Interaction-induced anomalous transport behavior in one dimensional optical lattice

Zi Cai\textsuperscript{1}, Lei Wang\textsuperscript{1} \textsuperscript{\textcopyright} X. C. Xie\textsuperscript{2,1}, and Yupeng Wang\textsuperscript{1}\textsuperscript{1}

\textit{Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, P. R. China and}

\textit{Department of Physics, Oklahoma State University, Stillwater, Oklahoma 74078, USA}

(Dated: November 18, 2009)

The non-equilibrium dynamics of spin impurity atoms in a strongly interacting one-dimensional (1D) Bose gas under the gravity field is studied. We show that due to the non-equilibrium preparation of the initial state as well as the interaction between the impurity atoms and other bosons, a counterintuitive phenomenon may emerge: the impurity atoms could propagate upwards automatically in the gravity field. The effects of the strength of interaction, the gradient of the gravity field, as well as the different configurations of the initial state are investigated by studying the time-dependent evolution of the 1D strongly interacting bosonic system using time-evolving block decimation (TEBD) method. A profound connection between this counterintuitive phenomenon and the repulsive bound pair is also revealed.

PACS numbers: 03.75.Lm, 05.70.Ln, 05.60.Gg, 37.10.Jk

Recently, ultracold atoms in optical lattice have provided a perfect platform for simulating quantum many-body models in condensed matter physics\textsuperscript{11} \textsuperscript{2}. What’s more, the uniqueness of cold atomic system, such as the low dissipation rate as well as long coherence times, has opened exciting possibilities for studying non-equilibrium quantum dynamics of many-body systems. It is known that, due to the energy dissipation between the system and the environment, the properties of the many-body system in solid state physics is mainly determined by its ground state as well as its low-energy excited state. In the ultracold atomic systems, however, the extreme low dissipation rates there guarantees the conservation of the system energy and total particle number in a relatively long time. Therefore, not only the ground state but also the high energy excited state may contribute to the non-equilibrium dynamics of the many-body systems, which may exhibit novel phenomena\textsuperscript{3} \textsuperscript{4} \textsuperscript{5} \textsuperscript{6} \textsuperscript{7} \textsuperscript{8}.

Repulsively bound atom pairs is one of the most interesting and novel phenomena emerging from the non-equilibrium many-body physics in optical lattice\textsuperscript{9} \textsuperscript{10}. It is shown that though repulsive force separates particles in free space, under a periodic potential and in the absence of dissipation, a bound atom pairs could be stabilized by the strongly repulsive interaction due to the conservation of energy. This unconventional phenomenon provides a typical example of non-equilibrium physics determined by the high-energy excited state of the Hamiltonian rather than the ground state, and has no analogue in traditional condensed matter systems due to the rapid dissipation. In this Letter, we provide another example of these exotic non-equilibrium phenomena by studying the propagation of spin impurity atoms through a strongly interacting one-dimensional (1D) Bose gas under an external potential which decreases linearly along a particular direction. The ground state and the quench dynamics of the Bose-Hubbard model under linear external potential have been discussed previously\textsuperscript{11} \textsuperscript{12}. We show that if the initial state is prepared far away from the equilibrium ground state, the spin impurity atoms could propagate towards the direction the external linear potential increases, which means a particle with initial momentum zero moves upwards in a gravity field in our case. This unconventional phenomenon, similar to the repulsive bound atom pairs, is a result of the conservation of the energy. We would also discuss the profound connection between these two non-equilibrium phenomena.

First, we propose the experimental set-up of our non-equilibrium system. It is motivated by a recent experiment\textsuperscript{13}, where the quantum transport of spin impurity atoms through a Tonks-Girardeau gas is studied. The departure point of our experimental set-up is loading the \(^{87}\text{Rb}\) atoms with the hyperfine ground state \(|F = 1, m_F = -1\rangle\) into a 1D optical lattice, which is along z-direction. We assume that the interaction between these \(^{87}\text{Rb}\) atoms is very large and the filling factor is one, thus the ground state of the system is the Mott state\textsuperscript{14}. An additional harmonic magnetic trap is implemented to provide a vertical confinement for the atoms and prevent the atoms escaping from the optical lattice due to the gravity. The harmonic magnetic trap couples with the atoms via the magnetic dipole interaction, therefore the vertical confinement is purely magnetic.

To prepare the initial state, one pumps the Mott ground state into a non-equilibrium state by applying a pulse of radio frequency resonant with the energy gap between the two hyperfine spin states of \(^{87}\text{Rb}\) atom: \(|F = 1, m_F = -1\rangle\) and \(|F = 1, m_F = 0\rangle\) and inducing a transition \(|F = 1, m_F = -1\rangle \rightarrow |F = 1, m_F = 0\rangle\textsuperscript{15}. Below we denote the \(|F = 1, m_F = -1\rangle\) as trap atoms and \(|F = 1, m_F = 0\rangle\) as impurity atom. The spatial width and position of the pulse could be controlled experimentally\textsuperscript{15}. In our case, we constraint the pulse to only induce the transition on one site and produces one impurity, as shown in Fig.1 (general case containing more
interaction strength. We assume the intraspecies on-site interaction strength for $G/t = 0.5\text{,} U/t = 0\text{,} -2$ respectively. Notice the magnetic moment of the impurity atom $|F = 1\text{,} m_F = 0\rangle$ is zero thus it is not confined by the harmonic magnetic trap and experiences an external linear potential produced by gravity. The experimental set-up proposed here is different from that in Ref.[13] in the way that in our case, the bosons are loaded in a 1D optical lattice along the $z$-direction, rather than the Tonks-Girardeau gas loading in a continuous 1D space. Without the constraint of the periodic potential along the $z$-direction, an impurity atom in a gravity field would be accelerated downwards and finally escape from the system, as shown in Ref.[13]. In our case, however, the dynamics of the impurity atom becomes complex and nontrivial due to the optical lattice structure as well as the interaction between the impurity atom and the trap atoms. Without the interaction, the single particle dynamics is known as Bloch oscillation[16], which has been observed in ultracold atomic systems[17] [18].

The Hamiltonian in this system can be described by a 1D two-component Bose-Hubbard model in a linear external potential:

$$H = -t \sum_i (b_i^\dagger b_{i+1} + a_i^\dagger a_{i+1} + \text{h.c}) + U \sum_i n_i^a n_i^b + G \sum_i n_i^a n_i^b$$

(1)

where $a_i (b_i)$ is the annihilation operator for the impurity (trap) atoms. $U_{ab} = U$ is the interspecies on-site interaction strength. We assume the intraspecies on-site interaction $U_{aa}$ and $U_{bb}$ are repulsive much larger than $U_{ab}$, thus the boson could be considered as hard-core for the bosons with same species. $G = mga_0$ is the potential gradient of the gravity, where $m$ is the mass of $^{87}$Rb atom and $a_0$ is the lattice constant of the optical lattice. The energy scale of $G$ could be estimate as $\mu K$, which is in the same order of magnitude of $U$ and $t$. We assume that the energy scale of the gap between the $s$-band and $p$-band is much larger than that of the parameters $(t, U, G)$ in our Hamiltonian.(1), therefore all the atoms are confined within the $s$-band and no interband physics involved. As we analyzed above, only the impurity atoms experience the gravity potential while the trap atoms are still confined by the magnetic trap. The non-equilibrium initial state can be represented as: $| \uparrow \uparrow \cdots \downarrow \cdots \uparrow \rangle$, where $\uparrow (\downarrow)$ denotes the trap (impurity) atoms. The impurity atom is initially localized in the center of the optical lattice, while all the trap atoms are still in the Mott phase. Obviously, this initial state is not a eigenstate of the Hamiltonian.(1) thus it would evolve. The time evolution of the system is controlled by the parameters in Hamiltonian.(1). Below we would study the dynamics of the impurity atom and show how it depends on the parameters $(U/t, G/t)$ in Hamiltonian.(1) using the TEBD method[19]. Total number conservation is used to reduce the computational effort. A straightforward treatment of the two component HCB needs local dimension $d = 4$, to reduce the computational effort, unfold technique is used and thus the local dimension is reduced to $d = 2$. The pay off is that the chain length increases to $2L$ and next-nearest neighbor interactions are introduced. Swap technique[19][20] is used to deal with next-nearest neighbor interaction within TEBD method. Both the unfolded $(d = 2)$ and folded $(d = 4)$ algorithm are implemented and to cross check the results. In this work we deal with

![FIG. 1: (Color online) (a). Experimental setup. The initial state is prepared by applying rf pulse on single site, making boson atom transitions from $|F = 1\text{,} m_F = 1\rangle$ to $|F = 1\text{,} m_F = 0\rangle$ level. Bosonic atom in the latter level experiences gravity potential. (b)-(d). Evolution of density distribution of the spin impurity, for $G/t = 0.5\text{,} U/t = 0\text{,} 2\text{,} -2$ respectively.](image1)

![FIG. 2: (Color online) The COM of the spin impurity for (a). $G/t = 0.5$ with different interaction strengths, the $U/t$ values are indicated at right axis. (b) $U/t = 1$ with different gravity fields, which could be attained by changing the lattice spacing or choosing different type of trapped atoms.](image2)
chain length $L = 33$, and the spin impurity was created at the 17th site. Finite size effect has little effect to the conclusion since the Bloch oscillation physics confines the atom near its original position. In the course of real time evolution we take the truncation dimension $\chi = 80$ and time step $\Delta \tau = 0.05$, the convergence is checked by taking larger $\chi$.

The time evolution of density distribution of the impurity atom is shown in Fig. 1(b)-(d). The dependence of the motion of impurity atom’s center of mass (COM) on the interaction $(U)$ and potential gradient $(G)$ is shown in Fig. 2. If there is no interaction $(U = 0)$, the COM of the impurity atom does not move at all. This phenomenon could be understood from the dynamics of a single particle under a combination of periodic and a linear external potential. The presence of the external potential breaks the translational symmetry, render momentum $k$ not a good quantum number. However, by choosing the temporal gauge (the scalar potential $\phi = 0$), the external potential is taken into account by a time-dependent gauge field $A(t) = Gt$ and the momentum $k$ is replaced by $k - A(t)$. The noninteracting Hamiltonian can be rewritten in the momentum space as: $H(t) = \sum_k \epsilon_k - A(t)a_k^\dagger a_k$, where $k - A(t)$ is good quantum number. Suppose initially the particle locates on the point $x = 0$, the initial state can be represented in the momentum space as: $\langle x = 0 | t = 0 \rangle = \sum_k |k\rangle \left( e^{ikx} = 1 \text{ because } x = 0 \right)$, where $|k\rangle$ is the single particle eigenstate in the momentum space and the sum is over the first Brillouin zone. In the process of time evolution, all the $|k\rangle$ modes experience Bloch oscillation from different initial momentum. The localization of the COM is actually a consequence of the superposition of all the momentum modes $|k\rangle$ in our initial state, the Bloch oscillation in $|k\rangle$ and $|-k\rangle$ modes cancel with each other and the net effect is zero.

The single particle picture does not work when $U \neq 0$, thus we deal with the time evolution by TEBD. If $U > 0$, the COM of the impurity atom would move downwards until it reaches a steady quasi-equilibrium position, while interesting phenomenon emerges for $U < 0$. The COM of the impurity atom would move upwards though it is experiencing a gravity potential. We also find that the dependence of the motion of COM on $U$ is not monotone. Notice in both case of large $U$ and small $U$, the COM is always constrained around the original position. The maximum deviation of the COM away from original point occurs when $U/t = \pm 2$. The dependence of the dynamic of the COM on the gravity gradient $G$ is also nontrivial. We notice that for larger $G$, the COM of the impurity would drop to a higher a final quasi-equilibrium position. The period of the oscillation is approximately the Bloch period $2\pi/G$.

To understand the origin of the counter-intuitive phenomenon, we perform a Jordan-Wigner transformation to map our system into a interacting fermionic system (considering the hard-core nature for the intraspecies boson).

Then we use the particle-hole transformation on the trap atoms, thus the problem could be translated into a two-particle problem due to the half-filling condition in our initial state. The initial configuration in Fig. 1(a) could be considered as two particles (an impurity atom and a trap hole) located on the same site (doublon) of the lattice. Below we mainly focus on the attractive condition $(U < 0)$ in original model, which could be mapped into a two-particle problem with repulsive interaction $(U > 0)$ under the particle-hole transformation. If $\tilde{U} \gg t$, the dynamics of this two-particle problem reminds us of the physics in the the repulsively bound atom pairs [9] [10]. The initial state is a doublon state with a high energy $\tilde{U}$. If the two particles are separated, the loss of the interaction energy $(\tilde{U})$ should be compensated by the increasing of the kinetic energy of the single particle to preserve the total energy of the system. However, in the periodic lattice structure, the kinetic energy of a single particle has a maximal value $(2t)$. Therefore, when $\tilde{U} \gg t$, a doublon would be stabilized by the strong repulsive interaction, fig. 4(c). In our case, interesting thing happens for smaller U, where the gravity field play a key role. It is possible that the loss of the interaction energy could be compensated by the increasing of the gravity potential energy of the impurity atom to preserve the total energy, as shown in fig. 4(b). The energy transfer between the interaction energy and gravity potential energy results in the anomalous dynamics of the impurity atom.

To verify this qualitative picture, we again use TEBD to study the two particle dynamics from the given initial doublon state. The result is shown in Fig. 3. We introduce the variance of the COM of the impurity atom, defined as $Var = \langle \sum_i i^2 n_i^2 \rangle - \langle \sum_i i n_i^2 \rangle^2$, to characterize the
Translate back into spin impurity language, the impurity atom and a trap hole bind together to form an exciton (which is the doublon in the two-particle picture) for both large attractive and repulsive interaction. For the noninteracting case, the exciton dissolves immediately and Bloch oscillation physics dominates. The intermediate interacting strength, the impurity atom will move upwards or downwards depending on the sign of the interaction. The sketch phase diagram is shown in Fig. 4. Notice that there is crossover instead of phase transition between different regions. The general principle guiding the time evolution of the strongly interacting systems is that the system always evolves toward a maximum entropy state with the constraint of the conservation of good quantum numbers (such as energy and total particle number)\[21, 22]\). So the competition between the energy and entropy play a key role in determining the properties in the final quasi-equilibrium steady state.

Finally, we would discuss the dynamic of the impurity atom evolving from two different initial configurations, we focus on the attractive condition to show the dependence of the anomalous phenomenon on the initial configuration we choose. The first case is that the filling factor in the initial state is not one, which means the impurity would propagate in an environment of the quasi-superfluid of the trap atoms. The attractive interaction between the impurity and the BEC atoms leads to a polaron\[23\], and its transport properties have been studied previously\[24\]. We choose the initial state as a quasi-superfluid with 31 hard-core bosons filled in the 1d lattice with 33 sites. We can find that the COM of the impurity atom does not move upwards, different from that in the Mott initial state. This phenomenon can also be understood by the particle-hole transformation on the trap atoms. In this case, the trap hole is not localized in the initial configuration due to the quasi-superfluidity of the trap atoms, which means there is no high-energy doublon initial state. The energy transfer picture is no longer available, thus the anomalous transport phenomenon disappears. Actually, we can always prepare a Mott plateau region in lattice by adding an external harmonic trap potential, even the filling factor is not one, and the “Negative Mass” phenomena will still appear. The other configuration is to apply a pulse of radio frequency on more than one site and produce many impurity atoms in the initial configuration. The initial state is chosen as five impurity atoms (from site 15 to site 19) located in the middle of the lattice while all other site is filled with trap atoms. We can find in this case the COM can still move upwards in the attractive interaction and the main result of this paper is not qualitatively changed by this multi-impurity effect.

ACKNOWLEDGMENT

The work is supported by NSFC, the Knowledge Innovation Project of CAS, the National Program for Basic Research of MOST. XCX is supported by US-DOE and US-NSF. LW thank Xi Dai and Yuan Wan for helpful discussions. We thank X.-M. Cai for bring Ref\[13\] into our attention.
[1] M. Greiner, O. Mandel, T. Esslinger, T. W. Hansch and I. Bloch. Nature. 415, 39 (2002).
[2] R. Jördens, N. Strohmaier, K. Günter, H. Moritz, T. Esslinger. Nature. 445, 204 (2008).
[3] T. Kinoshita, T. Wenger and D. S. Weiss. Nature. 440, 900 (2006).
[4] M. Rigol, Phys. Rev. Lett. 103, 100403 (2009).
[5] S. R. Manmana, S. Wessel, R. M. Noack and A. Muramatsu. Phys. Rev. Lett. 98, 210405 (2007).
[6] E. Altman and A. Auerbach. Phys. Rev. Lett. 89, 250404 (2002).
[7] C. Kollath, A. M. Lauchli and E. Altman. Phys. Rev. Lett. 98, 180601 (2007).
[8] G. M. Bruun, O. F. Syljuasen, K. G. L. Pedersen, B. M. Andersen, E. Demler and A. S. Sorensen, arXiv:0907.0652.
[9] K. Winkler, G. Thalhammer, F. Lang, R. Grimm, J. H. Denschlag, A. J. Daley, A. Kantian, H. P. Büchler and P. Zoller. Nature. 441, 853 (2006).
[10] A. J. Daley, A. Kantian, H. P. Büchler, P. Zoller, K. Winkler, G. Thalhammer, F. Lang, R. Grimm and J. Hecker Denschlag. arXiv:cond-mat/0608721.
[11] S. Sachdev, K. Sengupta, and S. M. Girvin. Phys. Rev. B 66, 075128 (2002).
[12] K. Sengupta, S. Powell, and S. Sachdev. Phys. Rev. A 69, 053616 (2004).
[13] S. Palzer, C. Zipkes, C. Sias, and M. Köhl. Phys. Rev. Lett. 103, 150601 (2009).
[14] T. Stöferle, H. Moritz, C. Schori, M. Köhl, and T. Esslinger. Phys. Rev. Lett. 92, 130403 (2004).
[15] I. Bloch, T.W. Hänsch and T. Esslinger. Phys. Rev. Lett. 82, 3008 (1999).
[16] F. Bloch, Z. Phys. 52, 555 (1929).
[17] M. BenDahan, E. Peik, J. Reichel, Y. Castin and C. Salomon. Phys. Rev. Lett. 76, 4508 (1996).
[18] S.R. Wilkinson, C. F. Bharucha, K.W. Madison, Q. Niu and M. G. Raizen. Phys. Rev. Lett. 76, 4512 (1996).
[19] G. Vidal. Phys. Rev. Lett. 91, 147902 (2003); Phys. Rev. Lett. 93, 040502 (2004); Y.-Y. Shi, L.-M. Duan, and G. Vidal. Phys Rev A 74, 4 (2006).
[20] I. Danshita and P. Naidon. Phys Rev A 79, 1 (2009).
[21] M. Rigol, V. Dunjko, V. Yurovsky, M. Olshanii. Phys. Rev. Lett. 98, 050405 (2007).
[22] M. Cramer, C. M. Dawson, J. Eisert and T. J. Osborne, Phys. Rev. Lett. 100, 030602 (2008).
[23] M. Bruderer, A. Klein, S. R. Clark and D. Jaksch. Phys. Rev. A 76, 011605(R) (2007).
[24] M. Bruderer, A. Klein, S. R. Clark and D. Jaksch. New J. Phys. 10, 033015 (2008).