AN ANALYTIC STUDY OF THE ITINERARY OF A HOLE IN ONE DIMENSIONAL ISING ANTIFERROMAGNET

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ABSTRACT
As the hole propagates in a finite one dimensional antiferromagnetic background, a mobile spinon is created. The magnetic energy needed to sustain the spinon states is $J_z$, and that required to sustain the none spinon states is $J_z/2$. Between the interval of creation and subsequent annihilation of a spinon, the energy of a hole is relatively constant and of magnitude $J_z$. Hence, the magnetic energy expended by the itinerant hole oscillates between $J_z$ and $J_z/2$. This spinon is found to be $N$ times slower than the hole. This weak coupling between the hole and the spinon tends to confine the hole in a linear rising potential. However, contact with the result obtained in the thermodynamic limit is established as the hole can break lose at this limit and propagate freely.

Keywords: Ising antiferromagnet, spin-charge separation, confinement, spinon and hole.

INTRODUCTION
Strongly correlated systems is one of the most intensively studied areas of research in condensed-matter physics [1]. The term “strong correlation” describes the state of affair when the interaction energy $U$ dominates in controlling the motion of the electron [2]. Due to this strong Coulomb repulsion ($U$), electrons in these systems remain localized in their respective sites. Any attempt for an electron to hop to a neighbouring site thereby reducing its kinetic energy ($t$) will amount to double occupancy of some sites which cost $U$. The presence of this large $U$ characterizes these systems as unconventional antiferromagnetic insulators, known as Mott insulators [3-5]. These insulators driven by strong coulomb repulsion are indeed different from the band insulators that are characterized by a full and empty one electron band. More so, the band insulator will require the state to be metallic at half filling. Understanding, controlling, and predicting the emergent complexity of strongly correlated electron systems is one of the most pressing challenges in condensed-matter physics [6]. It is known that under light doping, which removes electrons thereby producing mobile holes in the CuO$_2$ planes of these cuprates, the antiferromagnetic ordering is destroyed and the compound becomes superconducting [7].

There have been rigorous and intense researches on one and quasi-one dimensional (1D and quasi -1D) systems. The motivation for researches on 1D and quasi -1D systems is because of the intriguing phenomena that have been discovered theoretically and experimentally in them. For instance, the injection of a single hole into quasi-one dimensional Mott insulators such as Sr$_2$CuO$_2$ and SrCuO$_2$ has been known to give rise to Spin-charge separations [8-11]. This discovery therefore gives birth to two quasiparticles namely, holon (possessing only charge) and spinon (possessing only spin) [12]. More so, an experiment with Sr$_2$CuO$_2$ found an orbiton liberating itself from spinons and propagating through the lattice as a distinct quasi-particle with a dispersion of $\sim 0.2eV$ [13]. This observation of a free orbiton is another example of particle fractionalization known as Spin-orbital separation. In ref. [13], further fractionalization of spin and charge beyond the Luttinger-liquid paradigm was discovered.

The aim of the current work is to present an analytical and comprehensive study of the itinerary of a hole in one dimensional Ising antiferromagnet. The energy of one hole in the bulk limit of 1D Ising limit and some of its properties have been discussed by Sorella and Parola in Ref. [14]. However, in this current study, we hope to establish analytically the correlation between the mobile hole and the spinon produced as a result of the hole motion. The study will commence with the itinerary of a single in finite systems and later generalized to thermodynamic limit. It our hope that this analytic study will shed more light on some elusive aspect of hole dynamics and provide further evidence of spinon-holon decoupling in the thermodynamic limit. The rest of the paper is organized as follows: In section 2, the Ising 1D antiferromagnetic model as an effective Hamiltonian describing hole dynamics is presented. In section 3, we illustrate the dynamics of a hole in a finite chain. In section 4, we present an analytical study of the dynamics of a hole and a spinon. The magnetic energy expended per state by a hole is calculated in section 5. We present and the discuss the results obtained in section 6 and conclude in section 7.

2. One Dimensional Ising Antiferromagnet Model
The Ising ($t - J_z$) model is the strongly anisotropic limit of the $t - J$ model which captures some general properties of doped antiferromagnets (AF). The absence of spin fluctuations in the Ising model simplifies the analytical treatment of this problem and makes it possible to visualize the independent effect of a hole in an antiferromagnet. [12]. The destruction of the antiferromagnetic ordering in these Mott insulators when doped with a hole shows that a hole is not static but mobile. The central issue is whether a single hole can propagate freely (coherently) in an antiferromagnetic background. In ref [12] the following Hamiltonian was proposed for a single hole dynamics in finite systems:
$$H |R\rangle = -t(|R - 1\rangle + |R + 1\rangle) + \left( J_{z} |R\rangle - \frac{J}{2} \delta_{R,0} |R\rangle \right), \quad (1)$$

where $t$ is kinetic energy of the hole, $R$ is position vector of the hole and $J_{z}$ is the coupling constant. In the Bulk limit, close paths of the hole along the ring can be neglected [15]. On account of this, Sorella and Parola in Ref. [14] proposed the following Hamiltonian for the dynamics of a hole in the Ising limit of 1D cuprates:

$$H |R\rangle = -t(|R - 1\rangle + |R + 1\rangle) + \left( E_{N} + \frac{J}{2} \right) |R\rangle - \frac{J}{2} \delta_{R,0} |R\rangle, \quad (2)$$

where $E_{N}$ is the energy of the Neél state.

The translational invariance property of the $t - J_{z}$ model is often used to reduce the size of the Hilbert space of a single hole. This means that any one hole state with definite momentum $k$ and spin $\uparrow$ can be written as

$$|\psi_{k}\rangle = \frac{1}{\sqrt{L}} \sum_{R=0}^{L-1} e^{-ikR} T_{L}^{k} c_{0,4}^{\uparrow} |\sigma_{0}\rangle, \quad (3)$$

where $|\sigma_{0}\rangle$ is a suitable spin state with the spin at the origin $R = 0$ fixed to $\downarrow$ and $T_{L}$ is the spin translation operator defined by the transformation property

$$T_{L} S_{R} T_{L}^{-1} = S_{R+1} \quad (4)$$

With translational symmetry, the Hilbert space of size $N(N-1)$ (where $N$ is the number of sites) is reduced by a factor of $N$ according to the equation

$$S_{N} = \frac{N(N-1)}{N} = N - 1 \quad (5)$$

3. The Dynamics of a Hole in Finite Chains

This section studies the dynamics of a hole in one dimensional antiferromagnets. This is carried out by careful examination of the motion of a hole in finite chains subject to periodic boundary conditions. A study of this dynamics is presented for the case of six-site chain containing five electrons and one hole as shown in Fig.1. This study will help provide information that will be useful for the analytical treatment of this hole problem in section 4.

Fig 1. A six-site chain with a hole. The system is subjected to periodic boundary conditions.

The two possible Neel states for the antiferromagnetic background without a hole are:

$$|\psi_{1}\rangle = |1 \uparrow, 2 \downarrow, 3 \uparrow, 4 \downarrow, 5 \uparrow, 6 \downarrow\rangle$$

$$|\psi_{2}\rangle = |1 \downarrow, 2 \uparrow, 3 \downarrow, 4 \uparrow, 5 \downarrow, 6 \uparrow\rangle$$

The starting point for this study is to inject a hole into either of the Neél states shown above. Thus, the hole can either propagate in the subspace of $S_{tot}^{z} = -1/2$ or $S_{tot}^{z} = 1/2$, corresponding to the removal of an up spin electron or a down spin electron respectively. The propagation of this hole in six-site chain in the subspace of $S_{tot}^{z} = 1/2$ is illustrated in Fig.2.
When a hole is created in an antiferromagnetic chain as shown in Fig. 2 and allowed to hop, a ferromagnetic link or bond is created at the birth site of the hole. It is important to study the dynamics of this spinon, the nature of the coupling between it and the hole and its effect on the hole motion. This issues will be addressed in the next section.

\[
\begin{align*}
|1,2 \uparrow,3 \downarrow,4 \uparrow,5 \downarrow,6 \uparrow\rangle & \rightarrow |1,2,3 \downarrow,4 \uparrow,5 \downarrow,6 \uparrow\rangle \\
3 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \uparrow,6 \uparrow\rangle \\
4 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \uparrow,6 \rangle \\
5 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \uparrow,6 \rangle \\
6 & \rightarrow |1 \downarrow,2 \uparrow,3 \downarrow,4 \uparrow,5 \downarrow,6 \uparrow\rangle \\
7 & \rightarrow |1 \downarrow,2 \uparrow,3 \downarrow,4 \uparrow,5 \downarrow,6 \rangle \\
8 & \rightarrow |1 \downarrow,2 \uparrow,3 \downarrow,4 \uparrow,5 \downarrow,6 \rangle \\
9 & \rightarrow |1 \downarrow,2 \uparrow,3 \downarrow,4 \uparrow,5 \downarrow,6 \rangle \\
10 & \rightarrow |1 \downarrow,2 \uparrow,3 \downarrow,4 \uparrow,5 \downarrow,6 \rangle \\
11 & \rightarrow |1 \downarrow,2 \uparrow,3 \downarrow,4 \uparrow,5 \downarrow,6 \rangle \\
12 & \rightarrow |1 \downarrow,2 \uparrow,3 \downarrow,4 \uparrow,5 \downarrow,6 \rangle \\
13 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
14 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
15 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
16 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
17 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
18 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
19 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
20 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
21 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
22 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
23 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
24 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
25 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
26 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
27 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
28 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle \\
29 & \rightarrow |1 \uparrow,2 \downarrow,3 \uparrow,4 \downarrow,5 \downarrow,6 \rangle
\end{align*}
\]

Fig. 2. The propagation of hole in six-site chain subject to PBC. Starting from its birth site \(|1,2 \uparrow,3 \downarrow,4 \uparrow,5 \downarrow,6 \uparrow\rangle\), a hole propagating on a six-site chain must hop eleven times to get to its final state.

4. Analytical Study of the Dynamics of a Hole and a Spinon

For a clearer picture of the dynamics of a single hole in 1D antiferromagnetic chains, there is need to development relevant equations that will provide a connection between the dynamics of the hole and that of the spinon. From these relations, one can analytically draw, for instance, an inference as to whether the hole motion is hindered or not by the motion of the spinon. Furthermore, contact with the thermodynamic expectations can also be made from this analytical treatment. The starting point of this analytical treatment is the dynamics of a hole in the Trugman loop, which describes the motion of a hole on a 2x2 square [16]. Trugman noted that the single hole needs not travel on a straight line, trailing string of flipped spins behind it. According to Trugman as shown in Fig. 3, it is possible for a hole to unwind the strings of flipped spins if it transverses a closed loop one and half times. In order words, it will find itself translated into a degenerate vacuum. Degenerate vacua are states that are degenerate in energy with \(|0\rangle\) (i.e. “strong of zero length” state or it birth state before propagating). Therefore, degenerate vacua are devoid of overturned spins (or flipped spins) and have the same energy as \(|0\rangle\).
This work now extends Trugman closed loop to include hole motion in an N even sites chain. This is achieved first by imposing periodic boundary conditions (PBC) on all N even sites. The topology of the geometry can be approximated as N sites on a circle of radius $R$ given by

$$R = \frac{N\alpha}{2\pi},$$

(6)

where $\alpha$ is the lattice constant. The number of revolution $n_r$ of the hole is given by

$$n_r = \frac{n_h}{N},$$

(7)

where $n_h$ is the number of hops. This means that for $N=4$ and $n_h=4$, $n_r=1$. Now, $N$ hops of the hole will produce strings of flipped spins with a spinon between two extreme spins. This spinon will be removed when the hole makes an additional $(N-2)$ hops, giving a total of $(2N-2)$ hops. The first degenerate vacuum will therefore be produced in $(2N-2)/N$ revolutions. This is in agreement with Trugman statement which states that if a hole traverses any simple closed curve two steps less than two full circuits, the net effect is to translate the hole two lattice spacings to a state with the same energy as the initial one. In the thermodynamic limit ($N \to \infty$), the first degenerate vacuum will occur after two revolutions. This means that it will unwind the strings and translate to its original site. For instance, let the hole occupy the first site in an $N$ even lattice sites, then the spin next to the last spin will occupy $(N-1)$th position. The new position of the hole after unwinding the strings is this $(N-1)$th position. Hence, for four-site chain, the hole will translate to the 3rd position, while for six-site chain, the hole position will be on the 5th site. The next degenerate vacuum will occur after $2(2N-2)/N$ revolutions or $(4N-4)$ hops. Thus, it takes the hole $N-1$ hops to create every new spinon. The total number of a single hole states denoted by $N_h$ is given by

$$N_h = N(N-1)$$

(8)

The number of hops require to generate the available degenerate vacua in a given finite system denoted by $N_d$ is given by

$$N_d = N_h - (2N - 2) = N^2 - 3N + 2$$

(9)

Therefore, the total number of degenerate vacua in a given chain excluding the birth site is
\[
D = \frac{N_d}{2N - 2} = \frac{N^2 - 3N + 2}{2N - 2}
\]

(10)

The total number of states that are none degenerate but contain no spinon is given by

\[
D_{\text{non}} = D + 1 = \frac{N^2 - N}{2N - 2}
\]

(11)

Therefore, total number of states devoid of ferromagnetic bond is obtained by summing eqns. (10) and (11). This gives

\[
D + D_{\text{non}} = N - 1
\]

(12)

The total number of states with spinon is given by

\[
N_h - (D + D_{\text{non}}) = N^2 - 2N
\]

(13)

5. Magnetic Energy Expended Per State by a Hole

Classically, it is possible to visualize a hole as a particle with a hopping amplitude \( t \), finite mass \( m \) and speed \( v = (2t/m)^{\frac{1}{2}} \). For lattice spacing of \( a = 1 \), the time taken for a hole to make a hop from its birth site is \( (m/2t)^{\frac{1}{2}} \). This first hop will produce a spinon. Once this spinon is formed, it will take another \( N - 1 \) hops to create a new spinon. The time taken to make these hops is \( (N - 1)(m/2t)^{\frac{1}{2}} \). Put differently, this time will elapse before a new spinon is formed. The ratio of the speed of the spinon to that of the hole is therefore \( 1/(N - 1) \). In other words, the hole is \( N - 1 \) times faster than the spinon.

The creation of every new spinon will cost the hole a magnetic energy of \( J_z/2 \). The destruction of the antiferromagnetic bond connecting pairs of spin as the hole propagates costs a magnetic energy of \( J_z/2 \). Therefore, states with a spinon will require a magnetic energy cost of \( J_z \) to sustain it, while states devoid of spinon will cost a magnetic energy of \( J_z/2 \). Between the interval of creation and subsequent annihilation of a spinon, the energy of a hole is relatively constant and of magnitude \( J_z \). Hence, the motion of the hole causes the ferromagnetic bond to oscillate between \( J_z \) and \( J_z/2 \).

Therefore, the total magnetic energy cost of the hole denoted by \( E_j \) for \( N_h \) hops is obtained by summing the magnetic energy contributions arising from (12) and (13)

\[
E_j = J/2(N - 1) + J(N^2 - 2N)
\]

(14)

Hence, the magnetic energy expended per state or the average magnetic energy \( E_j / N_h \) gives

\[
\frac{E_j}{N_h} = \frac{J_z(N^2 - 2N) + J_z/2(N - 1)}{N(N - 1)} = \frac{J_z}{2} \left[ \frac{N - 2}{N - 1} + \frac{1}{N} \right]
\]

(15)

For purely spinon states, magnetic energy expended per state as obtained from (13) is given by

\[
\frac{E_j}{N_h} = \frac{J_z(N - 2)}{N - 1}
\]

(16)

For states with degenerate vacua, we have

\[
\frac{E_j}{N_h} = \frac{J_z}{4} \left( \frac{N - 2}{N^2 - N} \right)
\]

(17)

For states with none degenerate states devoid of spinon, we have

\[
\frac{E_j}{N_h} = \frac{J_z}{4} \left( \frac{1}{N - 1} \right)
\]

(18)

6 Results and Discussions

This section presents and discusses the results arising from sections 4 and 5.
6.1. Numerical Result for Spinon and None Spinon States

In Table 1, the states with degenerate vacua are states that have the same energy as the “strong of zero length”. It cost the hole a magnetic energy of $J_z/2$ to create a degenerate vacua. These state are fewer compare with the none degenerate states. The states with degenerate vacua and some peculiar none spinon and none degenerate states constitute the none spinon states. Each of these states is created by an energy cost $J_z/2$. The spinon states are larger in number, and it cost the hole a magnetic energy of $J_z$ to create a spinon state. This large number of the spinon states enables the hole to maintain a constant energy for a relatively long time before moving to none spinon states and thus changing its energy.

Table 1. Numerical result for spinon, degenerate and none degenerate states.

<table>
<thead>
<tr>
<th>No. of sites</th>
<th>states with degenerate vacua</th>
<th>states with no spinon</th>
<th>states with spinon</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>1</td>
<td>3</td>
<td>8</td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>5</td>
<td>24</td>
</tr>
<tr>
<td>10</td>
<td>4</td>
<td>9</td>
<td>80</td>
</tr>
<tr>
<td>20</td>
<td>9</td>
<td>19</td>
<td>360</td>
</tr>
<tr>
<td>50</td>
<td>24</td>
<td>49</td>
<td>2400</td>
</tr>
<tr>
<td>100</td>
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<td>9800</td>
</tr>
<tr>
<td>200</td>
<td>99</td>
<td>199</td>
<td>39600</td>
</tr>
<tr>
<td>300</td>
<td>149</td>
<td>299</td>
<td>89400</td>
</tr>
<tr>
<td>400</td>
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<td>399</td>
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<td>638400</td>
</tr>
<tr>
<td>1000</td>
<td>499</td>
<td>999</td>
<td>998000</td>
</tr>
</tbody>
</table>

6.2. Magnetic energy cost per state as function of number of sites

The dependence of magnetic energy cost per state $E_N / N$ for spinon and none spinon states is shown in Figs.4-7 for $J_z = 0.1$. For small systems, as shown in Fig. 4, this dependence is obvious, but is immediately broken for large systems (thermodynamic limit). The same behaviour is observed for purely spinon states as shown in Fig. 5, except that the energy expended by the hole before stabilizing is higher. In Figs. 6-7, the energy expended by the hole decreases for small system and stabilizes for larger systems. This is expected because for very small systems, states with degenerate vacua and states devoid of spinon are very few as observed from Table 1. Hence, the magnetic energy expended per state shows a remarkable increase for small systems before attaining stability at large N. For comparison, the result obtained in ref [12] from the exact diagonalization of finite systems is shown in Fig. 8. As observed from Fig. 8, agreement between the current analytical and exact studies of ref [12] is made at large distances or large N (corresponding to the thermodynamic or bulk limit) when the energy of a hole become stable.
Fig. 4. Magnetic energy of hole as a function of the number of sites for states with spinon and none spinon states

Fig. 5. Magnetic energy of hole as a function of the number of sites for states with a spinon
Fig. 6. Magnetic energy of a hole as a function of the number of sites for none degenerate states devoid of spinon

Fig. 7. Magnetic energy of hole as a function of the number of sites for degenerate states
7. CONCLUSION

In this research work, it is shown that a spinon created as a result of the motion of a hole in finite one dimensional Ising antiferromagnetic chain is not static, but only N-1 times slower than the hole, where N is the number of site. Hence, the hole can be said to be weakly coupled to the ferromagnetic bond. For small N, this weak coupling tends to create a confining potential (a kind of string potential) along the path of the hole, pulling it to its birth site. However, in the thermodynamic (large N) limit, the hole can break away from this linear “string potential” and propagates as a free particle in agreement with experimental result in ref [10] and theoretical result by Sorella and Parola [14]. This fact can also be verified from the result obtained from magnetic energy per state (E/Nh) expended by the hole. It is observed that (E/Nh) increases steadily with N. For larger N, this increment becomes infinitesimally small. This behaviour shows that at large distances corresponding to large N, the hole become separated from the spinon and hence escape from the confining potential, propagating as a free particle in agreement with spin-charge separation expected in 1D [8,9,10,14,17,18].

REFERENCES


