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Instability of Nagaoka's Theorem within The Hubbard Model.

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Abstract

Within the t – U model, the so – called Hubbard model, a lattice of electrons is not completely ferromagnetic, especially at large U. Using the exact diagonalization technique, a numerical analysis carried out to determine the transition from an antiferromagnetic phase to a ferromagnetic phase on the t–J model, when a hole is allowed to move round the lattice, showed that as the J term decreases the ferromagnetism in the lattice becomes more stable, [5]. Hence the t – J model is a better model for studying magnetism than the t – U model. Investigation also revealed that the inclusion of the on-site Coulomb interaction term U, in the t – J model enhances ferromagnetic tendencies in the systems studied. In this work, Nagaoka's theorem on ferromagnetism has been extended beyond the Hubbard model where it was first studied to the t – J and t – U – J model.

1.0 Introduction

An important paradigm for the study of strongly interacting electrons in general, is the Hubbard model for interacting particles on a lattice. This is probably the simplest possible model that captures some of the behaviour of strongly correlated electrons, hence it is widely used to study various correlated driven effects [1].

It is believed that strong ferromagnetic interactions in some solids are generated by subtle interplay between quantum many-body effects and spin-independent Coulomb interactions between electrons. It is a challenging problem, however, to verify this scenario in the Hubbard model. Nagaoka's ferromagnetism is a well-known rigorous example of ferromagnetism in the Hubbard model. It deals with the limiting situation in which there is one electron less than the half-filled case, and the on-site Coulomb interaction is infinitely large [2].

Within the limit of the t – U model the lattice is not completely antiferromagnetic, especially at large U. Considering the ground state energy of two interacting electrons in a two sites system, $E_g = \frac{1}{2}(U - \sqrt{U^2 + 16t^2})$, it was observed [3] that at the extreme case where U is very large, we obtained an asymptotic graph, where the ground state energy for the singlet state (E_s) is approximately equal to the ground state for the triplet state (E_t) as $U \to \infty$. At this point, the lattice is either ferromagnetic or antiferromagnetic. It shows no transition as in Table 1.1 and Figure 1.1

However, rigorous evidence for itinerant ferromagnetism in this model is very limited. One of the most important results is Nagaoka's theorem [4]. The physical mechanism behind Nagaoka's theorem is the following. If $U = \infty$, the ground state of the t – U model is macroscopically degenerate. This degeneracy is lifted by the motion of the hole since it is energetically favorable for it to move in a background of fully aligned spins (provided the lattice allows for motion of the hole around loops). Now the t – J model is an approximation to the Hubbard model when the filling is slightly less than one fermion per site, i.e half-

filling again in the limit U >> t, which gives t >> J. The t – J model forbids doubly occupied sites, but includes their virtual effect by having the super-exchange interaction J between adjacent singly-occupied sites. It also includes the process of a fermion hopping to a neighboring empty site with matrix element t [1].

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Table 1.1 Singlet (E_s) and Triplet (E_t) energies as U varies, with the hopping integral t fixed.

t (hopping integral)	U (on-site coulomb repulsion)	Es (singlet state energy)	Et (triplet state energy)
2	1000	-0.016	0
2	3000	-0.00533	0
2	5000	-0.0032	0
2	7000	-0.00229	0
2	9000	-0.00178	0
2	20000	-0.0008	0
2	80000	-0.0002	0
2	100000	-0.00016	0

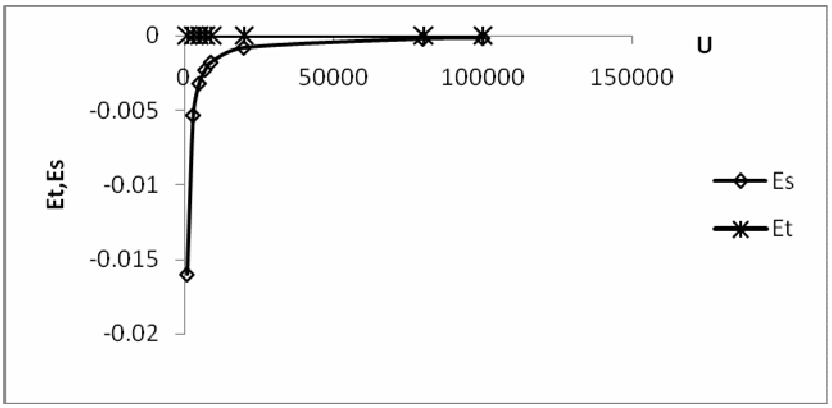

Fig. 1.1 A graph of the energies (E_s, E_t) versus U in the t – U model, showing no transition between E_s and E_t as $U \to \infty$.

However, rigorous evidence for itinerant ferromagnetism in this model is very limited. One of the most important results is Nagaoka's theorem [4]. The physical mechanism behind Nagaoka's theorem is the following. If $U = \infty$, the ground state of the t – U model is macroscopically degenerate. This degeneracy is lifted by the motion of the hole since it is energetically favorable for it to move in a background of fully aligned spins (provided the lattice allows for motion of the hole around loops). Now the t – J model is an approximation to the Hubbard model when the filling is slightly less than one fermion per site, i.e half-filling again in the limit U >> t, which gives t >> J. The t – J model forbids doubly occupied sites, but includes their virtual effect by having the super-exchange interaction J between adjacent singly-occupied sites. It also includes the process of a fermion hopping to a neighboring empty site with matrix element t [1].

2.0 Method

The effective Hamiltonian which governs the low-energy behavior of the Hubbard model for a nearly half-filled band in the U→∞ limit is the t – J model of itinerant fermions on the lattice

$$H^{t-j} = -t\left(\sum_{<ij>\sigma} a^{+}_{i\sigma} a_{j\sigma} + H.C. \right) + J \sum_{<IJ>} \left(S_i . S_j - \tfrac{1}{4} n_i n_j \right)$$

(2.1)

The occupation number of each site $\eta_i = a^{+}_{i\uparrow} a_{i\uparrow} + a^{+}_{i\downarrow} a_{i\downarrow}$ can be either 0 (a hole) or 1 (a spin), since double occupancy is forbidden by strong on-site Hubbard repulsion. The spin operator S_i is given in terms of the Pauli matrices $\sigma_{\alpha\beta}$

$$S_i = \tfrac{1}{2} \sum_{\alpha\beta} a^{+}_{i\alpha} \sigma_{\alpha\beta} a_{i\beta}$$

(2.2)

Since the spin exchange coupling constant $J=4t^2/U$ is positive, the on-site Hubbard interaction translates to an antiferromagnetic (AFM) super-exchange, which favors an AFM correlated ground state.

Nevertheless, in one extreme case this model has a ferromagnetic (FM) ground state, known as the Nagaoka state [4]. A fully polarized state minimizes the total energy of a single hole in an otherwise half-filled band, at least in the limit J→0. This is due to the hole kinetic energy which favors FM ordering. The nature of the ground state for finite J is therefore determined by the competition of this FM tendency with the AFM exchange.

Consider a 2 × 2 square lattice in the presence of a hole ie. when a hole is allowed to move in the lattice. The following basis states arising from the interactions from this new lattice structure were generated within the limit of the following conditions:

1. No double counting
2. No next nearest-neighbour interaction.
3. Interactions with only net spin-up are considered.

Since we are interested in the net spin-up states, hence the only contributing states are: $|1\rangle$ *to* $|6\rangle$ *and* $|7\rangle$. i.e

$$|1\rangle = |1\uparrow 1\downarrow 2\uparrow\rangle, |2\rangle = |1\uparrow 1\downarrow 3\uparrow\rangle, |3\rangle = |1\uparrow 2\downarrow 2\uparrow\rangle, |4\rangle = |2\uparrow 2\downarrow 3\uparrow\rangle, |5\rangle = |1\uparrow 3\uparrow 3\downarrow\rangle, |6\rangle = |2\uparrow 3\uparrow 3\downarrow\rangle, |7\rangle = |1\uparrow 2\uparrow 3\uparrow\rangle$$

The Hamiltonian for the t-J model is given by;

$$H = -t\left(\sum_{\langle ij\rangle\sigma} C^{+}_{i\sigma} C_{j\sigma} \right) + J \sum_{\langle ij\rangle} \left(s_i \cdot s_j - \frac{1}{4} n_i n_j \right)$$

(2.3)

Expanding the Hamiltonian (2.3) we have equation (2.4):

$$H = -t\left(C^{+}_{i\uparrow}C_{j\uparrow} + C^{+}_{j\uparrow}C_{i\uparrow} + C^{+}_{i\downarrow}C_{j\downarrow} + C^{+}_{j\downarrow}C_{i\downarrow}\right) + J\left\{\frac{1}{4}\left(C^{+}_{i\uparrow}C_{i\uparrow}C^{+}_{j\uparrow}C_{j\uparrow} - C^{+}_{i\uparrow}C_{i\uparrow}C^{+}_{j\downarrow}C_{j\downarrow} - C^{+}_{i\downarrow}C_{i\downarrow}C^{+}_{j\uparrow}C_{j\uparrow} + C^{+}_{i\downarrow}C_{i\downarrow}C^{+}_{j\downarrow}C_{j\downarrow}\right) + \right.$$

$$\left. \frac{1}{2}\left(C^{+}_{i\uparrow}C_{i\downarrow}C^{+}_{j\downarrow}C_{j\uparrow} + C^{+}_{i\downarrow}C_{i\uparrow}C^{+}_{j\uparrow}C_{j\downarrow}\right)\right\} - \frac{1}{4}\left(C^{+}_{i\uparrow}C_{i\uparrow}C^{+}_{j\uparrow}C_{j\uparrow} + C^{+}_{i\uparrow}C_{i\uparrow}C^{+}_{j\downarrow}C_{j\downarrow} + C^{+}_{i\uparrow}C_{i\uparrow}C^{+}_{j\downarrow}C_{j\downarrow} + C^{+}_{i\downarrow}C_{i\downarrow}C^{+}_{j\downarrow}C_{j\downarrow}\right)$$

(2.4)

3.0 Results

The results of acting with the Hamiltonian on the various states are summarized in equation (3.1)

$$H|1\rangle = H|1\uparrow 1\downarrow 2\uparrow\rangle = -t|2\rangle + t|3\rangle - \frac{J}{2}|1\rangle, \quad H|2\rangle = H|1\uparrow 1\downarrow 3\uparrow\rangle = -t|1\rangle + t|5\rangle - \frac{J}{2}|2\rangle$$

$$H|3\rangle = H|1\uparrow 2\uparrow 2\downarrow\rangle = +t|1\rangle - t|4\rangle - \frac{J}{2}|3\rangle, \quad H|4\rangle = H|2\uparrow 2\downarrow 3\uparrow\rangle = -t|3\rangle + t|6\rangle - \frac{J}{2}|4\rangle$$

(3.1)

$$H|5\rangle = H|1\uparrow 3\uparrow 3\downarrow\rangle = +t|2\rangle - t|6\rangle - \frac{J}{2}|5\rangle, \quad H|6\rangle = H|2\uparrow 3\uparrow 3\downarrow\rangle = +t|4\rangle - t|5\rangle - \frac{J}{2}|6\rangle$$

Setting up the Hamiltonian matrix, we obtain equation (3.2):

$$H = \begin{pmatrix} -\frac{J}{2} & -t & t & 0 & 0 & 0 & 0 \\ -t & -\frac{J}{2} & 0 & 0 & t & 0 & 0 \\ t & 0 & -\frac{J}{2} & -t & 0 & 0 & 0 \\ 0 & 0 & -t & -\frac{J}{2} & 0 & t & 0 \\ 0 & t & 0 & 0 & -\frac{J}{2} & -t & 0 \\ 0 & 0 & 0 & t & -t & -\frac{J}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad (3.2)$$

The minimum eigenvalue of this matrix is given by $E = \frac{1}{2}\left(-J - 2\sqrt{3}t\right)$

Hence the ground state energy of the lattice becomes $E_g = \frac{1}{2}\left(-J - 2\sqrt{3}t\right)$

A numerical analysis carried out to determine the transition of an anti-ferromagnetic phase to a ferromagnetic phase is given in Table 3.1 and Figure 3.1.

Table 3.0: Singlet (E_s) and Triplet (E_t) energies in the t –J model for various values of t and J.

t (hopping integral)	J (NN exchange interaction)	E_s (singlet state energy)	E_t (triplet state energy)
-50.00	100.00	36.60	0
-40.00	90.00	24.28	0
-30.00	80.00	11.96	0
-20.00	70.00	-0.36	0
-10.00	60.00	-12.68	0
0.00	50.00	-25.00	0
10.00	40.00	-37.32	0
20.00	30.00	-49.64	0
30.00	20.00	-61.96	0
40.00	10.00	-74.28	0

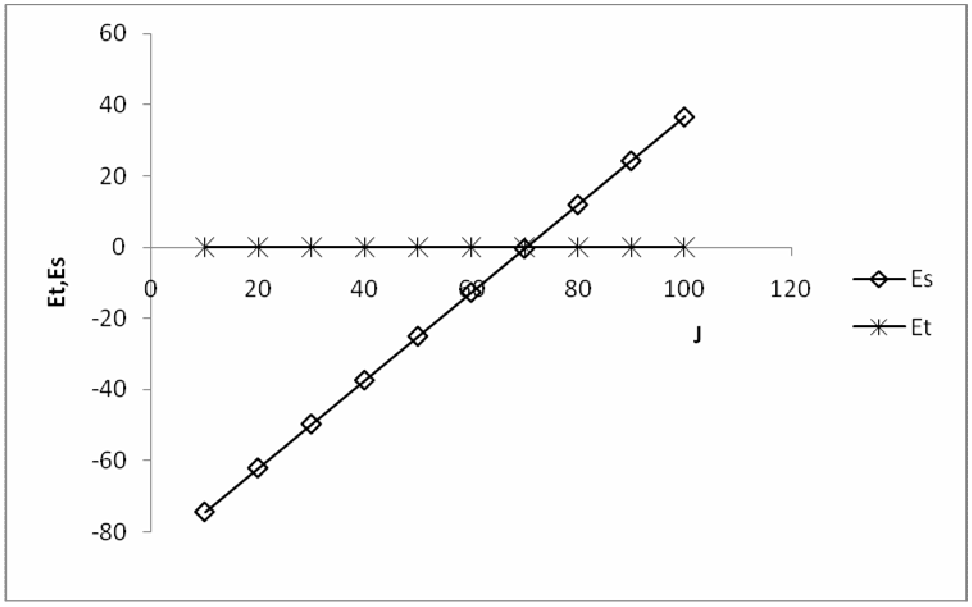

Fig.3.0: A graph of the energies (E_s, E_t) versus J in the t – J model, showing the transition between E_s and E_t as J increases.

Let us consider the original t – u – J model represented by (3.3) and let us examine its influence on ferromagnetic transition.

$$\hat{H} = \hat{t} + \hat{u} + \hat{J} =$$

$$-t\sum_{\langle i\,j\rangle\sigma} C_{i\sigma}^{+}\, C_{j\sigma} + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + J\sum_{\langle i\,j\rangle}\left[S_i^z\, S_j^z - \frac{n_i n_j}{4} + \frac{1}{2}\left(S_i^{+}S_j^{-} + S_i^{-}S_j^{+}\right)\right]$$

$$where \quad S_i^z = \frac{1}{2}\left(n_{i\uparrow} - n_{ij}\right),\ S_i^{+} = C_{i\uparrow}^{+}C_{i\downarrow},\ S_i^{-} = C_{i\downarrow}^{+}C_{i\uparrow}$$

$$\therefore S_i^z S_j^z = \frac{1}{2}\left(n_{i\uparrow} - n_{i\downarrow}\right)\cdot\frac{1}{2} + \left(n_{j\uparrow} - n_{j\downarrow}\right) + \frac{1}{2}\left(C_{i\uparrow}^{+}C_{i\downarrow}C_{j\downarrow}^{+}C_{j\uparrow} + C_{i\downarrow}^{+}C_{i\uparrow}C_{j\uparrow}^{+}C_{j\uparrow}\right),\ \frac{n_i n_j}{4} = \frac{1}{2}\left(n_{i\uparrow}n_{j\uparrow} + n_{i\uparrow}n_{j\downarrow} + n_{i\downarrow}n_{j\uparrow} + n_{i\downarrow}n_{j\downarrow}\right)$$

$$S_i^{+}S_j^{-} + S_i^{-}S_j^{+} = \left(C_{i\uparrow}^{+}C_{i\downarrow}C_{j\downarrow}^{+}C_{j\uparrow} + C_{i\downarrow}^{+}C_{i\uparrow}C_{j\uparrow}^{+}C_{j\uparrow}\right)$$

$$H = -t\left(C_{i\uparrow}^{+}C_{j\uparrow} + C_{j\uparrow}^{+}C_{i\uparrow} + C_{i\downarrow}^{+}C_{j\downarrow} + C_{j\downarrow}^{+}C_{i\downarrow}\right) + U\left(C_{i\uparrow}^{+}C_{i\uparrow}C_{i\downarrow}^{+}C_{i\downarrow} + C_{j\uparrow}^{+}C_{j\uparrow}C_{j\downarrow}^{+}C_{j\downarrow}\right) + J\left[\frac{1}{4}\left(C_{i\uparrow}^{+}C_{i\uparrow}C_{j\uparrow}^{+}C_{j\uparrow} - C_{i\uparrow}^{+}C_{i\uparrow}C_{j\downarrow}^{+}C_{j\downarrow} - C_{i\downarrow}^{+}C_{i\downarrow}C_{j\uparrow}^{+}C_{j\uparrow}\right.\right.$$

$$\left.\left. + C_{i\downarrow}^{+}C_{i\downarrow}C_{j\downarrow}^{+}C_{j\downarrow}\right) + \frac{1}{2}\left(C_{i\uparrow}^{+}C_{i\uparrow}C_{j\downarrow}^{+}C_{j\downarrow} + C_{i\downarrow}^{+}C_{i\uparrow}C_{j\uparrow}^{+}C_{j\downarrow}\right) - \frac{1}{4}\left(C_{i\uparrow}^{+}C_{i\uparrow}C_{j\uparrow}^{+}C_{j\uparrow} + C_{i\uparrow}^{+}C_{i\uparrow}C_{j\downarrow}^{+}C_{j\downarrow} + C_{i\downarrow}^{+}C_{i\downarrow}C_{j\uparrow}^{+}C_{j\uparrow} + C_{i\downarrow}^{+}C_{i\downarrow}C_{j\downarrow}^{+}C_{j\downarrow}\right)\right]$$

$$+ \frac{1}{2}\left(C_{i\uparrow}^{+}C_{i\downarrow}C_{j\downarrow}^{+}C_{j\uparrow} + C_{i\downarrow}^{+}C_{i\uparrow}C_{j\uparrow}^{+}C_{j\downarrow}\right)$$

(3.3)

The results of applying the Hamiltonian (3.3) on the basis states are given by (3.4)

$$H|1\rangle = H\left|1\uparrow 1\downarrow 2\uparrow\right\rangle = -t|2\rangle + t|3\rangle + u|1\rangle - \frac{J}{2}|1\rangle,\quad H|2\rangle = H\left|1\uparrow 1\downarrow 3\uparrow\right\rangle = -t|1\rangle + t|5\rangle + u|2\rangle - \frac{J}{2}|2\rangle,$$

$$H|3\rangle = H\left|1\uparrow 2\uparrow 2\downarrow\right\rangle = +t|1\rangle - t|4\rangle + u|3\rangle - \frac{J}{2}|3\rangle,\quad H|4\rangle = H\left|2\uparrow 2\downarrow 3\uparrow\right\rangle = -t|3\rangle + t|6\rangle + u|4\rangle - \frac{J}{2}|4\rangle,$$

$$H|5\rangle = H\left|1\uparrow 3\uparrow 3\downarrow\right\rangle = +t|2\rangle - t|6\rangle + u|5\rangle - \frac{J}{2}|5\rangle,\quad H|6\rangle = H\left|2\uparrow 3\uparrow 3\downarrow\right\rangle = +t|4\rangle - t|5\rangle + u|6\rangle - \frac{J}{2}|6\rangle,$$

$$H|7\rangle = H\left|1\uparrow 2\uparrow 3\uparrow\right\rangle = 0.$$

(3.4)

The Hamiltonian matrix formed from the interaction is presented in (3.5)

$$H = \begin{pmatrix} u - \frac{J}{2} & -t & t & 0 & 0 & 0 & 0 \\ -t & u - \frac{J}{2} & 0 & 0 & t & 0 & 0 \\ t & 0 & u - \frac{J}{2} & -t & 0 & 0 & 0 \\ 0 & 0 & -t & u - \frac{J}{2} & 0 & t & 0 \\ 0 & t & 0 & 0 & u - \frac{J}{2} & -t & 0 \\ 0 & 0 & 0 & t & -t & u - \frac{J}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

(3.5)

Table 3.2: Singlet (E_s) and Triplet (E_t) energies as J and t vary, with the on-site Coulomb repulsion U fixed.

t (hopping integral)	U (on-site coulomb repulsion)	J (NN exchange interaction)	Es (singlet state energy	Et (triplet state energy)
-50.0	50.0	100.0	86.6	0.0
-40.0	50.0	90.0	74.3	0.0
-30.0	50.0	80.0	62.0	0.0
-20.0	50.0	70.0	49.6	0.0
-10.0	50.0	60.0	37.3	0.0
0.0	50.0	50.0	25.0	0.0
10.0	50.0	40.0	12.7	0.0

20.0	50.0	30.0	0.4	0.0
30.0	50.0	20.0	-12.0	0.0
40.0	50.0	10.0	-24.3	0.0

As the value of U (the Coulomb interaction strength) increases from 50 to 70, the transition point decreases as shown in Fig. 3.3.

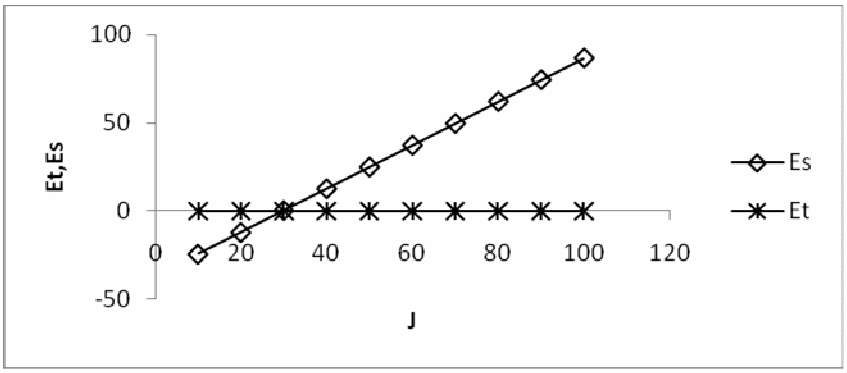

Fig. 3.2 A graph of the energies (E_s, E_t) versus J in the t – u – J model, showing the transition between E_s and E_t as J is varied and U fixed at a value of 50. The transition occurs at about J = 30.

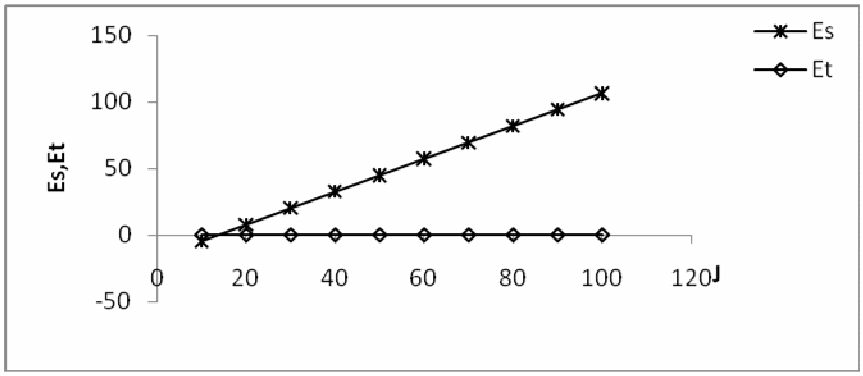

Fig. 3.3 A graph of the energies (E_s, E_t) versus J in the t – U – J model. The value of U hs been increased from 50 to 70 here and the transition point has now occurred at the reduced value of J ≈ 10.

4.0 Conclusion.

From this work, strickly within the t – U model, Fig.1.0 reveals that the singlet state energy approached the triplet state energy, without crossing, as $U \rightarrow \infty$. The physical meaning of this graph as $U \rightarrow \infty$, is that the lattice is not completely antiferromagnetic or ferromagnetic, which indicates that it is unstable. But when the t – J model is used for the case of a nearly half-filled band (i.e when a hole is allowed to move in the lattice), a completely different graph that is ferromagnetically stable is obtained (see Fig. 3.1). Also, from Figures 3.2 and 3.3, it is observed that as the value of U increases from 50 to 70 the transition point decreases. Hence we can say that the, t – J and t – U – J models are better models for demonstrating Nagaoka's theorem.

References

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