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Motion of a Distinguishable Impurity in the Bose Gas: Arrested Expansion Without a Lattice and Impurity Snaking

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We consider the real-time dynamics of an initially localized distinguishable impurity injected into the ground state of the Lieb-Liniger model. Focusing on the case where integrability is preserved, we numerically compute the time evolution of the impurity density operator in regimes far from analytically tractable limits. We find that the injected impurity undergoes a stuttering motion as it moves and expands. For an initially stationary impurity, the interaction-driven formation of a quasibound state with a hole in the background gas leads to arrested expansion—a period of quasistationary behavior. When the impurity is injected with a finite center-of-mass momentum, the impurity moves through the background gas in a snaking manner, arising from a quantum Newton’s cradlelike scenario where momentum is exchanged back and forth between the impurity and the background gas.

Introduction.—With recent experimental advances in the field of cold atomic gases, the physics of the one-dimensional Bose gas is receiving an increasing amount of attention [1–15]. These systems, in which one has unprecedented isolation from the environment and fine control of interparticle interactions, are excellent tools for examining novel phenomena arising from strong correlations.

One such phenomenon which has piqued both theoretical [8,14,16–21] and experimental [19,22] curiosity is the expansion dynamics of a gas of cold atoms. A number of surprising and interesting effects have been observed, of which arrested expansion (or self-trapping) [16–18] is particularly relevant to this Letter. A gas (bosons [19] or fermions [23,24]) is released from a confining potential and allowed to expand on the lattice. Under this time evolution, “bimodal” expansion is observed: the sparse outer regions of the cloud rapidly expand while the dense central region spreads only very slowly. This can be partially understood by considering the limit of strong interactions: doubly occupied sites are high-energy configurations which, thanks to the lattice imposing a finite bandwidth and energy conservation, cannot release their energy to the rest of the system and decay [18].

With these recent experimental advances [25] has also come the ability to examine systems in which there is a large imbalance between two species [6,7,9,26–29], a natural starting point for the study of impurity physics. This gives insight into a diverse range of problems [29], including the physics of polaron [27,30] as well as the x-ray edge singularity [31,32] and the orthogonality catastrophe [33]. The physics of impurities also plays an important role in the calculation of edge exponents in dynamical correlation functions [34] and in understanding the nonequilibrium dynamics following a local quantum quench [13,35,36].

The experimental study of the out-of-equilibrium dynamics of a single impurity in the one-dimensional Bose gas has revealed rather rich physics, including how an impurity spreads when accelerated through a Tonks-Girardeau gas [6] as well as how interactions affect oscillations in the size of a trapped out-of-equilibrium impurity [9]. Numerous theoretical investigations have addressed the Tonks-Girardeau regime, from a static point impurity [37,38] to a completely delocalized (e.g., plane wave) impurity [39–44]. Theoretical study of the continuum problem is challenging away from the Tonks-Girardeau limit; results have thus focused on lattice models, such as the Bose-Hubbard model [8,45].

In this Letter we consider the out-of-equilibrium dynamics of an initially localized impurity in the Lieb-Liniger model. Using a combination of exact analytical results and numerical computations, we show that an impurity injected into the ground state of the Lieb-Liniger model undergoes a snatching sequence of rapid movement or expansion followed by arrested expansion. For an initially stationary impurity, this is caused by the interaction-driven out-of-equilibrium formation of a quasibound state of the impurity with a hole in the background gas. This quasibound state is robust under time evolution for long periods of time. For an impurity with a finite initial center of mass (c.m.) momentum, the stuttering sequence results in the impurity “snaking” through the background gas; the impurity exchanges momentum back and forth with the background gas through a quantum Newton’s cradlelike mechanism [3]. The results we present are relevant to experiments (see, e.g., Ref. [6]) and should be observed under reasonable conditions.
The two-component Lieb-Liniger model.—We consider two species of delta function interacting bosons confined to a ring of length $L$. The Hamiltonian of the two-component Lieb-Liniger model (TCLLM) is given by

$$
H = \int_0^L dx \sum_{j=1,2} \frac{\hbar^2}{2m} \frac{d}{dx} \Psi_j^\dagger(x) \frac{d}{dx} \Psi_j(x) + \int_0^L dx \sum_{j=1,2} c \Psi_j^\dagger(x) \tilde{\Psi}_j^\dagger(x) \Psi_j(x) \Psi_j(x),
$$

(1)

where herein we set $\hbar = 2m = 1$, $c$ is the interaction parameter, and the boson operators obey the canonical commutation relations $[\Psi_j(x), \Psi_l^\dagger(y)] = \delta_{jl} \delta(x - y)$ with $j, l = 1, 2$ denoting the species. As in the case of the one-component Lieb-Liniger model [46–48] the generalization to multiple particle species remains integrable provided all species interact identically [49,50].

The TCLLM can be solved by the Bethe ansatz [49,50], giving access to some of its basic physical properties (see, e.g., [51–53] and references therein). An $N$-particle eigenstate containing $N_1$ particles of species 1 is characterized by a set of $N$ momenta $\{q_j\}_N = \{q_1, \ldots, q_N\}$ and a set of $N_1$ species rapidities $\{\lambda_j\}_{N_1} = \{\lambda_1, \ldots, \lambda_{N_1}\}$. These momenta and rapidities satisfy the nested Bethe ansatz equations

$$
e^{iq_jL} = -\prod_{l=1}^N \left( q_j - q_l + ic \right) \prod_{l=1}^{N_1} \left( q_j - \lambda_l - ic \right),$$

(2)

$$\prod_{i=1}^N \frac{\lambda_k - q_i - ic}{\lambda_k - q_i + ic} = -\prod_{i=1}^{N_1} \frac{\lambda_k - \lambda_i + ic}{\lambda_k - \lambda_i - ic},$$

(3)

where $j = 1, \ldots, N$ and $k = 1, \ldots, N_1$. The eigenstate $|\{q\}_N;\{\lambda\}_{N_1}\rangle$ has energy $E_q = \sum_j q_j^2$ and momentum $K_q = \sum_j q_j$.

The initial state.—We study the dynamics of an impurity starting from the state

$$|\Psi(Q)\rangle = \frac{1}{N} \int_0^L dx e^{iQx} e^{-(1/2)(x-x_0)/(\alpha_0)^2} \Psi_1^\dagger(x) |\Omega\rangle,$$

(4)

where $|\Omega\rangle$ is the $N_2 = N - 1$ particle ground state of the one-component Lieb-Liniger model, $Q$ is the c.m. momentum of the impurity, and $N_1$ normalizes the state. The study of such a state is partially motivated by the experiments performed in Refs. [6,9], which study the dynamics of an impurity in a background gas.

The initially localized impurity of Ref. [6] is prepared by illuminating a trapped one-component Bose gas with a radio-frequency pulse; this causes transitions between the $|F, m_F\rangle = |1, -1\rangle$ hyperfine state of the trapped gas and the $|1, 0\rangle$ state (the impurity). Because of the magnetic trap, transitions occur only within a spatially localized region, the thinness of which is Fourier limited by the pulse duration. The resulting impurity contains up to three particles and is accelerated through the gas by gravity, as the $|1, 0\rangle$ state does not experience the magnetic trap.

On the other hand, the impurity in Ref. [9] is prepared by first tuning the interspecies interaction to zero and then using a species-dependent trap and light blade to shape the impurity. Following this preparation, the interspecies interaction is turned on, the impurity is released from the trap and light blade, and its expansion is studied.

To distill the intrinsic dynamics of the impurity, our scenario varies slightly from experiments [6,9]: we study an impurity injected into a constant-density background gas in the absence of an external potential (such as a magnetic trap and gravity). Similar approximations have been applied in the well-studied yrast states [54–58].

Time evolution protocol.—Our aim is to compute the impurity density profile when the initial state (4) is time evolved according to the Hamiltonian (1) $\rho_1(x, t) = \langle \Psi(Q)|e^{iHt}\Psi_1^\dagger(x)\Psi_1(x)e^{-iHt}|\Psi(Q)\rangle$. This is a nontrivial problem as the initial state (4) is not an eigenstate of the Hamiltonian. We use the integrability of the TCLLM to numerically evaluate the density profile using recently derived results for matrix elements of local operators [53]. Because of a dearth of results for matrix elements in the TCLLM, we are restricted to studying the density of the impurity and we cannot examine the background gas [59].

The essential idea is the following: we insert complete sets of eigenstates between each time evolution operator and the initial state in $\rho_1(x, t)$. By orthogonality, we sum over the Bethe states with $N_1 = 1$ and $N_1 + N_2 = N$. The momenta and rapidities characterizing these states satisfy the nested Bethe ansatz equations (2), (3). The density profile of the impurity will then be given by

$$\rho_1(x, t) = \sum_{|\{q\}_N;\{\lambda\}_{N_1}\rangle} \langle \Psi(Q)|\{p\};\{\lambda\} \langle \{p\};\{\lambda\} |\Psi_1^\dagger(0)\Psi_1(0)|\{k\};\mu\rangle \times \langle \{k\};\mu|\Psi(Q)\rangle e^{i(E_k^0 - E_0k)l} e^{i(K_k - K_0)x},$$

(5)

where $\{q\} \equiv \{q\}_N$. The overlap of the initial state with a Bethe state can be expressed as $\mathcal{N}(\{k\};\mu|\Psi(Q)\rangle = \int_0^L dx e^{iQx} e^{-(1/2)(x-x_0)/(\alpha_0)^2} \langle \{k\};\mu|\Psi_1^\dagger(0)\Psi_1(0)|\Omega\rangle$, where $K_0$ is the momentum of the ground state $|\Omega\rangle$. So, in order to compute (5) we require two ingredients: the matrix elements of the creation operator $\Psi_1^\dagger(0)$ and the density operator $\Psi_1^\dagger(0)\Psi_1(0)$ on the Bethe states. These matrix elements have been derived from the algebraic Bethe ansatz [53,60]. Required results are summarized in the Supplemental Material [61].

Readers interested in our scheme for numerically evaluating the expansion (5) can consult Ref. [69]. An important point to note is that the expansion (5) contains an infinite number of terms. We truncate the Hilbert space by selecting the Bethe states which have the largest overlap with the
initial state (4). To quantify the truncation error, we compute the saturation of the sum rule

$$\sum_{\{k\}_{N,\mu}} |\langle \Psi(Q) | \{k\}_{N,\mu} \rangle|^2 = 1,$$

and we present numerical values for this with our results. We are limited to small numbers of particles $N \lesssim 10$ and we have to keep $\sim 10^4$--$10^5$ states to saturate the sum rule to 2 decimal places.

The noninteracting limit.—In the noninteracting limit, the time evolution of the initial state (4) is a single particle problem. The time-dependent density profile can be calculated exactly (we take $L \to \infty$ as $\rho_i(x, t)_{t=0} = (a_0/\sqrt{\pi}) \exp[-a_0^2(x + 2Q t)^2/(a_0^4 + r^4)]/\sqrt{a_0^4 + r^4}$. The noninteracting density profile remains Gaussian at all times, with a time-dependent width and amplitude.

Arrested expansion: $Q = 0$.—In Fig. 1 we present results for the time evolution of the impurity density profile (5) for $N = 8$ bosons on the circumference $L = 40$ ring starting from the initial state (4) with $x_0 = L/2$, $a_0^2 = 1.125$, and interaction parameter $c = 10$. We measure time in units of $t_F = 1/E_F$, where $E_F = (\pi N/L)^2$ is the Fermi energy in the $c \to \infty$ limit. The Hilbert space is truncated to 25 150 states, leading to a sum rule saturation of 0.9858 (i.e., to 1.4%). Upon time evolution the wave packet spreads, maintaining its Gaussian shape as in the noninteracting case. However, at time $t \sim 2t_F$ the wave packet stops spreading and only undergoes small-amplitude breathing oscillations. This arrested expansion is an example of prethermalization [70–77]. The system relaxes in a two-step process, first approaching a quasistationary nonequilibrium state (the arrested expansion) before the subsequent equilibration. Two-step relaxation has been observed in the one-dimensional Bose gas following a global quantum quench [78–80].

We can qualitatively reproduce aspects of this behavior with a mean field (MF) decoupling of the interaction term

$$\Psi_j(x) \Psi_j^\dagger(x) \Psi_j(x) \Psi_j^\dagger(x) \approx \rho_j(x, t) \Psi_j^\dagger(x) \Psi_j(x) + j \leftrightarrow l.$$ (7)

At a MF level the impurity profile is a time-dependent repulsive one-body potential for the background gas. The region under the impurity then excludes particles in the background gas, resulting in the formation of a “hole.” This hole in the background gas acts as a confining (attractive) one-body potential for the impurity in the MF and the two form a quasibound particle-hole pair [81], much like an exciton in the electron gas (see, e.g., Ref. [82]). This is different to the self-trapping scenario on the lattice—there, the “doublons” are stable as the large interaction energy cannot be converted into kinetic energy due to particle number conservation and the finite bandwidth. In the continuum, dynamical arrest is driven by the formation of the impurity-hole quasibound state and is not observed for an indistinguishable impurity [61].

At later times ($t \gtrsim 7t_F$), the impurity eventually broadens. This broadening occurs in a sequence of steps of expansion or arrested expansion, while the impurity undergoes small-amplitude breathing oscillations [61]. The slow decay of the density at later times may be related to the subdiffusive equilibrium behavior reported in Ref. [35]. However, finite-size effects and our choice of observables obscure the characteristic logarithmic decay of subdiffusion.

The snaking impurity: $Q \neq 0$.—Finally, we consider the time evolution of the initial state (4) with nonzero c.m. momentum $Q$. Our prescription for computing the time evolution is identical to the $Q = 0$ case; in Fig. 2 we present results for the impurity density profile for the same set of parameters as in Fig. 1 with $Q = \pi$. We see rather surprising behavior: the impurity moves in a snaking

FIG. 1. Time evolution of the impurity density of the initial state (4) with $Q = 0$, $x_0 = L/2$, and $a_0^2 = 1.125$ on the $L = 40$ ring for a system of $N = 8$ particles with interaction parameter $c = 10$. The Hilbert space is truncated to 25 150 states, leading to the sum rule (6) equaling 0.9858. Inset: Time evolution of the maximum of the density $\rho_i(x, t)$. Constant time cuts can be found in the Supplemental Material [61].

FIG. 2. The dynamics of the impurity density (5) from the initial state (4) with $a_0^2 = 1.125$ and $Q = 40\pi/L$. We use 21 507 states to study a system of $N = 8$ bosons on the length $L = 40$ ring with interaction parameter $c = 10$, resulting in the sum rule (6) equaling 0.981. Plots of constant time cuts are presented in the Supplemental Material [61].
momentum and the process repeats. In support of this
more with the impurity. (iv) The impurity gains c.m.
particles in the background gas and creating excitations
Fig. 2: (i) The impurity moves to the left, scattering
interactions with the background gas[83].

We have the following picture for the behavior shown in
a number of interaction strengths: $X(t)$ shows regions of
rapid movement, followed by (approximately) stationary
plateaus. Only at $t \lesssim t_F/3$ does the c.m. move as in the
noninteracting case, $X(t)_{c=0} = X(0) - 2Qt$. The sharpness
of the plateaus and transient regions are governed by the
interplay between the delocalization of the impurity and its
interactions with the background gas [83].

We have the following picture for the behavior shown in
Fig. 2: (i) The impurity moves to the left, scattering
particles in the background gas and creating excitations
with finite momentum. (ii) The impurity continues to
scatter with the background until it imparts most (or all)
of its c.m. momentum. (iii) The excitations in the back-
ground gas propagate around the ring and then collide once
more with the impurity. (iv) The impurity gains c.m.
momentum and the process repeats. In support of this
picture is the behavior of the c.m. position plateau with
system size $L$: the time for leaving the plateau $\tau_p$ is
(approximately) linearly dependent on $L$. $\tau_p$ is also related
to the initial momentum $Q$ of the impurity; for large $Q$,
$\tau_p \sim 1/Q$ (an excitation with momentum $Q$ has velocity
$\sim Q/m$). This $Q$ dependence reflects the momentum
impacted by the impurity to excitations in the background
gas, which then propagate around the ring [84].

In contrast, when the impurity is injected with a finite
c.m. momentum, the quantum stutter is clearly seen in the
motion of the impurity, which snakes through the back-
ground gas (see Figs. 2 and 3). We can picture this as a
quantum Newton’s cradle [3] on the ring: the injected
impurity scatters particles in the background gas until it

FIG. 3. The time evolution of the center of mass $X(t)$ [Eq. (8)]
for the initial state (4) with $a_0^2 = 1.255$, $Q = \pi$ for $N = 8$
particles on the length $L = 40$ ring with interaction parameter
c = 5, 10, 20 (points), and a noninteracting point particle with
mass $m = 1/2$ and velocity $Q/m$ (line). Inset: velocity of the
center of mass $V(t) = \Delta X(t)/\Delta t$ (cf. Ref. [39]).
loses most of its c.m. momentum. These scattered excitations then propagate around the ring and subsequently collide with the impurity, causing it to move once again. This process repeats, leading to the stuttering, snaking motion of the c.m. Quantum flutter, the exchange of momentum back and forth between a delocalized impurity and the background gas, has been studied in the Tonks-Girardeau regime \cite{39-44}. The momentum of the impurity in the long-time limit was computed by means of the DE and found to be small, but nonzero.

Our results are of direct relevance to experiments in cold atomic gases; the observed physics should not be reliant upon the integrability of the model (see, e.g., Refs. \cite{40} and \cite{61}) and should survive finite temperature \cite{87}. The results discussed here may also be useful in elucidating the properties of the TCLLM at finite temperature, where it is likely that impuritylike solitons arise \cite{88,89}. Finally, this Letter provides a nontrivial check and validation of cutting-edge theoretical results for the matrix elements of the TCLLM in the extreme imbalance limit \cite{53,60}.

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\begin{thebibliography}{99}


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Recently, new results for matrix elements in the TCLLM were obtained [60]. We hope to incorporate these results in future works and note that these new expressions remove our limitation of only studying the impurity density.

See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.116.145302, which includes Refs. [48,53,60,62–68], for (i) a summary of the matrix elements required in our computations; (ii) a description of the dynamics of an indistinguishable impurity in the one-component Lieb-Liniger model; (iii) a study of the lattice mean field description of the problem; (iv) additional data including constant time cuts and longer times; (v) supporting evidence for the “quantum Newton’s cradle on the ring” scenario; (vi) a study of the interaction-dependence of the center of mass motion; (vii) further details of our diagonal ensemble computations.

See [61] for data showing that the length of time for which the c.m. coordinate is approximately stationary is determined by the total system size $Q$ and the momentum $Q$ of the impurity.

For further details on our computations in the diagonal ensemble, see [61].

We show results in this case in [61].

In [61] we show that for weak interactions the impurity has almost completely delocalized by the second plateau, leading to a flat and stationary c.m. On the other hand, with strong interactions the spreading of the impurity is hindered, and on the second plateau the impurity is still well localized. Slight spreading of the (almost) stationary impurity leads to the drifting of the c.m. observed in Fig. 3.

See [61] for a mean-field analysis in a discretized model which shows this picture captures the correct physics.

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See [61] for data showing that the length of time for which the c.m. coordinate is approximately stationary is determined by the total system size $L$ and the momentum $Q$ of the impurity.

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