Spontaneous quantum walk reversal of bosonic Mott insulator defects

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(Dated: January 24, 2020)

Quantum walks of interacting particles may display non-trivial features due to the interplay between the statistical nature and the many-body interactions associated to them. We analyze the quantum walk of interacting defects on top of an uniform bosonic Mott insulator at unit filling in an one dimensional graph. While the quantum walk of single particle defect shows trivial features, the case of two particles exhibits interesting phenomenon of quantum walk reversal as a function of additional onsite three-body attractive interactions. In the absence of the three-body interaction a quantum walk of pairs of particles is obtained and as the strength of the three-body interaction becomes more and more attractive, the independent particle behavior in quantum walk appears. Interestingly, further increase in the three-body interaction leads to the re-appearance of the quantum walk associated to a pair of particles. This quantum-walk reversal or re-entrant phenomenon is studied using the real-space density evolution, Bloch oscillation as well as two-particle correlation functions.

Introduction: Dynamical systems often exhibit exotic physical phenomena due to the quantum nature of the particles. Understanding such phenomena in complex systems has been a topic of great interest both from theoretical and experimental point of view. Quantum walk(QW) is one of such phenomena which is the quantum analogue of the classical random walk has attracted enormous attention in recent years due to its relevance to physical and biophysical applications [1]. The underlying physics arising from the wave-function overlap enables quantum mechanical particle to access various paths to optimize the motion on a graph showing a linear propagation of correlation limited by the Lieb-Robinson bound [2]. This very idea of optimization is considered to be the key to develop efficient quantum algorithms. In the last decade, the quantum walks have been observed in various systems such as trapped ions, neutral atoms, photons in photonic and waveguides, biological systems etc [3–10] in the single particle level. Considerable efforts have been made to understand the effect of interactions on the QW of more than one indistinguishable particles in various systems such as quantum gases in optical lattice [11], correlated photon pairs [12,13] and superconducting qubits [14,15]. In the interacting systems, the combined effect of quantum correlation and interaction may yield novel scenarios in the phenomenon of quantum walks as a result of the Hanbury-Brown and Twiss(HBT) interference and Bloch oscillation [11] [12,16,23].

In recent years, remarkable progress has been made in the experimental front in various systems to understand the quantum many-body effects of interacting particles. The ease of controlling the system parameters has paved the path to understand several complex phenomena in nature. One of such systems is the famous Bose-Hubbard model which deals with the dynamics of bosons in periodic potentials [24]. Despite its simplicity, it has been shown to exhibit various fundamental properties such as the famous phase transition from a superfluid(SF) phase where the bosons are completely delocalized over the entire lattice to a localized Mott insulator(MI) phase [25]. The experimental observation of this SF-MI transition [26] in optical lattices with ultracold bosons has opened up a new avenue to explore numerous novel scenarios based on different variants of the Bose-Hubbard model in terms of higher order local interactions [27–29], long range interactions [30–33], artificial magnetism [34–36], cavity QED [37,38], non-equilibrium phenomena [39] etc. Recently, it has been shown that the multi-particle QW in interacting systems like the Bose-Hubbard model can be utilized for quantum computation [40,41].

In this paper we investigate the continuous time QW of two interacting defects located initially at the same site on top of an perfect one dimensional Mott insulator at unit filling as shown in the top panel of Fig. 1. Motivated by the recent experimental progress in various systems such as cold atoms and circuit QED setups, we try to uncover the physics due to the enhancement of quantum effects in an interacting multi-particle system. Moreover, we consider an additional on-site three-body interaction which may allow access to novel dynamical quantum phen-
nominal. The model which describes this system under consideration is the modified Bose-Hubbard model which is given by:

\[ \mathcal{H} = -J \sum_{\langle i,j \rangle} (a_i^\dagger a_j + H.c.) + \frac{U}{2} \sum_i n_i(n_i - 1) + \frac{W}{6} \sum_i n_i(n_i - 1)(n_i - 2) \]

where \( a_i^\dagger \) (\( a_i \)) is the creation(annihilation) operator and \( n_i = a_i^\dagger a_i \) is the number operator at \( i \)th site. Here, \( J \) is the hopping matrix element and \( U(W) \) is the two(three)-body onsite interaction energy. In the following, we discuss the QW of the MI defects in the presence of attractive three-body interaction \( W \).

This scenario considered here is completely different from the quantum-walk of interacting bosons already discussed in the literature. The very difference is that the quantum walkers interact with themselves as well as with the background bosons of the MI state. Although the interactions experienced from the background bosons in the MI state are uniform throughout the lattice, we will show that this background plays an important role in revealing interesting physics. Before going to the details in the following section we briefly mention our important findings here. We show that for fixed values of \( U \), increase in \( W \) results in the phenomenon of QW reversal as depicted in Fig. 2(a-c). To be more specific, we find that initially the defects pair up and perform QW when \( W \) is vanishingly small. As the value of \( W \) increases, the pair tends to dissociate into mobile defects and the system exhibits independent particle QW. Further increase in \( W \) results in an interesting phenomena of re-entrant QW of the defect pairs which will be discussed in detail in the following.

Our starting point is a perfect MI state at unit filling with two defects created at the central site in an one dimensional periodic potential i.e. \( |\Psi(0)\rangle = (a_0^\dagger)^2|\text{MI}_1\rangle = \ldots |1 1 3 \rangle \ldots \). The MI state is a result of large onsite repulsion \( U \) compared to the hopping amplitude \( J \). Note that in the process of quantum-walk there is a ballistic expansion of the particle wave function i.e. the probability of finding the particle at a specific distance from the starting point grows proportional to the diffusion time \( t \).

In contrast, for the classical case the probability grows diffusively as \( \sqrt{t} \). Our focus is to understand the signatures of the QW from the particle density propagation which is defined as the expectation value \( n_i(t) = \langle a_i^\dagger a_i \rangle \) with the time evolved state \( |\Psi(t)\rangle \) and the two particle correlation function \( \Gamma_{ij} = \langle a_i^\dagger a_j^\dagger a_j a_i \rangle \) at fixed time which are accessible in recent experiments. Due to the large number of particles involved in the system, exact solution of the Schrödinger equation with the Bose-Hubbard model is difficult. Hence, the dynamical evolution of the initial state is done by using the Time-Evolving Block Decimation(TEBD) method using the Matrix Product States(MPS) \cite{55} with maximum bond-dimension of 500.

This method is well suited for one-dimensional systems with local interactions \cite{54}. In our calculation we scale all the physical quantities by setting \( J = 0.2 \).

Before addressing the QW of a pair of defects we will show the QW of a single defect for completeness. The initial state in this case is \( |\Psi(0)\rangle = a_0^\dagger |\text{MI}_1\rangle = \ldots |1 1 2 1 1 \ldots \rangle \). A single particle on top of an MI background will experience an uniform interaction and hence the system is identical to the QW of single particle in an empty lattice. Hence, one expect a typical ballistic expansion of \( \langle n_i \rangle \) over the time \( t \) during the process of evolution as shown in Fig. 2(a). We also compute the propagation of single defect entanglement entropy \( S = \text{Tr}(\rho \log \rho) \) which shows a light-cone like spread of the information as depicted in Fig. 2(b), where \( \rho \) is the reduced density matrix.

**Quantum walk of two interacting defects:** In this section we discuss the QW of two interacting defects in detail. As mentioned before we start from the initial state with two defects on top of a perfect Mott insulator. Then we analyze the time evolution with \( J = 0.2 \) and \( U = 10 \) which makes the ratio \( U/J = 50 \). With this ratio the two-particle repulsion between the bosons are very strong. We study the QW of such a system by systematically varying the three-body attraction \( W \) from vanishingly small to a very large value compared to \( U \) which is shown in Fig. 2(a-g). It can be seen that for \( W = -0.5U \), the density evolution shows a slow propagation of the quantum walker although it is ballistic in nature. This indicates the QW of a massive composite particle in contrast to the independent particle QW. At this point by switching on three-body interaction, the density distribution gradually spreads and moves towards the boundaries of the lattice at a faster rate. At some intermediate values of \( W \) around \( W < -U \), two different cones appear in the QW. In this regime of interaction, the signatures of light and heavy particle QW are visible. Exactly at \( W = -U \), the system exhibits a QW similar to that of the non-interacting particles(compare with Fig. 2).

Interestingly, further increase in \( W \) after

\[ \text{FIG. 2: (Color online)(a) Time evolution of } \langle n_i \rangle \text{ of a single defect with } J = 0.2 \text{ and } U = 10 \text{ on an MI background of length } L = 29 \text{ sites. (b) Propagation of entanglement entropy } S \text{ shows the linear spread of information.} \]
$W = -U$ slowly traces back to the original scenario (i.e. $W = -0.5U$) where we see the feature similar to the QW of a massive particle. In other words the change in $W$ in one direction introduces a re-entrant QW phenomena in the system.

At this state it is difficult to ascertain about the different situations shown in Fig. 3(a-g). So, in order to understand the nature of these two extreme situations we exploit the physics of the Bloch oscillation which is the periodic breathing motion of particle in position space. This is an interesting manifestation of particle motion in a periodic potential subjected to an external force [23]. This external force can be incorporated in model (1) as a constant tilt or gradient of the form $H_{\text{tilt}} = \lambda \sum_i n_i$. Under the influence of this tilt potential, the particle undergoes a Bloch oscillation with period $\tau = 2\pi/\lambda$. We solve the model(1) with this additional term $H_{\text{tilt}}$ and study the density evolution for various values of $W$ as considered in Fig. 3(a-g) with a tilt of $\lambda = 0.02 \times 2\pi$. Interestingly, we see distinctly different features in the Bloch oscillations and a reversal phenomena as shown in Fig. 3(h-n). It is interesting to note that for small and large values of $W$ the time period of oscillation are half that of the one at $W = -U$ (which corresponds to a independent particle type evolution). Note that the frequency doubling in this case is a typical signature of the Bloch oscillation of a pair of particles as already discussed in Ref. [11, 55, 56]. For intermediate values of ($W > -U$ and $W < -U$) there exists two types of oscillations with two different time periods. In this regime, it appears that both single and double occupancy state are energetically favorable. From this signature it is now easy to ascertain that the system exhibits a QW of a bound pair in the beginning when $W = -0.5U$ and gradually the pair tends to dissociate and the defects perform QW independently at $W \sim -U$. Counter intuitively, for larger values of $W$ the QW of pair reappears showing a reversal of QW phenomena as a function of $W$.

From the above analysis it is evident that the quantum walker is a pair of defects for small and large values of $W$ compared to $U$. The pair which appears for $W = 0$ can be thought of as a repulsively bound pair on top of the MI state which is similar to the one observed in the quantum gas experiment by Winkler et al. [57]. In this case the MI phase acts as a uniform background and hence the defect pair experiences uniform repulsions from all the sites. In such a case the velocity of the walker becomes extremely small as can be seen from the Fig. 3 (upper panel). However, when the value of $W$ increases, the effective local interaction reduces gradually due to the attractive nature of $W$. Hence, the repulsively bound pair tends to dissociate into single particles and therefore, we see enhanced group velocity of propagation which corresponds to independent particle QW. However, the mechanism for the QW of pair in the large $W$ regime is completely different from the one for vanishing $W$. In this regime, the pairing of defects is due to the combined effect of the interactions $U$ and $W$. This is altogether a different kind of mechanism to establish repulsively bound pairs which can be understood as follows. When $W$ is very large and attractive compared to the other energy scales of the system then ideally the system prefers to form a trimer (three particle bound state). This trimer may consists of the two defect bosons and one from the MI background. However, because of the uniform repulsion from all the sites due to the MI state the two defects may rather prefer to move freely throughout the system as bound pair [58]. It is to be noted that although the pair formation mechanism for both the cases ($W = 0$ and $\neq 0$) are different, the signatures in the quantum walk are identical in nature.

At this stage, to further substantiate the physics presented above we utilize the two-particle correlator $\Gamma_{i,j}$ defined before which sheds light on the quantum coherence of the two particles. It is well known that if two particles perform QW together, then HBT interference occurs which strongly depends on the statistical nature of the particles. However, in the present case, since the
quantum walkers originate from the same site, the HBT interference are forbidden. We compute $\Gamma_{i,j}$ after an evolution time of $t = 11.25(\text{units of } 1/J)$ for different values of $W$ as shown in the bottom panel of Fig. 4(a-g). We have considered a reduced basis to define the two particle correlator $\Gamma_{ij}$ and number operator $n_i$ where we subtract the contributions from the MI$_2$ background. The mapping between the initial and the reduced on-site basis reads $\{|n\rangle\} \rightarrow \{|n-1\rangle\}$ for $n > 0$. The correlation functions (particle densities) of each plot of Fig. 4 are normalized by their largest respective values so that each plot can share the same scale from 0 to $\Gamma_{\text{max}}$ (or zero to one). One can clearly see that when the ratio $W/U$ is very small the diagonal weights of the correlation matrix are dominant indicating the QW of repulsively bound pair (Fig. 4(a)). Increasing the value of $W/U$ to a very large limit recovers the similar behavior in the correlation matrix corresponding to a QW of bound pair. However, at intermediate regime of the ratio $W/U$, the off-diagonal weights of the correlation matrix start to increase and eventually showing the signature of independent particle QW as shown in Fig. 4(d). In the top panel of Fig. 4 we plot the normalized densities $\langle n_i \rangle$ which shows features complementing the two particle correlation behavior.

**Conclusions:** We analyses the QW of two interacting defects on a perfect MI$_2$ state in the context of the Bose-Hubbard model with both two-body repulsive and three-body attractive interactions. By fixing the onsite two-body interaction at a finite value and varying the three-body interaction from zero to large value we predict the phenomenon of QW reversal. We show that the two defects on top of the MI phase pair up and perform QW for small and large values of $W$. At intermediate strength of $W$, the defects behave like independent walkers in the QW. We rigorously discuss this process in the time evolution of real-space density distribution, Bloch oscillation and also two particle correlation function. This results shows a spontaneous QW reversal process in Mott insulator defects.

The above findings are based on a simple Bose-Hubbard model with two and three-body interactions and one of the immediate platform where one can think of observing this re-entrant phenomena is quantum gas experiment in optical lattices. The simultaneous existence of both two and three-body interactions has been observed in recent experiment in optical lattices [59].

Several theoretical proposals have been made to engineer and tune the three-body interaction in optical lattices [30, 31, 33, 60]. Moreover, recent observation of QW with single-site addressing in interacting ultracold atoms in optical lattices [11] have broadened the scope by many-fold. On the other hand quantum simulations in circuit QED systems have attracted enormous attention in recent years due to the flexibility to design and control strong non-linearities and interactions with microwave radiation and artificial atoms. Very recently, strongly correlated quantum walks with a 12-qubit superconducting circuit has been observed in experiment [15]. In practice two-level artificial atoms are considered in the quantum simulations with circuit QED setups. However, a recent experimental proposal shows that it is possible to control the two and three-body interactions by considering a fluxonium qubit [61] where the first and second excitation levels are of equal energy and the third one can be controlled by detuning it from the first two. This scenario results in a two- and three-body interacting Bose-Hubbard model. In such a scenario the above predicted physics of QW reversal can be observed in the current state-of-the-art experiments based on quantum gases in optical lattice or circuit QED systems. This result also opens up directions to study other interesting quantum mechanical phenomena such as the HBT interference effects [11, 13, 16, 21] in such multi-body interacting quantum walks of defects.

**Acknowledgments**

We thank David Carpentier, Abhishek Dhar and Kanhaiya Pandey for useful discussions. We acknowledge useful suggestions from Daniel Jaschke and Arya Dhar related to the open source OSMPS software. The
computational simulations were carried out using the Param-Ishan HPC facility at Indian Institute of Technology - Guwahati, India. T.M. acknowledges DST-SERB for the early career grant through Project No. ECR/2017/001069.

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