THE DYNAMICS OF A HOLE IN TWO DIMENSIONAL MOTT INSULATORS

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ABSTRACT

This paper presents a detailed and quantitative study of the dynamics of strongly correlated electron systems with one hole less than half-filling. This study is carried out by investigating the propagation of a hole in finite Systems of eight and ten sites tilted square clusters within the t-J_z model using exact diagonalization (ED) method. The result obtained from (ED) study of the doped tilted square cuprates at Nagaoka limit, weak and strong coupling regimes agrees excellently with the result obtained by ref. [1] in Lanczos and Mote Carlo study of 4x4 cluster. The well-known intermediate coupling result for the string picture is effectively reproduced for N=10 in agreement with ref. [1] who used N=64 and ref. [2] who used N=256 for the pure t-J model. The difference between the result obtained in the intermediate regime by ref. [1] and this current study may likely be due to the difference in the system size.

1. INTRODUCTION

The behaviour of the cuprates unlike the conventional superconductors is known to be governed by strong electronic interactions. This has spurred interest in the field of strongly correlated electron systems with the hope that it will unravel the mystery behind superconductivity in the cuprates and possibly solve the problems inherent in these materials. The cuprates are also classified as Mott insulators with dominant physical processes (charge transport, antiferromagnetic exchange…..) that participate in the formation of the superconducting condensate located in the copper-oxygen planes [3-5]. At half filling, hopping of electrons is highly forbidden due to the strong onsite electronic repulsion. The magnetic properties of these half-filled (undoped) systems are well described by the isotropic spin-1/2 Heisenberg model [6-8]. It has been observed that under light doping, which removes electrons thereby producing mobile holes in the CuO_2 planes, antiferromagnetic ordering is destroyed and the compound becomes superconducting [1]. A study of hole motion in a classical Neel state in two dimensions by ref [9-11] concluded that the motion of the hole is confined. By considering quantum spin fluctuations and some complicated paths, a single hole was made mobile [12-15]. But recent discovery of string excitations in ARPES studies of cuprates seems to be in support of the string picture proposed by ref. [11] in the intermediate coupling regime [16,17,2]. It is therefore obvious that there is lack of consensus regarding the dynamics of a hole in an antiferromagnet. This field is still evolving with theoretical and experimental researches geared towards addressing some of the problems of this hole dynamics. This work employs the exact diagonalization method with well constructed tilted square clusters of eight and ten sites to study the coherent and incoherent propagation of a hole in an antiferromagnet. The ultimate goal of this paper is to see if a single hole motion on relatively small system size systems within the t-J_z can reproduce the known dominant results.

2. DERIVATION OF AN EFFECTIVE HOLE HAMILTONIAN IN 2D

The Ising Hamiltonian ($t - J_Z$ model) obtained by removing the spin flip term from the generalized $t - J$ model is given by

$$H = -t \sum_{\langle i,j \rangle \sigma} \left[C_{i\sigma}^{\dagger} C_{j\sigma} + C_j^{\dagger} C_{i\sigma} \right] + J_z \sum_i S_i^Z S_j^Z \tag{1.0}$$

where t is the kinetic energy term, $c_{i\sigma}^{+}(c_{j\sigma})$ are the creation (annihilation) operators, $J_Z = 4t^2/U$ is the antiferromagnetic exchange coupling parameter between spins on sites i

and j, $S_i^z = \frac{1}{2}\left(c_{i\uparrow}^{\dagger}c_{i\uparrow} - c_{i\downarrow}^{\dagger}c_{i\downarrow}\right)$ is the spin operator in the z direction and the symbol $\langle i, j\rangle$ means that hoppings are constrained to nearest neighbour site. Eq. (1.0) is with an understood restriction to unoccupied and singly occupied sites.

The energy of a single hole on a tilted $\sqrt{N}\times\sqrt{N}$ square lattice is given by

$$\in_h = \langle\varphi|H|\varphi\rangle - E_N = E_{oh} + \frac{J_z N}{2} \tag{2.0}$$

where E_N is the energy of the Neél state, N is the number of sites and E_{oh} is total energy of the system in the presence of a hole. The single hole Hamiltonian can therefore be constructed as follows

$$H' = H - E_{oh} \tag{3.0}$$

As the hole propagates in an antiferromagnetic background, destroying the Neél ordering of the spin, ferromagnetic links are produced. Since the cost of each ferromagnetic bond is $J_z/2$, the magnetic part of H' acting on a class $|\phi\rangle$ takes the form

$$H'_{J_Z}|\phi\rangle = \frac{J_Z}{2}\sum_{\langle i,j\rangle}(i, j)|\phi\rangle + J_Z|\phi\rangle \tag{4.0}$$

where $(i, j) = (n_{i\sigma}n_{i\sigma'})\delta_{\sigma'\sigma}$ and $i \neq j$. The last term in eqn. (4.0) is due to the four antiferromagnetic links that were destroyed once a hole is created in a Neél state. Since the system is translationally invariant, Eq. (4.0) gives

$$H'_{J_Z}|\phi\rangle = \frac{1}{\sqrt{N}}\left[\left(E_Z + J_Z\right)|R_1\rangle + \left(E_Z + J_Z\right)|R_2\rangle + \ldots + \left(E_Z + J_Z\right)|R_N\rangle\right] \tag{5.0}$$

where R_1 R_2... R_N are members of the class $|\phi\rangle$ generated by the translational operator T given by

$$|\phi_{K=0}\rangle = \frac{1}{\sqrt{N_{R_i}}}\sum_{r=0}^{N-1} e^{-iKr}T^r|R_i\rangle \tag{6.0}$$

Further simplification of eqn. (5.0) gives

$$H'_{J_Z}|\phi\rangle = (E_Z + J_Z)|\phi\rangle \quad (6.0)$$

where

$$E_Z = \frac{J_Z}{2}\sum_{\langle i,j\rangle}(i,j) \quad (7.0)$$

On adding the hopping term in H' to Eq. (1.0), the complete single hole

Hamiltonian acting on a state $|\phi_n\rangle$ gives

$$H'|\phi_n\rangle = -t\left[|\phi_{n+\pm\hat{x}}\rangle + |\phi_{n+\pm\hat{y}}\rangle\right] + (E_Z + J_Z)|\phi_n\rangle \quad (8.0)$$

where $\pm\hat{x}$, $\pm\hat{y}$ are unit vectors in the directions $\pm x$, $\pm y$ and n=0,1..., N_h-1. Here, N_h is the number of state in the reduced Hilbert space. It is given by

$$N_h = \frac{2(N-1)!}{N[(N/2-1)!]^2} \quad (9.0)$$

3. THE TOPOLOGY OF EIGHT AND TEN SITES TILTED SQUARE CLUSTERS

The topology of eight and ten sites tilted clusters are respectively shown in Fig. 1 and Fig. 2.

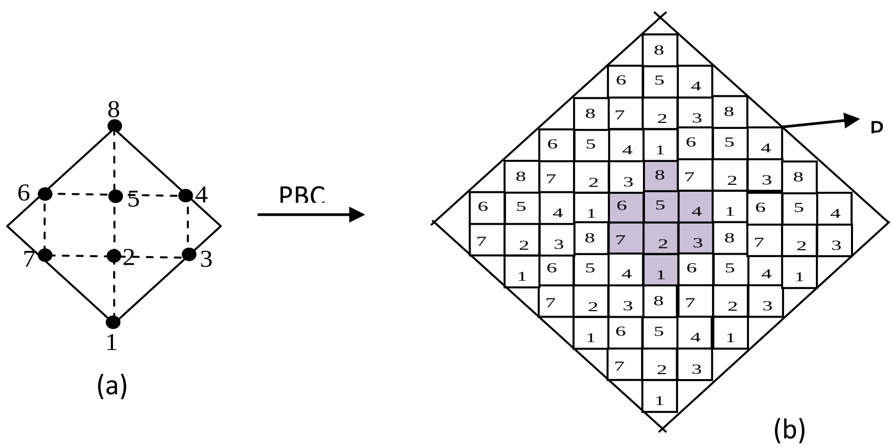

Fig. 1. The topology of an eight sites tilted square cluster. Fig (a) is the original cluster without periodic boundary conditions (PBC). Fig. (b) is obtained when periodic boundary conditions is imposed on the open cluster.

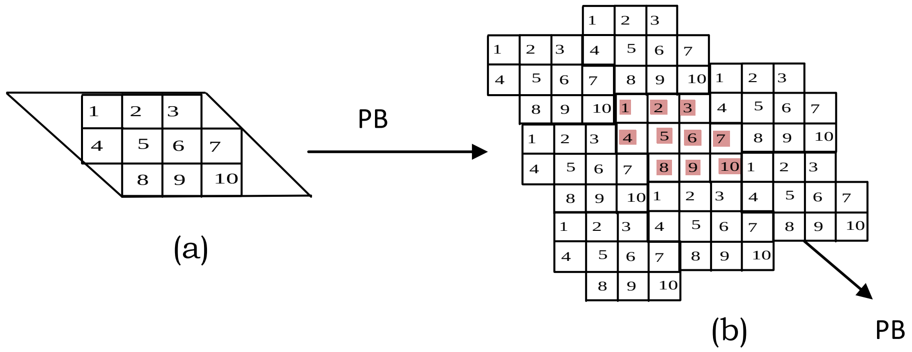

Fig. 2. The topology of a ten sites tilted square cluster. Fig. (a) is the original cluster without periodic boundary conditions (PBC). Fig. (b) is due to periodic PBC.

The number of antiferromagnetic links N_{AL} in any 2-dimensional cluster is given by

$$N_{AL} = 2N \qquad (10.0)$$

where N is the number of sites. Therefore, for an eight sites tilted cluster, N_{AL} =16. These links are.

(1,2), (1,6),(1,8), (1,4), (2,3), (2,5),(2,7), (3,4)

(3,6), (3,8),(4,5), (4,7), (5,6), (5,8),(6,7), (7,8)

where for instance (1,2) refers to the antiferromagnetic link $1\uparrow - 2\downarrow$ or $1\downarrow - 2\uparrow$. The number of antiferromagnetic links for 10 sites tilted cluster is 2x10=20. These links are

(1,2), (1,4),(1,8), (1,10), (2,3), (2,5),(2,9), (3,4)(3,6), (3,10),

(4,5), (4,7), (5,6), (5,8),(6,7), (6,9),(7,8),(7,10), (8,9),(9,10)

By using Eq. (9.0), the size of the Hilbert space for eight site tilted square can be reduced from 280 to 35 and that for ten site tilted square can be reduced from 1260 to 260.

4. RESULTS AND DISCUSSION

This section presents numerical exact diagonalization results for $\sqrt{8}\times\sqrt{8}$ and $\sqrt{10}\times\sqrt{10}$ clusters. The results obtained for the energy of the hole E_h/t at various values of the magnetic coupling constant J_z/t is presented in the Table 1. For comparison, the string picture by ref. [11] and the results obtained by ref.[1,18] on a 4x4 square cluster by both the Lanczos technique (LT) and quantum Monte Carlo (QMC) method are also included in Table 1. These results will be discussed under the following regimes namely, Nagaoka's limit, weak coupling, intermediate coupling and strong coupling.

Table 1. Exact numerical ground state (GS) energy of a hole for N=8 and N=10 tilted clusters. Comparison is made between the results obtained by exact diagonalization (ED) method and the numerical results from quantum Mote Carlo(QMC) and Lanczos Technique (LT) [1,18]

J_Z/t	EXACT E/t (N=8)	EXACT E/t (N=10)	LT E/t (N=16)	QMC E/t (N=16)	STRING PICTURE
0.00	-4.00000	-4.00000	-4.00000	-4.0000	-3.46410
0.01	-3.96431	-3.95454	-3.92530	-3.9254±0.0001	-3.33692
0.02	-3.92866	-3.90927	-3.85187	-3.8516±0.0002	-3.26222
0.05	-3.82196	-3.77466	-3.63864	-3.6384±0.0004	-3.09223
0.10	-3.64507	-3.55445	-3.30627	-3.306±0.001	-2.87379
0.20	-3.29528	-3.13113	-2.75419	-2.755±0.002	-2.52703
0.40	-2.61658	-2.36632	-2.07192	-2.084±0.009	-1.97660
0.60	-1.97872	-1.72806	-1.56082	-1.551±0.008	-1.51492
0.80	-1.40104	-1.20773	-1.11920	-1.131±0.008	-1.10284
1.00	-0.89746	-0.77112	-0.72325	-0.709±0.009	-0.72410
1.50	0.08869	0.12443	0.13728	0.145±0.003	0.12631
2.00	0.86658	0.87790	0.88237	0.883±0.007	0.88538
2.50	1.55199	1.55623	1.55808	1.557±0.002	1.58302
3.00	2.18634	2.18817	2.18902	2.185±0.003	2.23533
4.00	3.36844	3.36889	3.36914	3.368±0.002	3.44027

I. NAGAOKA'S LIMIT

In this limit, a hole is not confined in a linear potential, and so it can propagate freely through the antiferromagnetic background without losing energy. On account of this, the number of broken bonds or aligned spin pairs increases, amounting to increase in the size of the polaron. This will eventually gives rise to a ferromagnetic ground state of ($2S^{max}$ +1)-fold degenerate with energy E_h=-4t or E_h/t=-4, where S^{max} = (N-1)/2 and N is the number of sites. This limit called the Nagaoka's polarized state occurs at J_z/t=0 [19]. This limit is captured by both N=8 and N=10 as shown in Table 1

II. WEAK COUPLING REGIME (J_Z<<t)

According to Dagotto et al (1989), in this regime, E_h takes the form

$$E_h = -4t + \frac{J_z}{2}\left[L^2 - 1 + \frac{1}{L^2 - 1}\right] \tag{11.0}$$

where L is the length of the side of the square. The ED result in this regime and that obtained from Eq. (11.) are shown in Table 2. For comparison, the result obtained by ref. [1] with the Lanczos technique (LT) on 4x4 cluster is also included. These two presentations are in excellent agreement, showing that the weak coupling regime is well captured by the system size studied. Fig. 3 gives a graphical illustrations of the hole energy in this regime. For sufficiently small value of J_Z/t as shown in Fig. 3, the energy of the hole for any number of sites is expected to converge to a common value. Consequently, E_h will become less dependence on J_z. Also, the kinetic energy of the hole is well minimized since the magnetic energy cost is small. As J_z becomes smaller, the number of flipped spins increases as the hole propagates. Consequently, the size of the polaron is increased.

Table 2. Result for weak coupling regime

	ED Result		From Eq. (11.0)		LT
J_Z/t	E_h/t(N=8)	E_h/t(N=10)	E_h/t(N=8)	E_h/t (N=10)	E_h/t(N=16)
0.00002	-3.99993	-3.99991	-3.99993	-3.99990	-3.99984
0.00004	-3.99986	-3.99982	-3.99986	-3.99980	-3.99968
0.00006	-3.99979	-3.99973	-3.99979	-3.99970	-3.99952
0.00008	-3.99971	-3.99964	-3.99971	-3.99960	-3.99936
0.00010	-3.99964	-3.99954	-3.99964	-3.99950	-3.99920
0.00020	-3.99929	-3.99909	-3.99929	-3.99899	-3.99839
0.00040	-3.99857	-3.99818	-3.99857	-3.99798	-3.99679

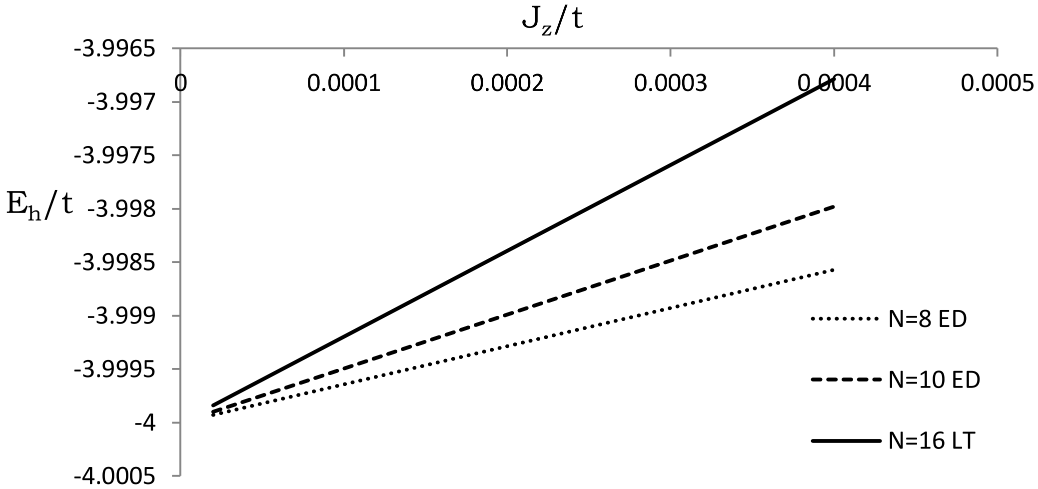

Fig.3. Energy of a hole in the Weak coupling regime

III. STRONG COUPLING REGIME ($J_z/t>>1$ OR $J_z>>t$)

In this regime, the motion of the hole becomes highly incoherent due to increase in linear rising potential that tends to confine the hole to its original site. This is because an increase in J_z will increase the amount of magnetic energy paid by the hole in destroying antiferromagnetic bonds and creating new ferromagnetic bonds. Hence, in the strong coupling regime, the hole may be treated as a localized particle, and to second order in t/J_z, the hole energy according to ref. [1] becomes

$$E_h = J_z - \frac{8t^2}{3J_z} \qquad (12.0)$$

The results obtained from the ED of N=8 and N=10 and that from Eq. (12.0) as presented in Table 3 are in reasonable agreement. This behaviour of E_h at this regime is also visible in Fig.4. It shows that in the strong coupling regime, the energy of a hole is independent of the system size in accordance with Eq. (12). For comparison, the result obtained by ref. [1] with the Lanczos technique (LT) on 4x4 cluster is also included. Since the hole is strongly confined in this regime, the number of “anti-Neel spins’’ which is a measure of the size of the polaron decreases significantly.

Table 3. Result for Strong coupling regime

J_z/t	N=8 (ED)	N=10 (ED)	From eqn.38
4.0	3.36844	3.36889	3.33333
5.0	4.48558	4.48573	4.46667
6.0	5.56682	5.56688	5.55556
7.0	6.62627	6.62630	6.61905
8.0	7.67156	7.67158	7.66667
9.0	8.70717	8.70718	8.70370
10.0	9.73588	9.73588	9.73333

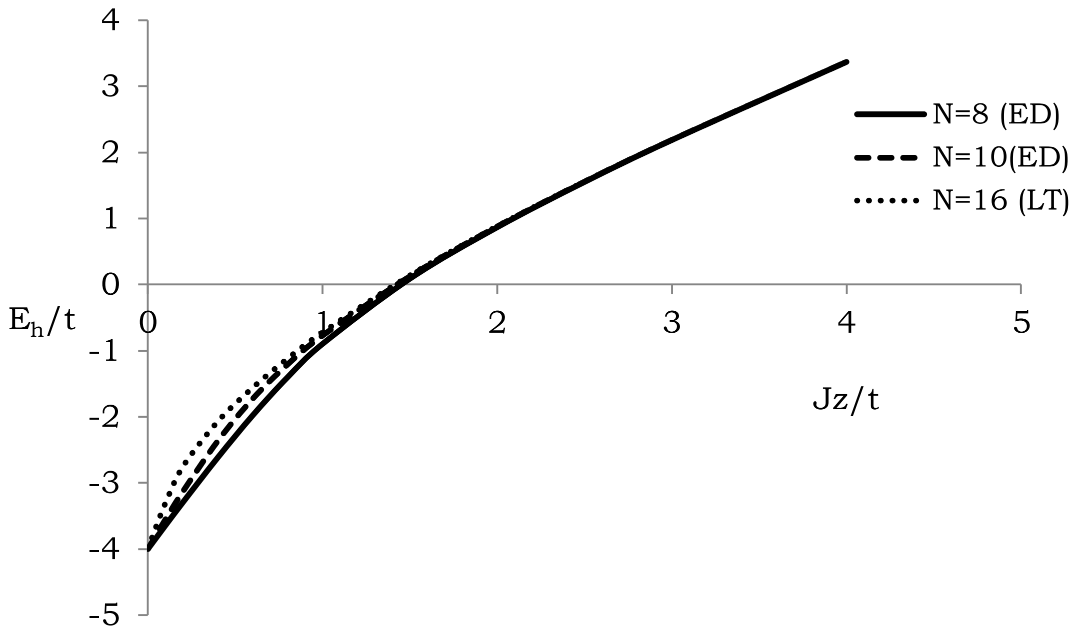

Fig.4. Energy of a hole in the strong coupling regime

IV. INTERMEDIATE COUPLING

If a hole is prevented from propagating through winding paths (Trugman loops), then we have a hole motion on a Bethe lattice. This is the approximation used by ref. [11] to obtain the result in the last column of Table 1. This approximate result known as the string picture and valid at the intermediate region $5\times10^{-3} \le J_z/t \le 1$ is giving by.

$$E_h/t \approx -2\sqrt{3} + 2.74(J_z/t)^{2/3} \tag{13.0}$$

As t-J models of the high-T_c materials typically assume J=0.1eV [20] and t=0.3eV [21], this regime therefore captures the intermediate-coupling region ($J_z/t \sim 1/3$), which is of greatest interest. This intermediate regime as shown in Fig.5 is investigated for N=8 and N=10 in the range $0.01 \le J_z/t \le 1$, and comparison is made with N=16 and string estimate. The behaviour of the graphs for both N=8 and N=10 is similar to that of N=16 and the string estimate. This shows that a power law description of E_h in this regime is present in N=8 and N=10. In the region $5\times10^{-3} \le J_z/t \le 1$, the curve for N=10 can be approximately fitted to give

$$E_h/t \approx -3.999 + 3.228(J_z/t)^{2/3} \tag{14.0}$$

Similar power law behaviour can also be obtained for N=8. A QMC result for 8x8 square lattice in this regime by ref. [1] gave a fit given by

$$E_h/t \approx -3.63 + 2.93(J_z/t)^{2/3} \tag{15.0}$$

The difference of 0.369 and 0.298 observed in the constant term and coefficient of $(J_z/t)^{2/3}$ respectively between eqn. (14) and (15) is obviously due to the difference in cluster size studied. Within this intermediate regime, the energy of a hole E_h is approximately linear in $(J_z/t)^{2/3}$. This approximate linear behaviour is captured in the plot of E_h versus $(J_z/t)^{2/3}$ for N=10 as shown in Fig.5.

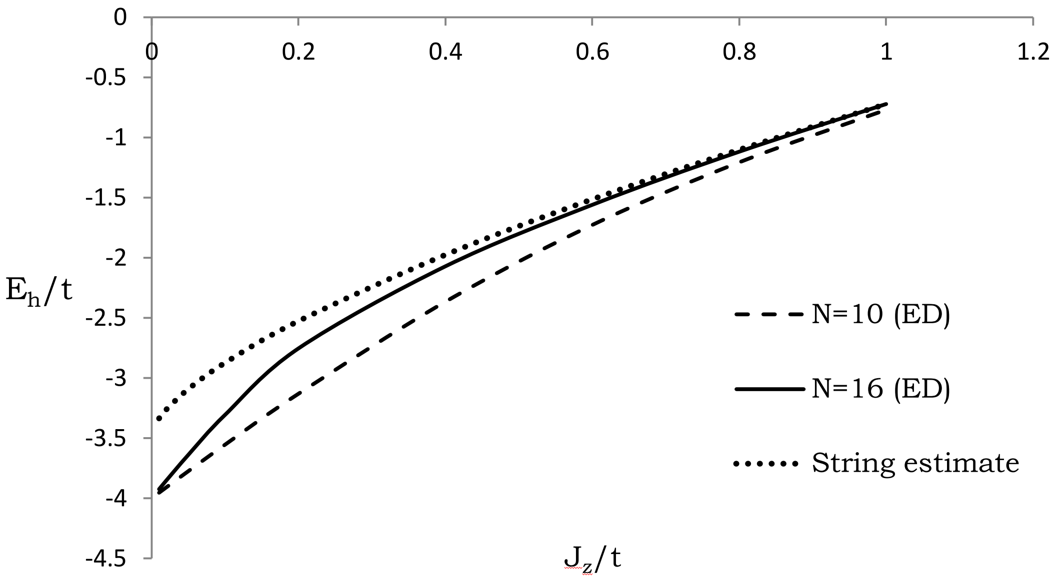

Fig. 5. Intermediate coupling result for N= 10 compared with N= 16 and the string estimate.

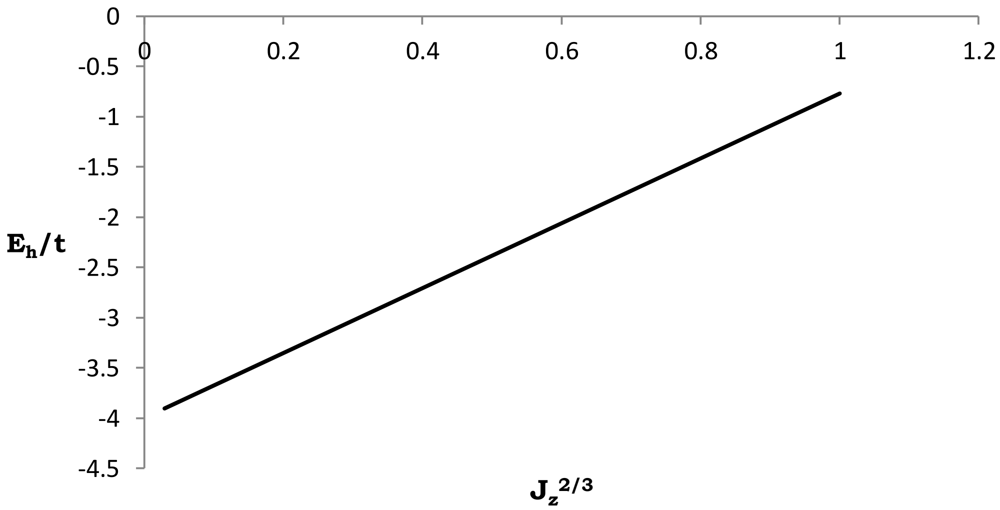

Fig.6. Linear behaviour of E_h with $J_z^{2/3}$.

5. EXPERIMENTAL REALIZATION OF STRING EXCITATION IN THE INTERMEDIATE REGIME IN 2D CUPRATES

Recent high resolution ARPES studies of $Ca_2CuO_2Cl_2$ taken along the cut (0,0) to (π,π) as shown in Fig.7 has revealed the presence of dispersive feature at higher energies (peak II and III) that merges with the quasiparticle band (peak I) at lower energies [16,17]. The energy of the three peaks as identified by ref.[22]Manousakis and Liu (1992) on 16×16 lattice by perturbation approach in the regime $0.02 \le J \le 0.4$ and $K = (\pi/2, \pi/2)$ is in agreement with the string excitation of the t-J_Z model obtained in this paper. The string energies for these peaks as well as the one obtained in this thesis are

$$E_I = -3.28 + 2.16 J^{0.667} \tag{16}$$

$$E_{II} = -3.28 + 5.46 J^{0.667} \tag{17}$$

$$E_{III} \approx -3.28 + 7.81 J^{0.667} \tag{18}$$

$$E_h / t \approx -3.999 + 3.228 (J_z / t)^{0.667} \tag{19}$$

ref. [2] has also reproduced Eqs. (16), (17) and (18) from the spectral function of a hole in a quantum antiferromagnet (the pure t-J model) for J/t=0.3 from (0, 0) to (π, π) as shown in Fig.8. He therefore concluded that the string excitation is responsible for the transfer of spectral weight from the quasiparticle peak to the high energy peaks as the Γ Point is approached.ref[1,22] have also observed similar feature in the t-J model. The t-J_z model is therefore robust enough to capture the dynamical properties of a hole in a quantum antiferromagnetic background in the region of small coupling.

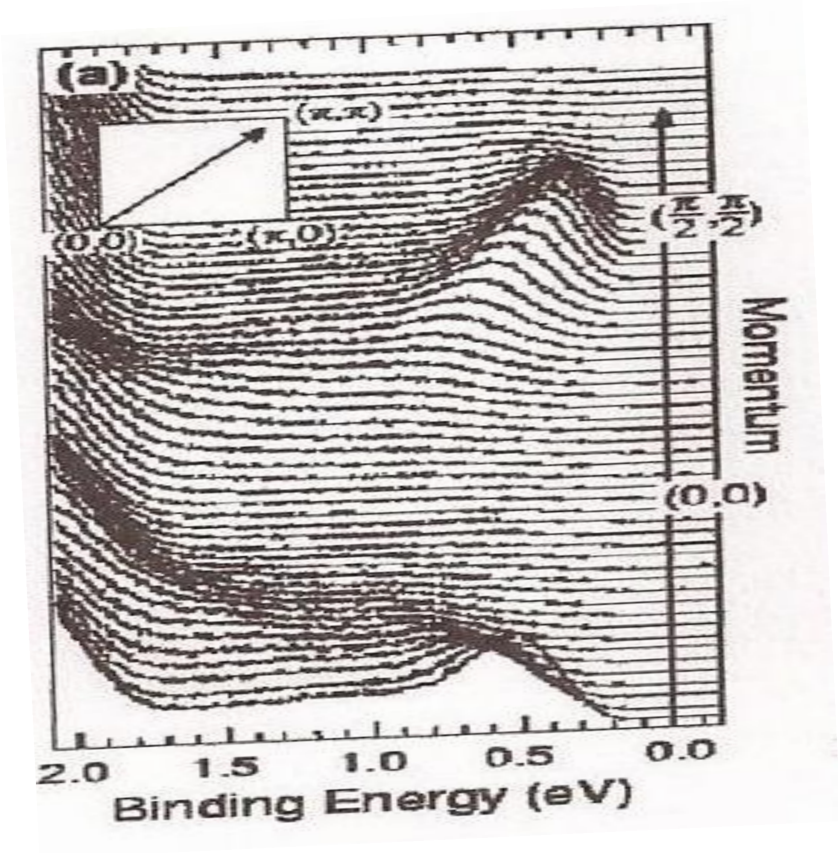

Fig.7. Experimentally determined spectra function of $Ca_2CuO_2Cl_2$ with ARPES

(Source: [16])

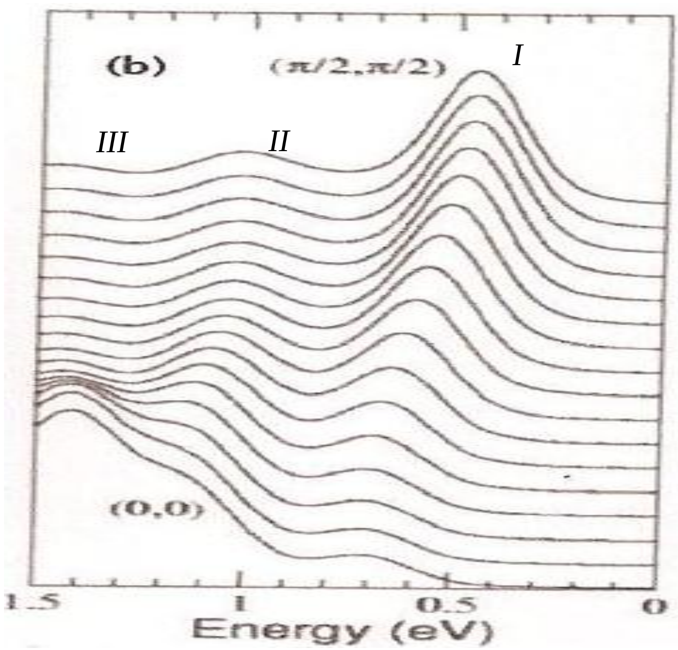

Fig.8. Spectra function obtained from t-J model for J/t=0.3 from (0,0) to (π,π)

(Source: [2])

6. CONCLUSION

We have in this study employ the exact diagonalization method to investigate the dynamical properties of a hole on N=8 and N=10 tilted clusters within the $t - J_Z$ model. The behaviour of one hole on N=8 and N=10 tilted clusters is not at variance with the results obtained from 4x4 square cluster by ref.[1]. Most importantly, the results obtained at strong and weak coupling regimes from these tilted clusters agreed excellently with theirs. The string energy obtained in the intermediate coupling for N=10 is in agreement with that obtained from Quantum Monte Carlo simulation of N=64 by ref.[1]. The small disagreement in this regime arising from the constant term in the hole energy and the coefficient of $(J_z/t)^{2/3}$ may be due to finite size effect.

This string excitation observed in this thesis are responsible for the transfer of spectra weight from the low energy quasiparticle peak to higher energy peaks as observed in the ARPES data from $Ca_2CuO_2Cl_2$ [16,17]. The agreement between the results obtained in this thesis and that obtained theoretically and experimentally in the region of small coupling (J/t<<1) suggests that the $t - J_Z$ model is robust enough to capture the dynamical properties of a hole in a quantum antiferromagnetic background. Furthermore, in the limit of J/t<<1, the spin-relaxation time is much longer than the characteristic time for hoping. As a result, the rate at which the spins are being flipped by the hole is faster than the rate at which they are being repaired by the spin flip term in the t-J model. Finally, the string energy obtained in this study from N=10 tilted cluster provides evidence that the occurrence of these string excitations is independent of system size.

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