the coulombic interaction that exists between the conduction electrons. Extensions of the actual KLM given by equation (1), have to be done with the inclusion of the on-site coulombic interaction term, U. With the inclusion of the U term, the Hamiltonian (1) becomes

$$H = -t \sum_{i\sigma} (C_{i\sigma}^+ C_{i+1\sigma} + H.C.) + J \sum_i S_{if} \cdot S_{ic} + U \sum_i \left(C_{i\uparrow}^+ C_{i\uparrow} - \frac{1}{2} \right) \left(C_{i\downarrow}^+ C_{i\downarrow} - \frac{1}{2} \right) \dots\dots\dots(2)$$

Equation (2) is known as the kondo lattice model with coulombic interaction between the conduction electrons (KLMC) [11].

The KLMC Hamiltonian was used to investigate the ground state properties in the lattices studied in this paper. With these tools, it is possible to study the KLMC systems of 2 electrons on 2 sites and 2 electrons on 3 sites, 3 electrons on 3 sites, 2 electrons on 4 sites and 4 electrons on 4 sites.

3 Calculations

Results for a system of 2 electrons on a 2- site (1-D) lattice system using the kondo lattice model with coulombic interaction between conduction electrons (KLMC) are given below.

For two electrons on two (2) sites we have six states i.e

$$S = {}^{2N}C_n = {}^4C_2$$

$$S = \frac{(2N)!}{n!(2N-n)!} \text{ where}$$

N = number of site = 2

n = number of electrons = 2

$$S = \frac{(2 \times 2)!}{2!(2 \times 2 - 2)!} = 6 \text{ basis states}$$

Generating the states, we have explicitly

$$\left. \begin{aligned} |1\rangle &= |1 \uparrow 1 \downarrow\rangle \\ |2\rangle &= |2 \uparrow 2 \downarrow\rangle \\ |3\rangle &= |1 \uparrow 2 \downarrow\rangle \\ |4\rangle &= |1 \downarrow 2 \uparrow\rangle \\ |5\rangle &= |1 \uparrow 2 \uparrow\rangle \\ |6\rangle &= |1 \downarrow 2 \downarrow\rangle \end{aligned} \right\} \quad (3)$$

Using the Hamiltonian (2) to act on the states (3) the following were obtained;

$$\left. \begin{aligned} H |1\rangle &= t |4\rangle - t |3\rangle \\ H |2\rangle &= t |4\rangle - t |3\rangle \\ H |3\rangle &= -t |1\rangle - t |2\rangle + \frac{3}{2} J |3\rangle - U |3\rangle \\ H |4\rangle &= t |1\rangle + t |2\rangle + \frac{3}{2} J |4\rangle - U |4\rangle \\ H |5\rangle &= \frac{3}{2} J |5\rangle - U |5\rangle \\ H |6\rangle &= \frac{3}{2} J |6\rangle - U |6\rangle \end{aligned} \right\} \quad (4)$$

The Hamiltonian Matrix obtained from the summary of the interaction in (4) above is given by (5)- THE singlet states matrix and (6) – the triplet states matrix.

$$H = \begin{pmatrix} 0 & 0 & -t & t \\ 0 & 0 & -t & t \\ -t & -t & 3J/2 - U & 0 \\ t & t & 0 & 3J/2 - U \end{pmatrix} \quad (5)$$

$$H = \begin{pmatrix} 3J/2 - U & 0 \\ 0 & 3J/2 - U \end{pmatrix} \quad (6)$$

The ground state energies for both the singlet E_s and the triplet E_t are given by (7) and (8) respectively.

$$E_s = \frac{1}{4} \left(3J - \sqrt{64t^2 + (3J - 2U)^2} - 2U \right) \quad \dots \quad (7)$$

$$E_t = \frac{3J}{2} - 2U \quad \dots \quad (8)$$

The ground states energies for both singlet E_s and Triplet E_t for the system of 2 electrons on 3- sites (1-D), 3 electrons on 3- sites (1-D), 2 electrons on a 4- site (1-D) and 4 electrons on 4- sites (1-D) lattice system using the kondo lattice model with coulombic interaction between conduction electrons (KLMC) are given in Table A while that for the Kondo Lattice Model for the cases considered for KLMC are given in Table B [12].

TABLE A: The lowest energies of both the Singlet and the Triplet states for 2 electrons on 3- sites, 3 electrons on 3- sites, 2 electrons on 4- site and 4 electrons on 4- sites for $t=J=U=1.0$.

Cases	E_s (the singlet state energy)	E_t (the triplet state energy)
2 electrons on 3- sites	0.000	0.086
3 electrons on 3- sites	-0.164	1.750
2 electrons on 4- sites	0.000	1.736
4 electrons on 4- sites	0.001	-0.148

TABLE B: The lowest energies of both the Singlet and the Triplet states for 2 electrons on 3- sites, 3 electrons on 3- sites, 2 electrons on 4- site and 4 electrons on 4- sites for $t=J=1.0$.

Cases	E_s (the singlet state energy)	E_t (the triplet state energy)
2 electrons on 3- sites	-0.066	2.250
3 electrons on 3- sites	-1.869	0.086
2 electrons on 4- sites	0.000	1.736
4 electrons on 4- sites	-0.095	-0.050

4.0 Discussion Of Results

4.1 Kondo Lattice Model with Coulombic Interaction (KLMC)

When t is varied between 0.01 and 0.10 in Table 1 and Figure 1, keeping J and U constant, the PM state was favored. In the absence of U , increase in t favors the PM ground state, while a reduction in t favors the FM phase.

The effect of the hopping integral term, t , on the KLMC was noticed from Table 2 and Figure 2. It was discovered that the t favours, enhances and stabilizes Paramagnetic states in this lattice. It is significant to state here that as the value of t is decreased, the tendency for the lattice to become ferromagnetic is quickened since the transition point has been lowered. From Table 3 and Figure 3., keeping interaction term U constant, i.e. $U=J=1$, there was stability of the PM ground state as t is gradually increased from $t=1.00$ to $t=10.00$.

From Table 4 and Figure 4, the increase of the hopping integral term, t , enhances and stabilizes the PM phase. This was observed at $t = 0.20$. This particular result was achieved at a constant value of the coulombic interaction term, $U = 1.00$. It was also observed in Table 5 and Figure 5, that the increase of the hopping integral term t , favors the stability of the PM ground state. This means that as t increases, it enhances the PM phase of the Kondo lattice model at half – filling.

4.2 Kondo Lattice Model (KLM)

The effect of the hopping integral term, t , on the KLM was observed from Tables 6 and Figures 6. It was discovered that the t favours, enhances and stabilizes ferromagnetic states in this lattice. It is significant to state here that as the value of t is decreased, the tendency for the lattice to become ferromagnetic is quickened since the transition point has been lowered.

For Table 6, t decreases from $t = -0.80$ to $t = -1.70$ and the transition occurs at point $t = -1.00$. From the table 7 and figure 7, a decrease in t , i.e., from $t = -1.01$ to $t = -1.10$, stabilizes the FM state. This is achieved keeping $J=1$ constant.

It was also observed from tables 8, and figures 8, that as the value of the hopping integral term, t , is decreased, the ferromagnetic phase is being favored and becomes more stable. This stability was easily observed at $t = -0.70$.

It was also observed in table 9 and figures 9 that the increase of the hopping integral term t , favors the stability of the PM ground state. Physically, this means that as t increases, it enhances the FM phase of the Kondo lattice model at half – filling.

5.0 Conclusions

5.1 Kondo Lattice Model with Coulombic Interaction (KLMC)

The nature of the ground state for half filling, slightly away from half filling and quarter filling were considered. The results obtained here show that the KLMC for low u , has a PM ground state at half-filling. This later transits to a FM ground state for the cases of slightly away from half-filling and quarter filling.

The stability of the PM phase of the KLMC for half filling in larger systems increases as t becomes large ($t > 0.01$) when J and U are kept constant.

In conclusion, a direct one-to-one correlation of the ground state properties of the KLMC was made. From our observation, when U is kept small and constant and t increases, the KLMC is paramagnetic. At this condition according to Guerrero and Carruzzo, the KLMC is metallic. Conversely, the decrease in t lead to a Ferromagnetic ground state as being observed in Table 4 and Figure 4. Guerrero and Carruzzo found out that for large values of U , there is no metal-insulator transition as t is varied, showing the dependence of t on U .

Therefore, as t becomes large ($t > 0.01$), the ground state properties of the KLMC is paramagnetic and metallic. When $t < 0$, the ground state properties transits to ferromagnetic (as indicated in Tables 1 to 5) and an insulator[8]. The insulator state was determined by Guerrero and Carruzzo which they observed that the spin gap is suppressed and becomes very small when the hopping term, t , is increased.

5.2 Kondo Lattice Model (KLM)

From our observation, when $U=0$ and as t increases, the KLM is paramagnetic. The stability of the PM phase of the KLM for half filling in larger systems increases as t increases when J is kept constant and $U=0$. Guerrero and Carruzzo found out that for $U=0$, small t lead to a destruction of the spin gap and in turn lead to a metal even at low temperature when $t > 0.25$.

ACKNOWLEDGMENTS

We are grateful to Professor J.O.A. Idiodi for useful communication during the course of this work.

Appendix

TABLE 1: The lowest energies of both the Singlet and the triplet states obtained numerically as the hopping integral term, t , is varied and other parameters remaining constant i.e., $J=2$, and $U=1$.

t (the hopping integral)	J (the exchange interaction term)	U (the coulombic interaction term)	E_s (the singlet state energy)	E_t (the triplet state energy)
0.01	2.00	1.00	-0.0002	1.000
0.02	2.00	1.00	-0.0008	1.000
0.03	2.00	1.00	-0.0020	1.000
0.04	2.00	1.00	-0.0040	1.000
0.05	2.00	1.00	-0.0050	1.000
0.06	2.00	1.00	-0.0070	1.000
0.07	2.00	1.00	-0.0100	1.000
0.08	2.00	1.00	-0.0130	1.000
0.09	2.00	1.00	-0.0160	1.000
0.10	2.00	1.00	-0.0198	1.000

TABLE 2:The lowest energies of both the singlet and the triplet states obtained numerically as the hopping integral term, t , is varied and other parameters remaining constant i.e., $U=1$ and $J=1$.

t (the hopping integral)	J (the exchange interaction term)	U (the coulombic interaction term)	E_s (the singlet state energy)	E_t (the triplet state energy)
1.00	1.00	1.00	0.75	0.75
2.00	1.00	1.00	-0.66	0.75
3.00	1.00	1.00	-1.25	0.75
4.00	1.00	1.00	-1.69	0.75
5.00	1.00	1.00	-2.07	0.75
6.00	1.00	1.00	-2.41	0.75
7.00	1.00	1.00	-2.71	0.75
8.00	1.00	1.00	-2.99	0.75
9.00	1.00	1.00	-3.25	0.75
10.00	1.00	1.00	-3.49	0.75

Table 3 : The lowest energies of both the singlet and the triplet states obtained numerically as the hopping integral term, t , is varied and other parameters remaining constant i.e., $J=1$ and $U=1$.

t (the hopping integral)	J (the exchange interaction term)	U (the coulombic interaction term)	E_s (the singlet state energy)	E_t (the triplet state energy)
1.20	1.00	1.00	0.75	0.75
2.20	1.00	1.00	0.75	-0.66
3.20	1.00	1.00	0.75	-1.25
4.20	1.00	1.00	0.75	-1.69
5.20	1.00	1.00	0.75	-2.07
6.20	1.00	1.00	0.75	-2.41
7.20	1.00	1.00	0.75	-2.71
8.20	1.00	1.00	0.75	-2.99
9.20	1.00	1.00	0.75	-3.25
10.20	1.00	1.00	0.75	-3.49

Table 4 :The lowest energies of both the singlet and the triplet states obtained numerically as the hopping integral term, t , is varied and other parameters remaining constant i.e., $U=1$ and $J=1$.

t (the hopping integral)	J (the exchange interaction term)	U (the coulombic interaction term)	E_s (the singlet state energy)	E_t (the triplet state energy)
0.10	1.00	1.00	0.00	-0.27
0.20	1.00	1.00	0.00	-0.01
0.30	1.00	1.00	0.00	0.17
0.40	1.00	1.00	0.00	0.39
0.50	1.00	1.00	0.00	0.61
0.60	1.00	1.00	0.00	0.84
0.70	1.00	1.00	0.00	1.06
0.80	1.00	1.00	0.00	1.28
0.90	1.00	1.00	0.00	1.51
1.00	1.00	1.00	0.00	1.73

Table 5 : The lowest energies of both the singlet and the triplet states obtained numerically as the hopping integral term, t , is varied and other parameters remaining constant i.e., $U=J=1$.

t (the hopping integral)	J (the exchange interaction term)	U (the coulombic interaction term)	E_s (the singlet state energy)	E_t (the triplet state energy)
2.00	1.00	1.00	0.220	0.457
3.00	1.00	1.00	0.224	0.471
4.00	1.00	1.00	0.230	0.479
5.00	1.00	1.00	0.233	0.488
6.00	1.00	1.00	0.234	0.491

TABLE 6: The lowest energies of both the Singlet and the Triplet states obtained numerically as the hopping integral term, t , is varied and other parameters remaining constant i.e., $J=1$.

t (the hopping integral)	J (the exchange interaction term)	E_s (the singlet state energy)	E_t (the triplet state energy)
-0.80	1.00	2.250	1.881
-0.90	1.00	2.250	2.022
-1.00	1.00	2.250	2.250
-1.10	1.00	2.250	2.305
-1.20	1.00	2.250	2.447
-1.30	1.00	2.250	2.588
-1.40	1.00	2.250	2.729
-1.50	1.00	2.250	2.871
-1.60	1.00	2.250	3.012
-1.70	1.00	2.250	3.154

TABLE 7: The lowest energies of both the Singlet and the Triplet states obtained numerically as the hopping integral term, t , is varied and other parameters remaining constant i.e., $J=1$.

t (the hopping integral)	J (the exchange interaction term)	E_s (the singlet state energy)	E_t (the triplet state energy)
-1.01	1.00	0.00	0.07
-1.02	1.00	0.00	0.05
-1.03	1.00	0.00	0.04
-1.04	1.00	0.00	0.02
-1.05	1.00	0.00	0.01
-1.06	1.00	0.00	0.00
-1.07	1.00	0.00	-0.01
-1.08	1.00	0.00	-0.02
-1.09	1.00	0.00	-0.04
-1.10	1.00	0.00	-0.05

TABLE 8: The lowest energies of both the Singlet and the Triplet states obtained numerically as the hopping integral term, t , is varied and other parameters remaining constant i.e., $J=1$.

t (the hopping integral)	J (the exchange interaction term)	E_s (the singlet state energy)	E_t (the triplet state energy)
-0.50	1.00	0.00	0.38
-0.60	1.00	0.00	0.15
-0.70	1.00	0.00	0.00
-0.80	1.00	0.00	-0.28
-0.90	1.00	0.00	-0.51
-1.00	1.00	0.00	-0.73
-1.10	1.00	0.00	-0.95
-1.20	1.00	0.00	-1.18
-1.30	1.00	0.00	-1.40
-1.40	1.00	0.00	-1.63

TABLE 9: The lowest energies of both the Singlet and the Triplet states obtained numerically as the hopping integral term, t , is varied and other parameters remaining constant i.e., $J=1$.

t (the hopping integral)	J (the exchange interaction term)	E_s (the singlet state energy)	E_t (the triplet state energy)
2.00	1.00	-0.272	1.295
3.00	1.00	-0.310	1.342
4.00	1.00	-0.340	1.371
5.00	1.00	-0.412	1.431
6.00	1.00	-0.413	1.545

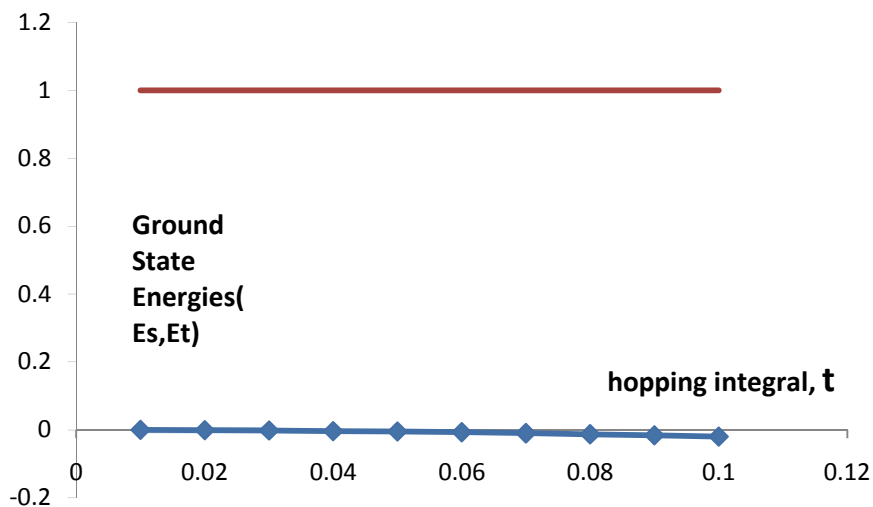


Fig 1: Lowest energies plotted against t for a system of 2 electrons on 2 sites (KLMC).

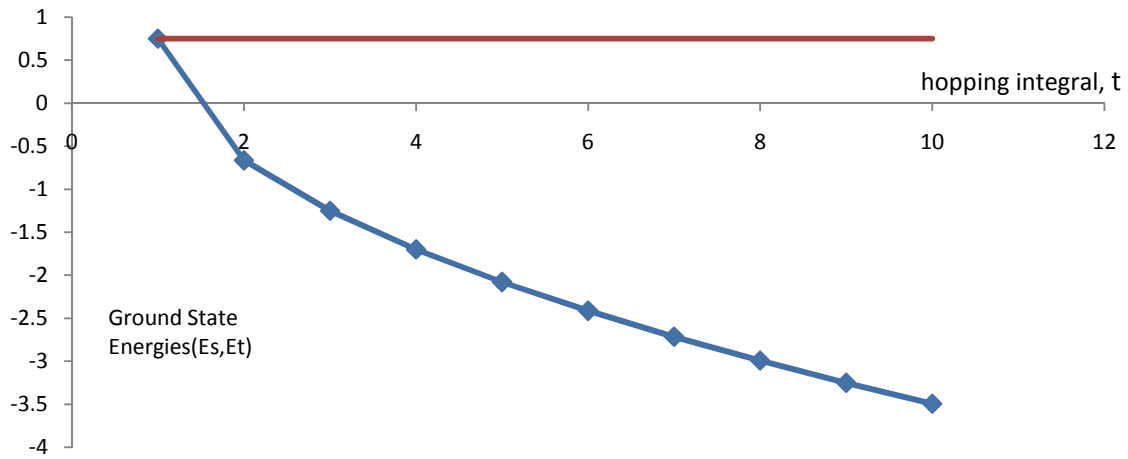


Fig 2: Lowest energies plotted against t for a system of 3 electrons on 3 sites (KLMC).

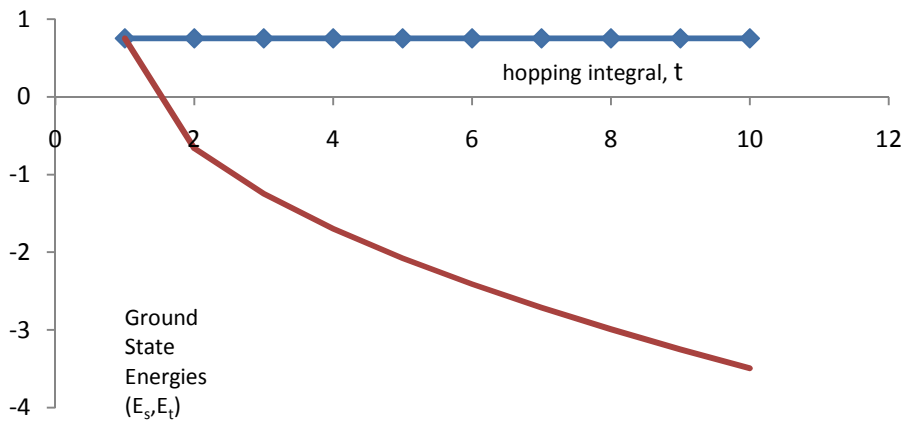


Fig 3: Lowest energies plotted against t for a system of 2 electrons on 3 sites (KLMC).

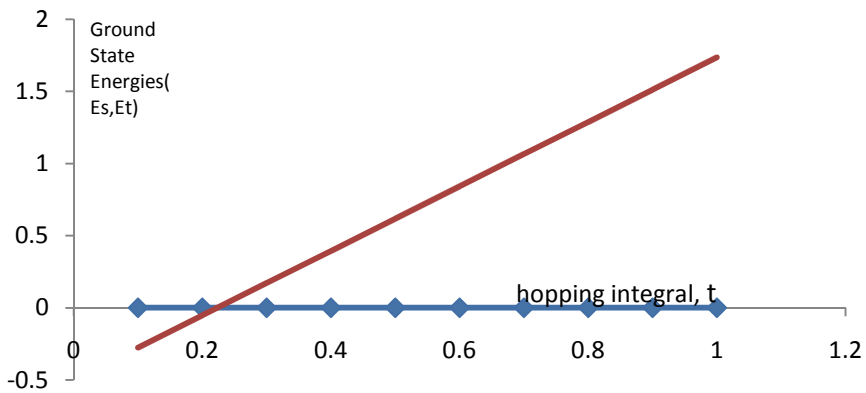


Fig 4 Lowest energies plotted against t for a system of 2 electrons on 4 sites (KLMC).

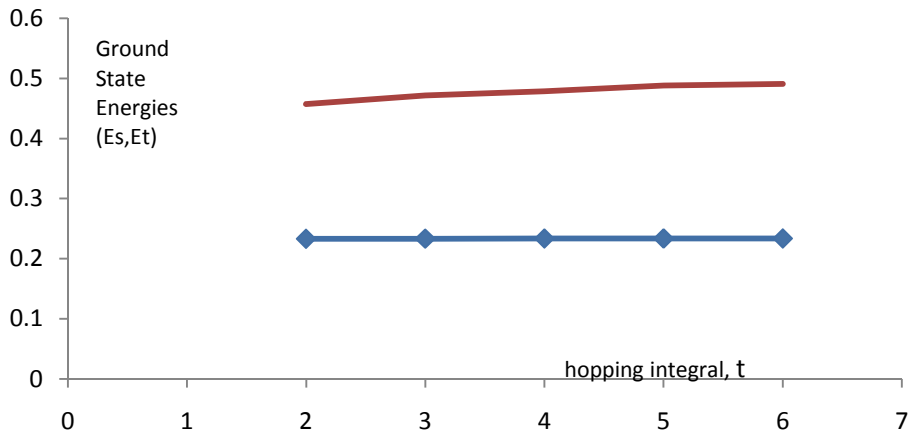


Fig 5: Lowest energies plotted against t for a system of 4 electrons on 4 sites (KLMC).

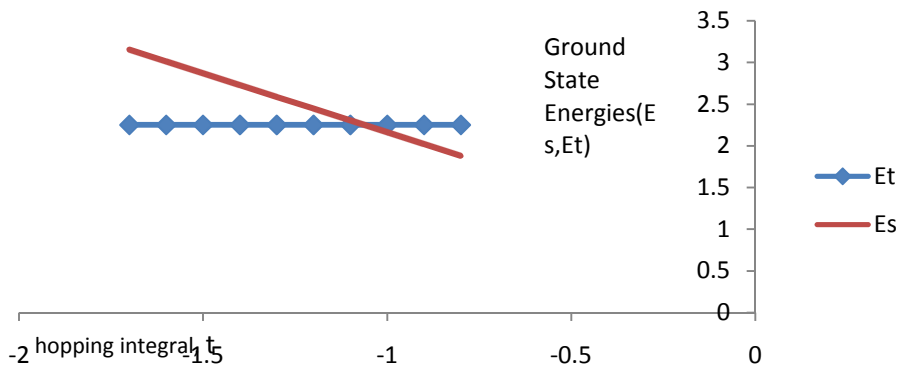


Fig 6: Lowest energies plotted against t for a system of 3 electrons on 3 sites (KLM).

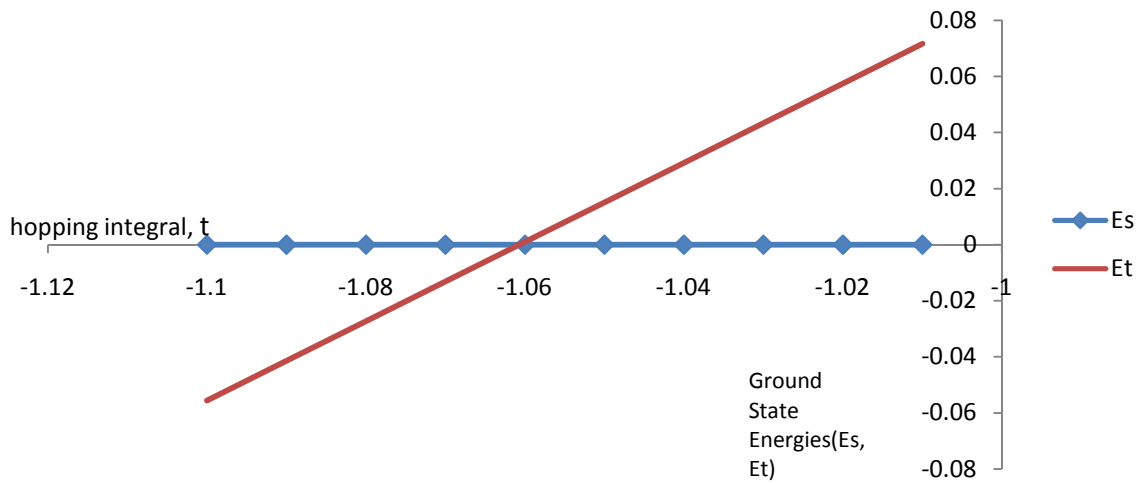


Fig 7: Lowest energies plotted against t for a system of 2 electrons on 3 sites (KLM).

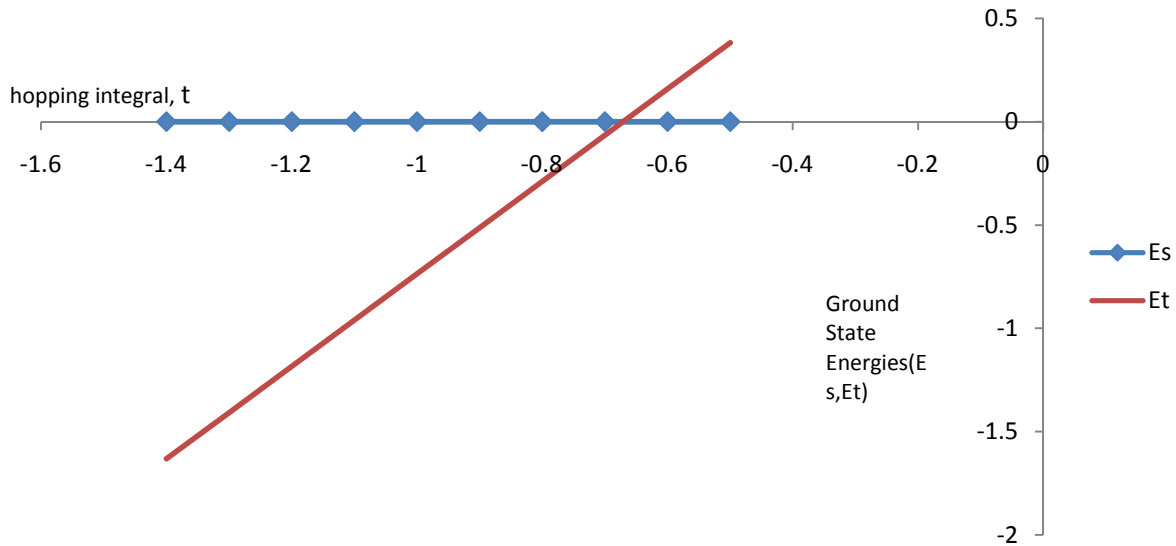


Fig 8: Lowest energies plotted against t for a system of 2 electrons on Sites (KLM).

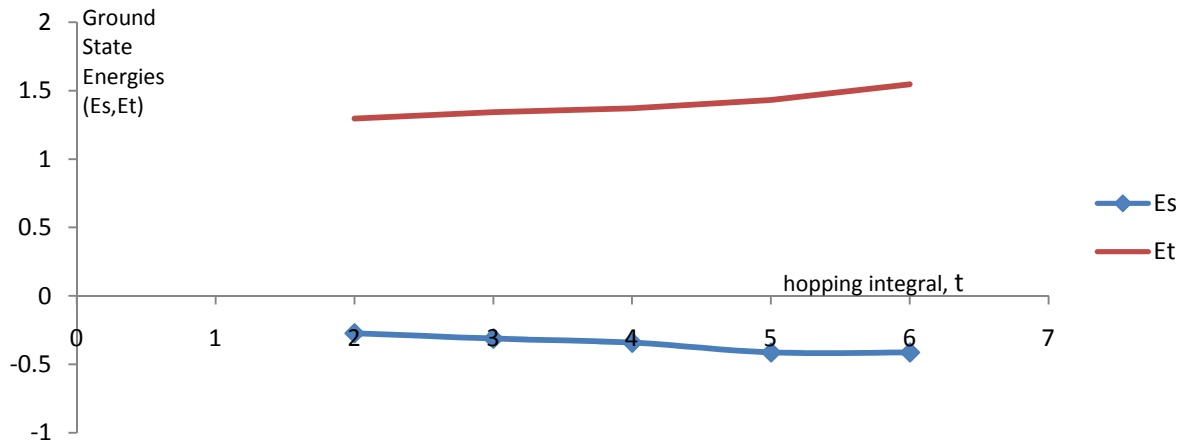


Fig 9: Lowest energies plotted against t for a system of 4 electrons on 4 Sites (KLM).

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