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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.

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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 polarons [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 stuttering 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

$$H = \int_0^L dx \sum_{j=1,2} \frac{\hbar^2}{2m} \partial_x \Psi_j^\dagger(x) \partial_x \Psi_j(x) + \int_0^L dx \sum_{j,l=1,2} c \Psi_j^\dagger(x) \Psi_l^\dagger(x) \Psi_l(x) \Psi_j(x), \quad (1)$$

where herein we set $\hbar = 2m = 1$, c is the interaction parameter, and the boson operators obey the canonical commutation relations $[\Psi_j(x), \Psi_l^\dagger(y)] = \delta_{j,l}\delta(x-y)$ 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 $\{q\}_N = \{q_1, \ldots, q_N\}$ and a set of N_1 species rapidities $\{\lambda\}_{N_1} = \{\lambda_1, \ldots, \lambda_{N_1}\}$. These momenta and rapidities satisfy the nested Bethe ansatz equations

$$e^{iq_jL} = -\prod_{l=1}^{N} \frac{q_j - q_l + ic}{q_j - q_l - ic} \prod_{m=1}^{N_1} \frac{q_j - \lambda_m - \frac{ic}{2}}{q_j - \lambda_m + \frac{ic}{2}}, \quad (2)$$

$$\prod_{l=1}^{N} \frac{\lambda_k - q_l - \frac{ic}{2}}{\lambda_k - q_l + \frac{ic}{2}} = -\prod_{l=1}^{N_1} \frac{\lambda_k - \lambda_l - ic}{\lambda_k - \lambda_l + ic}, \quad (3)$$

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

$$|\Psi(Q)\rangle = \frac{1}{\mathcal{N}} \int_0^L dx e^{iQx} e^{-(1/2)[(x-x_0)/(a_0)]^2} \Psi_1^\dagger(x) |\Omega\rangle, \quad (4)$$

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 $\mathcal{N}$ 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

$$\rho_1(x,t) = \sum_{\substack{\{k\};\mu \\ \{p\};\lambda}} \langle \Psi(Q)|\{p\};\lambda\rangle \langle \{p\};\lambda| \Psi_1^\dagger(0) \Psi_1(0) |\{k\};\mu\rangle \times \langle \{k\};\mu|\Psi(Q)\rangle e^{i(E_p - E_k)t} e^{i(K_p - K_k)x}, \quad (5)$$

where $\{q\} \equiv \{q\}_N$. The overlap of the initial state with a Bethe state can be expressed as $\mathcal{N}\langle\{k\};\mu|\Psi(Q)\rangle = \int_0^L dx e^{i(Q+K_k-K_\Omega)x} e^{-(1/2)[(x-x_0)/(a_0)]^2} \langle\{k\};\mu|\Psi_1^\dagger(0)|\Omega\rangle$, where K_Ω 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

$$\sum_{\{k\}_N;\mu} |\langle\Psi(Q)|\{k\}_N;\mu\rangle|^2 = 1, \tag{6}$$

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 $\rho_1(x,t)_{c=0} = (a_0/\sqrt{\pi}) \exp[-a_0^2(x+2Qt)^2/(a_0^4+t^2)]/\sqrt{a_0^4+t^2}$. 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

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

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

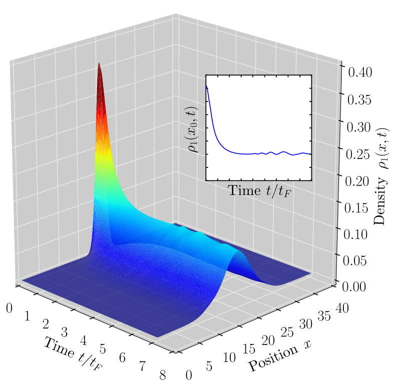

FIG. 1. Time evolution of the impurity density of the initial state (4) with $Q = 0$, $x_0 = L/2$, and $a_0^2 = 1.125$ on the $L = 40$ ring for a system of $N = 8$ particles with interaction parameter $c = 10$. The Hilbert space is truncated to 25 150 states, leading to the sum rule (6) equaling 0.9858. Inset: Time evolution of the maximum of the density $\rho_1(x_0,t)$. Constant time cuts can be found in the Supplemental Material [61].

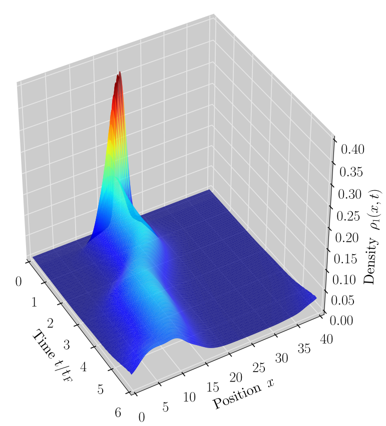

FIG. 2. The dynamics of the impurity density (5) from the initial state (4) with $a_0^2 = 1.125$ and $Q = 40\pi/L$. We use 21 507 states to study a system of $N = 8$ bosons on the length $L = 40$ ring with interaction parameter $c = 10$, resulting in the sum rule (6) equaling 0.981. Plots of constant time cuts are presented in the Supplemental Material [61].

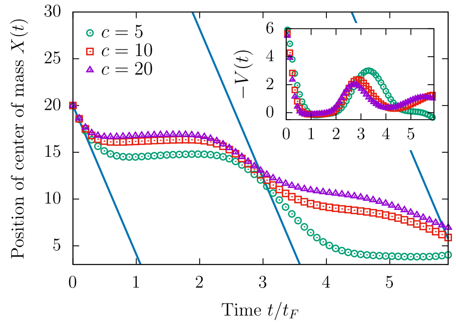

FIG. 3. The time evolution of the center of mass $X(t)$ [Eq. (8)] for the initial state (4) with $a_0^2 = 1.125$, $Q = \pi$ for $N = 8$ particles on the length $L = 40$ ring with interaction parameter $c = 5$, 10, 20 (points), and a noninteracting point particle with mass $m = 1/2$ and velocity Q/m (line). Inset: velocity of the center of mass $V(t) = \Delta X(t)/\Delta t$ (cf. Ref. [39]).

manner, repeatedly moving and expanding before becoming approximately stationary with arrested expansion. To quantify the nonuniform motion of the impurity further, we define the c.m. coordinate $X(t)$ as

$$X(t) = \frac{L}{2\pi} \arctan\left[\frac{\int_0^{2\pi} \mathrm{d}\theta \sin\theta \rho_1(\theta, t)}{\int_0^{2\pi} \mathrm{d}\theta \cos\theta \rho_1(\theta, t)}\right], \tag{8}$$

where $\theta = 2\pi x/L$. We plot the c.m. coordinate in Fig. 3 for 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 background 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 τ_p is (approximately) linearly dependent on L. τ_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 imparted by the impurity to excitations in the background gas, which then propagate around the ring [84]. This process can be thought of in terms of a quantum Newton's cradle [3] on a ring, with the impurity exchanging momentum back and forth with the background gas, resulting in the snaking motion shown in Fig. 2. In the Supplemental Material we show that this behavior is not realized on the lattice when we perform the MF decoupling (7) for the same set of parameters that capture some aspects of the $Q = 0$ behavior [61].

It is interesting to consider removing periodic boundary conditions: excitations produced by injecting the impurity will propagate towards the boundary and subsequently reflect, returning to once again scatter the impurity. This reflection of the excitations means that we expect the c.m. to snake back and forth about x_0 rather than around the ring. In the presence of a harmonic trap, the c.m. will travel in a snaking motion due to both the trap and collisions with the background excitations.

A question that has recently attracted attention is whether an injected impurity has finite momentum in the $t \to \infty$ limit (see, e.g., Refs. [39–44]). To address this, we compute the momentum of the impurity in the diagonal ensemble (DE) [85] $K_{\mathrm{DE}} = \sum_{\{k\};\mu} \langle \Psi(Q) | \{k\};\mu \rangle \langle \{k\};\mu | \Psi(Q) \rangle \times \sum_p \langle \{k\};\mu | p \Psi_{1,p}^\dagger \Psi_{1,p} | \{k\};\mu \rangle$, where $\Psi_{1,p} = 1/L \int dx e^{-ipx} \times \Psi_1(x)$. Doing so, we find $K_{\mathrm{DE}} \approx -0.022$ (for $N = 4$ particles on the length $L = 40$ ring), in keeping with general expectations from the study of the delocalized impurity in the Tonks-Girardeau limit [42–44]. We have also examined the density of the impurity in the DE to ascertain whether translational symmetry is restored in the long-time limit. Generically, we find that translational symmetry is not restored in the finite-size system due to a symmetry of the Bethe states under a change in sign of all the momenta and rapidities.

Conclusion.—In this Letter, we consider the nonequilibrium time evolution of a single localized impurity (4) injected into the ground state of the Lieb-Liniger model. In both the case of zero and finite c.m. momentum, we observe a "stuttering" behavior in the motion. In the first case (see Fig. 1), this quantum stutter manifests in the arrested expansion of the impurity (in the absence of a lattice). This arises from the out-of-equilibrium formation of quasibound impurity-hole pairs, which are stable for extended periods of time. This interaction-driven effect can be qualitatively captured by the MF decoupling (7): the impurity repels the background gas, leading to the formation of a hole that acts as a confining potential for the impurity. Eventually the impurity broadens in a sequence of rapid expansions and quasistationary periods, all the while undergoing small-amplitude breathing oscillations. This stuttering motion and the quasibound state formation highlights the importance of distinguishability, as this mechanism does not exist for an impurity of the same species as the background gas [86].

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 background 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 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 [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. [40] and [61]) and should survive finite temperature [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 [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 [53,60].

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