Breakdown of Integrability in a Quasi-1D Ultracold Bosonic Gas

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We demonstrate that virtual excitations of higher radial modes in an atomic Bose gas in a tightly confining waveguide result in effective three-body collisions that violate integrability in this quasi-one-dimensional quantum system and give rise to thermalization. The estimated thermalization rates are consistent with recent experimental results in quasi-1D dynamics of ultracold atoms.

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Thermalization does not occur in integrable systems [1], since the number of their integrals of motion equals exactly the number of their degrees of freedom, thus such a system always "remembers" its initial state in the course of its dynamical evolution. In an integrable system the finite spread of initial energy may lead only to relaxation towards the generalized Gibbs (or fully constrained thermodynamic) ensemble [2]. Strictly speaking, there is no thermalization in any *closed* system, but for nonintegrable systems the eigenstate thermalization hypothesis [3] holds, enabling *dephasing* to mimic relaxation to the thermal equilibrium.

The Lieb-Liniger model [4] of spinless bosons with contact (pointlike) interaction in one-dimension (1D) is a prime example of such an integrable system.

Ultracold atoms in strongly elongated traps with $\omega_r \gg \omega_z$ (ω_r, ω_z being the frequencies of the radial and longitudinal confinement, respectively) are an ideal system for studying 1D physics as long as both the temperature T and chemical potential μ are small compared to the energy scale given by the transverse confinement:

$$\mu < \hbar\omega_r, \qquad k_B T < \hbar\omega_r. \tag{1}$$

Strong inhibition of thermalization was observed in a beautiful experiment with bosons deep in the 1D regime [5]. However, recent experimental results for a weakly interacting Bose gas easily fulfilling the conditions of Eq. (1) [6–8] are in a good agreement with the thermal-equilibrium description of the 1D atomic ensembles.

In the present Letter we investigate the breakdown of integrability and thermalization in ultracold 1D bosons. The key observation is that a radially confined atomic gas is never perfectly 1D, and radial motion can be excited, either in reality or virtually even if Eq. (1) holds. Therefore we call such systems quasi-1D.

We start from identical bosons in a tight waveguide with radial frequency ω_r ($\omega_z = 0$), interacting via the pseudopotential $4\pi\hbar^2 m^{-1}\alpha_s\delta(\mathbf{r}-\mathbf{r}')$, where m is the atomic mass, and α_s the s-wave scattering length:

$$\hat{\mathcal{H}}_{3D} = \int d^3\mathbf{r}\Big[\hat{\psi}^\dagger(\mathbf{r})\Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \hat{H}^{(r)}\Big)\hat{\psi}(\mathbf{r}) + \frac{2\pi\hbar^2\alpha_s}{m}\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r})\Big], \tag{2}$$

$$\hat{H}^{(r)} = -\frac{\hbar^2}{2m}\Big(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\Big) + \frac{m\omega_r^2}{2}(x^2+y^2). \tag{3}$$

We expand the atomic field operator as follows:

$$\hat{\psi}(\mathbf{r}) = L^{-1/2}\sum_{n,\ell,k}\hat{a}_{\{n,\ell\}k}\varphi_{n,\ell}(x,y)\exp(ikz). \tag{4}$$

Here L is the quantization length and $\varphi_{n,\ell}(x,y)$ is the normalized eigenfunction of both the radial confinement Hamiltonian, $\hat{H}^{(r)}\varphi_{n,\ell}(x,y) = (n+1)\hbar\omega_r\varphi_{n,\ell}(x,y)$ and the z projection of the orbital momentum, $-i[x(\partial/\partial y) - y(\partial/\partial x)]\varphi_{n,\ell}(x,y) = \ell\varphi_{n,\ell}(x,y)$. The main quantum number $n = 0, 1, 2, \ldots,$ and the orbital-momentum z-projection quantum number ℓ is restricted by $|\ell| = \mathrm{mod}(n,2), \mathrm{mod}(n,2)+2, \ldots, n-2, n$ and thus has the same parity as the main quantum number. The atomic annihilation and creation operators $\hat{a}_{\{n,\ell\}k}$ and $\hat{a}^\dagger_{\{n,\ell\}k}$ obey the standard bosonic commutation rules.

If two colliding atoms are initially in the transverse ground state of the radial confinement (1D system), then their orbital-momentum quantum numbers after collision are restricted to $-\ell$ and $+\ell$.

For two-body collisions to contribute to thermalization, they have to lead to transverse excitations. The rate Γ_{2b} of population of the radially excited modes by pairwise atomic collisions can be estimated for a nondegenerate Bose gas, using Fermi's golden rule. For $k_B T < \hbar\omega_r$ this rate is

$$\Gamma_{2b} \approx 2\sqrt{2}\hbar n_{1D}\alpha_s^2(ml_r^3)^{-1}e^{-(2\hbar\omega_r/k_BT)} = 2\sqrt{2}\omega_r\zeta e^{-(2\hbar\omega_r/k_BT)}, \tag{5}$$

where n_{1D} is the linear density and $l_r = \sqrt{\hbar/(m\omega_r)}$ is the size of the transverse ground state. The dimensionless quantity $\zeta = n_{1D}\alpha_s^2/l_r$ combines two dimensionless parameters ($n_{1D}\alpha_s \propto \frac{\mu}{\hbar\omega_r}$ and α_s/l_r) which can be seen as characterizing a 1D system [9].

Equation (5) has a transparent physical interpretation: Γ_{2b} is related to the 3D atomic density, which is $\sim n_{1D}/l_r^2$, times the s-wave scattering cross section $\sim\alpha_s^2$, times the exponential Boltzmann factor for the fraction of atoms fast enough to scatter into higher radial modes, times the corresponding velocity of the collision, $\sim\hbar/(ml_r)$.

Calculating the numbers for the data in the ^{87}Rb experiments [7], $\alpha_s = 5.3$ nm, $n_{1D} = 50\ \mu\text{m}^{-1}$, $\omega_r/(2\pi) =$ 3 kHz, $T = 30$ nK ($\zeta \approx 0.007$) one obtains a collision rate of $\Gamma_{2b} \sim 0.02\ \text{s}^{-1}$, at least one order of magnitude too small for the time scale of the experiment.

If the kinetic energy of the collision is less than $2\hbar\omega_r$, then the radial modes can be excited only virtually and contribute to the system dynamics only in the second and higher orders of perturbation theory. If after the collision the radial motion state is $|\{n_1', \ell_1'\}, \{n_2', \ell_2'\}\rangle =$ $|\{0, 0\}, \{2p, 0\}\rangle$, then only one more collision is enough to quench the virtual excitation and return the system on the energy shell [Fig. 1, inset (a)]. Such a process yields an effective three-body collision already in the *second* order of perturbation theory.

In contrast processes involving a virtual excitation to $|\{n_1', -\ell\}, \{n_2', +\ell\}\rangle$, $\ell \neq 0$, shown in Fig. 1, inset (b), contribute only in the *third* order, and thus will be neglected.

The small parameter in our perturbation calculation is $n_{1D}\alpha_s$. To avoid complications related to the confinement-

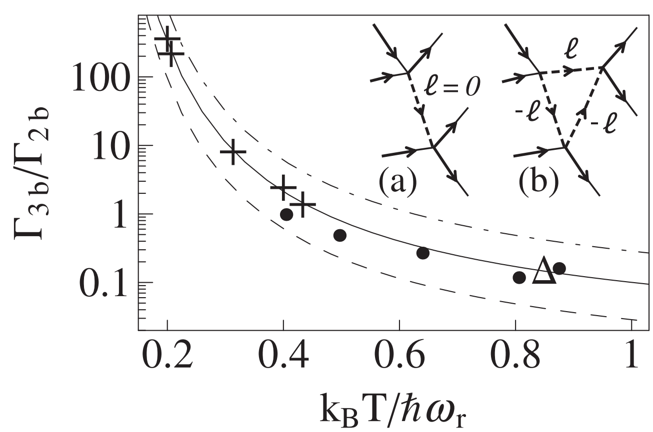

FIG. 1. Ratio between the scattering rates for the two routes to thermalization and breakdown of integrability in 1D systems: Γ_{2b} for two-body collisions leading to excited transverse states, and Γ_{3b} for the effective three-body collisions. Units on the axes are dimensionless. $\zeta = 0.002$ (dashed curve), 0.007 (solid curve), and 0.02 (dot-dashed curve). The points represent the predicted ratios for various sets of experimental parameters from [6] (points), [7] (crosses), and [8] (triangle). Inset: Feynman diagrams for the effective three-body processes in the second (a) and third (b) orders of perturbation theory. Solid and dashed lines correspond to atoms in the ground and excited states of the radial trapping Hamiltonian, respectively.

induced resonance in 1D scattering [10] we assume $\alpha_s \ll l_r$ [9]. We evaluate the matrix element

$$\langle\{0,0\},\{2p,0\}|\delta(x-x')\delta(y-y')|\{0,0\},\{0,0\}\rangle = (2^{p+1}\pi l_r^2)^{-1} \tag{6}$$

that corresponds to two atoms in the ground state of the incoming channel, one atom remaining in the same state, but the other one being excited to a state with zero orbital-momentum quantum number and even main quantum number $n = 2p$, $p = 0, 1, 2, \ldots$ (n and ℓ are required to have the same parity).

The result of Eq. (6) should not be confused with the matrix element where the outgoing channel is characterized by excitation of a higher radial mode of the *relative* motion of two atoms as discussed in [11], which equals to $(2\pi l_r^2)^{-1}$. The latter is a linear combination of the matrix elements corresponding to vertices of *both* types (a) and (b) in the inset to Fig. 1 and thus cannot be applied to the calculation of the second-order process.

Using the matrix element Eq. (6) we can rewrite Eq. (2) and by adiabatically eliminating the radially excited mode operators obtain the effective 1D Hamiltonian $\hat{\mathcal{H}}_{1D} =$ $\hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{1D}^{(3b)}$ with the three-body interaction

$$\hat{\mathcal{H}}_{1D}^{(3b)} = -\frac{2\xi\hbar\omega_r\alpha_s^2}{L^2}\sum \hat{a}_{k_1'}^\dagger \hat{a}_{k_2'}^\dagger \hat{a}_{k_3'}^\dagger \hat{a}_{k_1}\hat{a}_{k_2}\hat{a}_{k_3} \tag{7}$$

where the summation in Eq. (7) is taken over all the kinetic momenta obeying the conservation law $k_1' + k_2' + k_3' =$ $k_1 + k_2 + k_3$, $\hat{a}_k \equiv \hat{a}_{\{0,0\}k}$, and $\xi = 4\ln(4/3) \approx 1.15$. The relative contribution $(\xi - 1)/\xi$ of the virtual states with the excitation energy higher than $2\hbar\omega_r$ is remarkably small. Using Eq. (7) we then obtain the collision rate for the process shown in Fig. 1, inset (a):

$$\Gamma_{3b} = C_{3b}\hbar n_{1D}^2 m^{-1}(\alpha_s/l_r)^4 = C_{3b}\omega_r\zeta^2, \tag{8}$$

with $C_{3b} = (72\xi^2/\sqrt{3}\pi^2) \approx 5.57$. Comparison to the two-body rates for typical experiments is given in Fig. 1.

The result of Eq. (8) may seem counterintuitive at first: the collision rate is independent of temperature, and is proportional to ζ^2 and the radial confinement ω_r.

The physics behind the first observation is related to the fact that the collision kinetic energy is small compared to the virtual excitation energy [according to assumption Eq. (1)]. Consequently the composite matrix element of the second-order process should not depend (in leading order) on the velocities of colliding particles and hence on temperature [see Eq. (6)]. In addition the phase-space volume for the scattered particles is independent on the incoming momenta k_1, k_2, and k_3.

The rate of three-body elastic scattering must be proportional to the 3D density squared, $(n_{1D}/l_r^2)^2$. On the other hand, the scattering rate contains the square of the matrix element corresponding to the diagram in Fig. 1, inset (a), where each vertex is proportional to α_s, therefore this rate is proportional to α_s^4. The factor $\hbar/m$ provides the correct dimensionality (s^{-1}).

We can now compare the scattering rates for the two routes for thermalization and breakdown of integrability in 1D systems: thermally excited two-body collisions Γ_{2b} [Eq. (5)] or effective three-body collisions Γ_{3b} [Eq. (8)]. For $k_B T < \hbar\omega_r$ we find a simple scaling:

$$\frac{\Gamma_{3b}}{\Gamma_{2b}} \approx \frac{36}{\sqrt{6}\pi^2}\xi^2\zeta e^{2\hbar\omega_r/k_B T} \approx 1.97\zeta e^{2\hbar\omega_r/k_B T}. \tag{9}$$

For large ζ and small temperatures the scattering rate due to *virtual* excitations dominates, and can violate integrability even when thermalization processes due to simple two-body collisions are frozen out. A detailed comparison of the two rates and their relation to experimental parameters is given in Fig. 1. The scattering rate due to *virtual* excitations of the radial modes can dominate over real excitations for typical parameters of the recent experiment [7].

To quantify the thermalization due to the violation of integrability by the interaction (7), we consider a nondegenerate, weakly interacting [the Lieb-Liniger parameter [4] $\gamma = 2\alpha_s/(n_{1D} l_r^2)$ being much less than 1] gas of bosonic atoms [12] and write out the Boltzmann equation with a three-body collision integral [13], taking into account the indistinguishability of the particles:

$$\frac{d}{dt}f_k = \frac{72\xi^2\omega_r^2\alpha_s^4 m}{\sqrt{3}\pi^3\hbar}\int_{-K}^{K}\frac{dq}{\sqrt{K^2-q^2}} \times \int_{-\infty}^{\infty}dk'\int_{-\infty}^{\infty}dk''(f_{k_0-q}f_{k_+}f_{k_-} - f_k f_{k'} f_{k''}), \tag{10}$$

$$k_0 = \frac{k+k'+k''}{3}, \qquad k_\pm = k_0 + \frac{q}{2} \pm \frac{\sqrt{3}}{2}\sqrt{K^2-q^2},$$
$$K = \frac{2}{3}\sqrt{k^2+k'^2+k''^2-kk'-kk''-k'k''}. \tag{11}$$

To solve Eq. (10) we use the following *ansatz* for the perturbed momentum distribution

$$f_k(t) = \frac{n_{1D}}{\sqrt{\pi}k_{\mathrm{th}}}\exp(-k^2/k_{\mathrm{th}}^2)[1+\varepsilon_4(t)H_4(k/k_{\mathrm{th}})], \tag{12}$$

where $k_{\mathrm{th}} = \sqrt{2mk_BT}/\hbar$ and H_4 is the Hermite polynomial of the 4th order. We choose this form, since it is the simplest nontrivial perturbation that retains $\int dk k f_k = 0$. Linearizing Eq. (10) with respect to the perturbation amplitude $\varepsilon_4(t)$ we obtain the exponential solution $\varepsilon_4(t) = \varepsilon_4(0)\exp(-\Gamma_{[4]}^{3b}t)$ with the decrement

$$\Gamma_{[4]}^{3b} = C_{[4]}\hbar n_{1D}^2 m^{-1}(\alpha_s/l_r)^4 = C_{[4]}\omega_r\zeta^2, \tag{13}$$

where the numerical constant $C_{[4]} = (64\xi^2/3\sqrt{3}\pi^2) \approx 1.65$. Taking the perturbation proportional to a higher-order Hermite polynomial H_n leads only to a minor modification of the numerical prefactor, leaving the functional dependence on the parameters of the system unchanged (for example, $n = 5$ or 6 increases the thermalization rate by the factor 5/4 or 13/9, respectively). Figure 2 shows numerical values of $\Gamma_{[4]}^{3b}$ as a function of the 1D density of ^{87}Rb atoms and the radial trapping frequency.

Similarly, we calculate numerically the thermalization rate $\Gamma_{[4]}^{2b}$ for two-body collisions involving the *real* transitions between the ground and excited radial states. The velocity distribution of atoms in the ground and excited state was perturbed in the same way, as given by Eq. (12), the Boltzmannian distribution of overall populations between the levels being kept intact. In the parameter range of interest we find numerically $\Gamma_{[4]}^{2b} \approx (0.33 \pm 0.03)\Gamma_{2b}$, i.e., $\Gamma_{[4]}^{2b} \approx 0.93\omega_r\zeta\exp(-\frac{2\hbar\omega_r}{k_BT})$. The ratio of the thermalization rates for the two-body and three-body processes is very close to the respective ratio of the collision rates, shown in Fig. 1.

It is interesting to note that we find for both processes, the two-body collisions to real transverse states and the effective three-body processes via virtual excited states, that thermalization in 1D needs about 3 collisions which are able to distribute energy. This is very close to the 2.7 collisions required for thermalization in 3D [14].

For the typical parameters of an ultracold ^{87}Rb gas on an atom chip [7] ($\omega_r \approx 2\pi \times 3$ kHz, $n_{1D} \approx 50\ \mu\mathrm{m}^{-1}$) we obtain $\Gamma_{[4]}^{3b} \approx 2\ \mathrm{s}^{-1}$. This thermalization rate is temperature independent and much larger than the one calculated from the simple two-body collisions with the energy sufficient to excite radial modes $\Gamma_{[4]}^{2b} \approx 3 \times 10^{-3}\ \mathrm{s}^{-1}$ at the lowest temperatures measured (30 nK). The estimated $\Gamma_{[4]}^{3b}$ is consistent with the time needed for evaporative cooling of a ^{87}Rb gas on an atom chip well below $\hbar\omega_r$ [6,7].

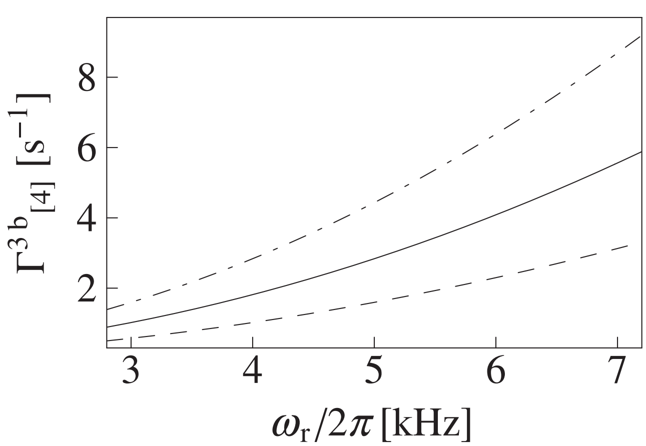

FIG. 2. Dependence of the rate $\Gamma_{[4]}^{3b}$ of thermalization induced by effective three-body collisions on the radial trapping frequency. $n_{1D} = 30\ \mu\mathrm{m}^{-1}$ (dashed curve), $40\ \mu\mathrm{m}^{-1}$ (solid curve), and $50\ \mu\mathrm{m}^{-1}$ (dot-dashed curve).

The thermalization rate $\Gamma_{[4]}^{3b}$ given by Eq. (13) applies for a weakly interacting, nondegenerate gas. Precise calculation of its counterpart $\Gamma_{[4]}^{3bG}$ in a general case (comprising also the intermediate and strongly interacting regimes as well as various degrees of degeneracy) is an extended problem, requiring numerical analysis of many particular cases and transcending far beyond the scope of the present Letter. However, taking into account that Eq. (7) can be written as $\hat{\mathcal{H}}_{1\mathrm{D}}^{(3b)} = -2\xi\hbar\omega_r\alpha_s^2 \int dz \hat{\psi}_{1\mathrm{D}}^{\dagger 3}(z)\hat{\psi}_{1\mathrm{D}}^3(z)$, where $\hat{\psi}_{1\mathrm{D}}(z) = L^{-1/2}\sum_k \hat{a}_k \exp(ikz)$, we can give a simple estimate of the ratio of these two rates $\Gamma_{[4]}^{3bG}/\Gamma_{[4]}^{3b} = \varrho(g_3/6)^2$. Here ϱ is a phase-space factor accounting for a possible deviation of the dispersion law of elementary excitation (from free particle to phonon in strongly correlated or crossover [15] regimes) and the decrease of the collision rate per atom in degenerate gases. However, we expect the influence of this factor be less dramatic than that associated with the local three-body correlation function $g_3 = \langle \hat{\psi}_{1\mathrm{D}}^{\dagger 3}(z)\hat{\psi}_{1\mathrm{D}}^3(z)\rangle/n_{1\mathrm{D}}^3$. The exact expression for g_3 in the whole range of the atomic repulsion strength ($0 < \gamma < \infty$) has been obtained recently [16] for a *degenerate* 1D Bose gas. For a nondegenerate weakly interacting Bose gas $g_3 = 6$. In the zero-temperature limit g_3 rapidly decreases from 1 to $16\pi^6/(15\gamma^6)$ as γ grows from 0 to values $\gg 1$.

This enables us to interpret qualitatively the experimental results of Ref. [5], where a degenerate ^{87}Rb gas in a two-dimensional optical lattice ($\omega_r \approx 2\pi \times 67$ kHz, $n_{1\mathrm{D}} \approx 10\ \mu\mathrm{m}^{-1}$) is split by a laser Bragg pulse into two groups with opposite kinetic momenta, which begin to oscillate in a weak trapping potential in z direction, colliding each half-period of the oscillation. Using the formula for g_3 from Ref. [16] and estimating $\varrho \sim 3$ [17], we find a thermalization rate under conditions of Ref. [5] to be of about 0.01 s^{-1} and 3×10^{-4} s^{-1} for $\gamma = 1.4$ and 3.2, respectively, which is consistent with the experimentally obtained respective lower bounds (2.6 and 25 s) to the thermalization time. The two-body collision rate decreases in a general case slower ($\propto\gamma^{-4}$) than $\Gamma_{[4]}^{3bG}$. In the case of [5] two-body collisions are suppressed because the collision energy is smaller than $0.5\hbar\omega_r$.

The *elastic* three-body processes considered in this Letter are essential for the possibility of obtaining very low temperatures in quasi-1D bosonic gases: as the temperature goes below the radial trapping energy, the "usual" two-body processes freeze out quickly, thus preventing further thermalization. However, the effective three-body collisions obey completely different scalings (e.g., independent of temperature) and allow for thermalization much deeper in the quasi-1D regime than previously believed, since thermalization via two-body collision ceases there. These three-body processes are associated with virtual excitations of radial modes, which can be dominant for $k_BT < \hbar\omega_r$. This mechanism is to a certain extent similar to the processes that allow for the dimer formation in atomic gases in tight waveguides ("quantum chemistry" in 1D) [18]. Our estimations of the relaxation rates are consistent with recent experimental observations [5–7]. The given scaling laws make the proposed three-body process accessible to experimental confirmation.

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