Integrability breakdown in longitudinally trapped, one-dimensional bosonic gases

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A system of identical bosons with short-range (contact) interactions is studied. Their motion is
confined to one dimension by a tight lateral trapping potential and, additionally, subject to a weak
harmonic confinement in the longitudinal direction. Finite delay time associated with penetration
of quantum particles through each other in the course of a pairwise one-dimensional collision in
the presence of the longitudinal potential makes the system non-integrable and, hence, provides a
mechanism for relaxation to thermal equilibrium. To analyse this effect quantitatively in the limit
of a non-degenerate gas, we develop a system of kinetic equations and solve it for small-amplitude
monopole oscillations of the gas. The obtained damping rate is long enough to be neglected in
a realistic cold-atom experiment, and therefore longitudinal trapping does not hinder integrable
dynamics of atomic gases in the 1D regime.

I. INTRODUCTION

One-dimensional systems (1D) [1,2] often provide suitable models to study the fundamental processes of quantum
dynamics, coherence and noise in interacting many-body systems. Integrability is one of such fundamental questions
most closely related to the 1D physics. In an integrable system [3,4], the number of integrals of motion is exactly equal
to the number of degrees of freedom. Thus the observables, which can be measured experimentally, namely, single-
particle (momentum and position distribution) or few-particle (correlation functions) ones retain the information on
the initial conditions forever. As a result, a quenched (i.e. suddenly driven off the equilibrium) integrable system
may undergo relaxation towards the generalized Gibbs (or fully constrained thermodynamics) ensemble [5], instead
of the thermal equilibrium state. A similar type of relaxation may be observed even in non-integrable systems [6].
Also local quantities of the Bose-Hubbard model are shown [7] to approach the thermal Gibbs state much faster
than non-local ones, such as the density-density correlation function. For a very wide class of non-integrable systems,
however, the eigenstate thermalization hypothesis [8] (see also [9]) may hold, enabling fast relaxation to thermal
equilibrium. Of course, the term “thermalization” with regard to closed (isolated from environment) systems means
that all experimentally measurable observables approach their thermal distributions; the information on the initial
conditions becomes contained in many-particle correlations (ultimately, in correlations involving all particles in the
system), whose measurement is not feasible in practice.

An uniform 1D system of indistinguishable bosons interacting with each other via pairwise delta-functional poten
tial is known to be integrable and described by the Lieb-Liniger model [10,11]. It can be, up to certain extent,
implemented in an ultracold-atom experiment in optical lattices [12,13] or on atom chips [14–17], provided that both
the temperature and mean interaction energy per atom are well below the excitation energy of the first excited state
of the radial trapping Hamiltonian. Under these conditions, the radial motion of atoms is confined to the ground state
of the radial trapping Hamiltonian. Ultracold atomic systems deeply in the 1D regime can be prepared in optical
lattices [15] and on atom chips [19]. However, in reality no system is perfectly 1D, but the actual question is, on
which timescale it can be described as 1D. For ultracold atoms under tight lateral confinement one-dimensionality
and, hence, integrability are lifted by atomic interactions causing virtual population of excited radial modes, even
if the energy of thermal motion is too low, and thermal excitation of the radial modes is strongly suppressed by a
Boltzmannian exponential factor. The role of the virtual radial excitations in the dynamics of ultracold atomic gases
in tight waveguides has been first noticed in the context of macroscopic flow of degenerate atomic gas through a
waveguide [20] and decay of mean-field solitons [21]. Microscopically, virtual radial excitations give rise to effective
3-body elastic collisions, which have been suggested as the source of thermalization in ultracold atomic gases on atom
chips [22] (see also Refs. [23,24]). Interestingly, if the interatomic repulsion is so strong that the system approaches
the Tonks-Girardeau limit, interatomic correlations reduce the rate of thermalizing collisions [23,25]. The latter
conclusion is in agreement with the results of the quantum “Newton cradle” experiment [18].

However, this is not the only source of non-integrability. An ultracold atomic cloud in a real experiment is also
confined longitudinally, although the ratio of the fundamental frequencies of the longitudinal ($\omega_\parallel$) and transversal
($\omega_\perp$) trapping may be as small as $\omega_\parallel/\omega_\perp \sim 10^{-3}$. Obviously, an ideal gas in 1D in the presence of harmonic confinement
is an integrable system, and so is the gas of impenetrable bosons [26]. However, the longitudinal confinement should
lift the integrability of the Lieb-Liniger model for any finite atomic interaction strength. Estimating the corresponding
relaxation rate is the subject of the present paper.
II. PHYSICAL MODEL

The Hamiltonian of the system of \(N\) identical bosons of mass \(m\) confined to 1D and also harmonically trapped in the longitudinal direction reads as

\[
\hat{H} = \sum_{j=1}^{N} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_j^2} + \frac{m^2 \omega^2}{2} x_j^2 + \frac{\hbar^2 c}{m} \sum_{i=j+1}^{N} \delta(x_j - x_i) \right].
\]  

(1)

Here \(c\) is the pairwise interaction strength. In the limit \(\omega \tau \to 0\) we recover the Hamiltonian of the Lieb-Liniger model \([10, 11]\). Virtual excitations of the radial modes \([20, 24]\) are not included into the model Eq. (1), therefore we can investigate the integrability breakdown solely due to the longitudinal confinement. The latter is assumed to be harmonic in order to distinguish the effect under study from dephasing of the atomic motion occuring in an anharmonic trap.

In what follows we consider a non-degenerate, weakly interacting 1D bosonic gas. The non-degeneracy means that the atomic motion can be viewed as quasi-classical propagation in the longitudinal direction of distinct wave packets localized of a size much smaller than the mean interatomic distance. However, as we noted in Sec. II the radial motion of atoms remains quantized, confined to the ground state of the radial trapping Hamiltonian. This is exactly the point, where our models differs from previous calculations of damping of excitations in a classical atomic gas in very elongated, but still three-dimensional (3D) traps \([27]\). In the latter case, (i) time delay in the process of scattering is neglected and (ii) collisions are essentially 3D and lead to scattering to a whole manifold of radial modes.

A collision of two atoms is not an instantaneous event, but entails a time delay in propagation of the two colliding wave packets. The delay time is \([28]\)

\[
\tau = \frac{1}{u} \frac{\partial \varphi}{\partial k_c},
\]

(2)

where \(u\) is the relative velocity of the collision (we assume here wave packet propagation in 1D with \(u > 0\), \(\hbar k_c = mu/2\) is the corresponding momentum (\(m/2\) is the reduced mass) and \(\varphi\) is the phase shift of the transmitted wave after 1D scattering on the given pairwise interaction potential. Having the formula \(\varphi = -\arctan[c/(2k_r)]\) for scattering on the contact (delta-functional) potential \([11]\), it is easy to obtain

\[
\tau = mc/\left[\hbar k_c(4k_r^2 + c^2)\right].
\]

(3)

Since in a weakly-interacting gas \(k_r \gg c\) for almost every collision,

\[
\tau \approx mc/(4\hbar k_r^3) = 2\hbar c/(m^2 u^3).
\]

(4)

Formally, Eq. 4 coincides with the classical expression \(\tau = [2/(mu^3)] \int_{-\infty}^{+\infty} dx U_{12}(x)\) for the delay time of a fast particle of mass \(m/2\) traversing the potential \(U_{12}(x)\) ["fast" meaning that the particle kinetic energy \(mu^2/4\) at \(x \to \pm \infty\) is much larger than the maximum value of \(U_{12}(x)\)]. Of course, in a case of the repulsive \((c > 0)\) delta-functional potential the classical description fails, but Eq. 4 holds also in the regime of quantum tunneling through a weak potential barrier. If the atomic interaction is attractive, we formally obtain \(\tau < 0\). However, the theoretical approach developed in Sec. III assumes \(\tau > 0\). Therefore we consider in this paper only gases with repulsive interactions \((c > 0)\).

The finite delay time does not change the statistical distribution of atomic velocities in an infinite waveguide in the thermodynamic limit. However, the situation becomes different for the trapped gases. The relative motion of two particles is assumed to be classical in the intervals between collisions, and the center-of-mass motion is always treated classically. Assume that at time \(t_0\) two particles with the velocities \(v_1(t_0) = v_{c1}\) and \(v_2(t_0) = v_{c2}\) collide at the point \(x_1(t) = x_2(t) = x_c\). We assume the following model: during the collision time \(\tau\), which depends on the absolute value of the relative velocity \(|v_{c1} - v_{c2}|\), the two atoms form a composite particle of mass \(2m\) moving in the potential \(m\omega^2 X^2\), \(X\) being the coordinate of the composite particle, with the initial conditions \(X(t_0) = x_c\), \(V(t_0) = X(t_0) = (v_{c1} + v_{c2})/2\). The kinetic energy of the relative motion is ascribed to an “internal degree of freedom” of the compound particle, thus ensuring energy conservation. After the time \(\tau\) the compound particle disintegrates, releasing two atoms at the point

\[
x_{1,2}(t_0 + \tau) = x_c \cos \omega|\tau| + \frac{v_{c1} + v_{c2}}{2\omega} \sin \omega|\tau|.
\]

(5)

The velocities of the particles are determined by the center-of-mass velocity and the relative-motion kinetic energy stored internally in the compound particle and released back at \(t = t_0 + \tau\):

\[
v_{1,2}(t_0 + \tau) = -\omega x_c \sin \omega|\tau| + \frac{v_{c1} + v_{c2}}{2} \cos \omega|\tau| \pm \frac{v_{c1} - v_{c2}}{2}.
\]

(6)
Since the atoms are identical, there is no one-to-one correspondence between the upper (lower) sign in front of the last term and the index (1 or 2) numbering the atoms. Although the total energy of the pair of the atoms is conserved exactly, the single-atom energies are not. They will be shifted by \( \pm \frac{m}{2}(v_{c1} - v_{c2})\left[\frac{1}{2}(v_{c1} + v_{c2})(1 - \cos \omega_\parallel \tau) + \omega_\parallel x_c \sin \omega_\parallel \tau\right] \).

### III. KINETIC EQUATIONS

To quantify the single-atom energy redistribution noticed in the previous section, we derive a set of kinetic equations describing 1D atomic collisions. We assume a two-component model: the system consists of single atoms characterized by a joint co-ordinate and velocity distribution function \( f(x, v, t) \) and diatomic compound particles representing atomic pairs, not actually bound but remaining close to each other during the delay time \( \tau \), which is considered as the effective collision duration. The distribution function of compound particles \( F(x, V, u, t) \) has, apart from the time \( t \), three arguments: \( x \) stands here for the compound particle co-ordinate (center of mass of two colliding atoms), \( V \) is the center-of-mass velocity, and \( u \) is the relative velocity of two atoms before the collision; \( u \) can be considered also as a label for “internal excitations” of a compound particle. Because of indistinguishability of the atoms, it is sufficient to consider only positive values of \( u \). We assume that the gas is dilute, i.e., only a small fraction of the atomic ensemble is simultaneously contained in compound particles. A rate of 1D collisions experienced by an atom with the velocity \( v \) is \( \int_{-\infty}^{\infty} dv' \left| v - v' \right| f(x, v, t)f(x, v', t) \), and each collision is followed by compound particle formation (it is impossible for two identical, interacting bosons to tunnel through each other in 1D without delay in propagation).

Also we assume that a compound particle does not experience collisions with other atoms during its lifetime. To make the set of kinetic equations simple, we assume (instead of a well-defined deterministic) time interval between formation and disintegration of a compound particle) that a compound particle undergoes exponential decay with the rate \( 1/\tau_u \). The lower index index \( u \) explicitly indicates the dependence \( \| \) of the delay time on the relative velocity \( u \) of the atoms before collisions. The products of the decay are two atoms emerging at the same point with the velocities \( V \pm u/2 \). The equality of the relative velocities before and after the collision is specific for motion in a harmonic potential, where the center-of-mass and relative-motion degrees of freedom are decoupled.

The corresponding set of kinetic equations now can be easily written:

\[
\frac{\partial}{\partial t} f(x, v, t) + v \frac{\partial}{\partial x} f(x, v, t) - \omega_\parallel^2 \frac{\partial}{\partial v} f(x, v, t) = - \int_{-\infty}^{\infty} dv' \left| v - v' \right| f(x, v, t)f(x, v', t) - \frac{1}{\tau_{\left|v-v'\right|}} F\left(x, \frac{v + v'}{2}, \left|v-v'\right|, t\right),
\]

(7)

\[
\frac{\partial}{\partial t} F(x, V, u, t) + V \frac{\partial}{\partial x} F(x, V, u, t) - \omega_\parallel^2 x \frac{\partial}{\partial V} F(x, V, u, t) = - \frac{1}{\tau_u} F(x, V, u, t) + u f\left(x, V + \frac{u}{2}, t\right) f\left(x, V - \frac{u}{2}, t\right).
\]

(8)

It belongs to a broad family of equation sets describing chemical reactions on the kinetic level \[29\]. It conserves the total number of atoms

\[
N = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dv \left[ f(x, v, t) + 2 \int_{0}^{\infty} du \ F(x, v, u) \right]
\]

(9)

and the total energy of the system

\[
E = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dv \ v \ f(x, v, t) + \int_{-\infty}^{\infty} dx \ int_{-\infty}^{\infty} dV \ int_{0}^{\infty} du \ \varepsilon_{cp} F(x, V, u, t),
\]

(10)

where \( \varepsilon_a = m(\omega_\parallel^2 x^2 + v^2)/2 \) and \( \varepsilon_{cp} = m(\omega_\parallel^2 x^2 + V^2 + u^2)/4 \) are the single-atom and compound-particle energies, respectively. Eqs. (7, 8) are also consistent with Newton’s second law \( d^2 X_N/dt^2 = -\omega_\parallel^2 X_N \) for the center of mass \( X_N = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dv \left[ f(x, v, t) + 2 \int_{0}^{\infty} du \ F(x, v, u, t)\right]/N \) of the \( N \)-atom system.
Eliminating $F(x,V,u,t)$, we arrive, by an exact transformation, to an equation for the distribution functions of atoms only:

$$\frac{\partial}{\partial t}f(x,v,t) + v \frac{\partial}{\partial x}f(x,v,t) - \omega^2 x \frac{\partial}{\partial v}f(x,v,t) =$$

$$- \int_{-\infty}^{\infty} dv' [v - v'] \left[ f(x,v,t)f(x,v',t) - f(x,v,t)f(x,v',t) \right]$$

$$\int_{0}^{\infty} ds e^{-s/T_{\parallel}} f(x,v,v^+_s,t-s)f(x,v^-_s,t-s),$$

(11)

where $x_s$ and $v^\pm_s$ are given by the right-hand side of Eq. (3) and Eq. (6), respectively, with the following substitutions: $x_s = x$, $v_{s1} = v$, $v_{s2} = v'$, and $\tau = -s$. If we approximate the exponential kernel in the right-hand-side of Eq. (11) by $\delta(s - \eta)$, $\eta \to 0^+$, this right-hand-side (the 1D collisional integral) becomes zero, and we obtain in this limit an equation of motion of a collisionless gas. The Maxwell-Boltzmann distribution

$$f_0(x,v,t) = \frac{N m_{\parallel}}{2 \pi T} \exp \left( - \frac{m_{\parallel}^2 x^2}{2T} - \frac{m v^2}{2T} \right)$$

(12)

is a stationary solution of Eq. (11). Here we set Boltzmann’s constant to 1 and thus measure temperature $T$ in energy units. We normalize $f_0$ in Eq. (12) to the total number of atoms $N$, since the interactions are week and the mean number of compound particles simultaneously present in the system is much less than $N$.

**IV. MONOPOLE MODE**

If a system state deviates from equilibrium only slightly, the typical time of return to the equilibrium is estimated from the linearized form of the kinetic equation [32]. Following the standard linearization scheme, we represent $f(x,v,t) = f_0(x,v,t) + f_1(x,v,t)$ where the small perturbation term $f_1$ describes the deviation from the equilibrium and is orthogonal to $f_0$:

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dv f_0(x,v,t) f_1(x,v,t) = 0.$$  

For the sake of definiteness, we consider one specific (monopole) 1D mode [31], and choose the perturbation term in the form

$$f_1(x,v,t) = f_0(x,v)[\Lambda(t)(v^2 - \omega^2_{\parallel} x^2) + B(t)\omega_{\parallel} xv].$$

(13)

If we completely neglect collisions in Eq. (11), we obtain the following linearized equations:

$$\dot{\Lambda} + 2\omega_{\parallel} B = 0, \quad \dot{B} - 2\omega_{\parallel} \Lambda = 0.$$  

(14)

In the next iteration, we substitute the solutions of Eq. (14) $\Lambda(t-s) = \Lambda(t) \cos 2\omega_{\parallel}s + B(t) \sin 2\omega_{\parallel}s$ and $B(t-s) = -\Lambda(t) \sin 2\omega_{\parallel}s + B(t) \cos 2\omega_{\parallel}s$ into the right-hand-side of Eq. (11) and finally obtain

$$\dot{\Lambda} + (2\omega_{\parallel} - \beta) B + \gamma \Lambda = 0, \quad \dot{B} - 2\omega_{\parallel} \Lambda = 0,$$

(15)

where

$$\beta = \frac{N m_{\parallel}^3}{64 \pi T^3} \int_{0}^{\infty} du u^5 e^{-m u^2/(4T)} \frac{2\omega_{\parallel} \tau_u}{1 + 4\omega_{\parallel}^2 \tau_u^2}$$

(16)

and

$$\gamma = \frac{N m_{\parallel}^3}{64 \pi T^3} \int_{0}^{\infty} du u^5 e^{-m u^2/(4T)} \frac{4\omega_{\parallel}^2 \tau_u^2}{1 + 4\omega_{\parallel}^2 \tau_u^2}.$$  

(17)

Solution of Eqs. (17) yields a complex eigenfrequency. Its real and imaginary parts give the oscillation frequency

$$\omega = 2\omega_{\parallel} \sqrt{1 - \beta/(2\omega_{\parallel}) - \gamma^2/(16\omega_{\parallel}^2)}$$

(18)

(we assume weak interactions, $\beta, \gamma \ll \omega_{\parallel}$, hence, the oscillations are not overdamped) and the decrement

$$\Gamma = \gamma/2$$

(19)
of the 1D monopole mode. Using the high-velocity limit Eq. (1) we calculate the leading terms of the two relevant parameters:

\[ \beta \approx \frac{\nu}{8\sqrt{\pi}} N \omega_\parallel, \]

\[ \gamma \approx \frac{\nu^2 \ln(1/\nu)}{12\pi} N \omega_\parallel, \]

where

\[ \nu = \frac{\hbar^2 c}{\omega_\parallel T \sqrt{m T}}. \]

The consistency of our solution requires \( \nu N \ll 1 \). The decrement of the monopole mode is smaller than the collision-induced correction to the oscillation frequency by a factor \( \sim \nu \ln(1/\nu) \). If we neglect \( \gamma \), Eqs. (18, 20, 22) yield the known result [31] for the monopole mode frequency in a 1D thermal gas. Note that dissipation has been introduced in [31] phenomenologically, and up to now only the damping via essentially 3D scattering [27] has been studied.

In the strongly interacting regime, one has to take, instead of Eq. (4), the opposite \( (k_r \ll c) \) limit of Eq. (3). Then \( \gamma \) decreases as \( c^{-4} \) as \( c \to \infty \), thus signifying integrability restoration for a longitudinally trapped gas in the Tonks-Girardeau limit [26].

We consider, as an example, a gas of \( N = 10^3 \) \(^{87}\)Rb atoms trapped at \( T = 1 \) \( \mu \)K in a highly elongated trap with the radial and longitudinal trapping frequencies \( \omega_\perp = 2\pi \times 67 \) kHz and \( \omega_\parallel = 2\pi \times 10 \) Hz (such a strong radial trapping needed to satisfy the one-dimensionality conditions can be achieved in optical lattices [18]). In this case \( \hbar^2 c/m = 2\hbar \omega_\perp a_s \) [32], where \( a_s = 5.3 \) nm is the atomic \( s \)-wave scattering length, and we obtain \( \nu \approx 2 \times 10^{-4} \). The collisional shift of the monopole mode frequency is, according to Eqs. (18, 20), approximately 0.4%. The decrement of this mode is \( \Gamma \approx 3 \times 10^{-4} \) s\(^{-1}\), which is too small to be measured experimentally.

The method developed in the present paper applies to non-degenerate 1D gases. However, by analogy with the results above, we can hazard a conjecture for the estimation of the decrement of the monopole mode also in the case of degenerate gas. Our guess is that the relation \( \Gamma \sim \nu \ln(1/\nu) \Delta \omega \) holds also in the latter case, but the parameter \( \nu \) has to be then estimated not from Eq. (22), but instead from the collisional shift \( \Delta \omega \sim \nu N \omega_\parallel \) of the monopole mode frequency (with respect to the frequency \( 2\omega_\parallel \) of this mode in an ideal gas). At maximum (in the Thomas-Fermi regime), \( \Delta \omega \sim \omega_\parallel \) [33] and, hence, \( \nu \sim 1/N \). Then we can roughly estimate the decrement as \( \Gamma \sim \ln(1/N) \omega_\parallel /N \). The time scale \( \Gamma^{-1} \), on which the integrability breakdown due to longitudinal trapping can be neglected, is long compared to a typical duration of an ultracold-atom experiment.

V. CONCLUSION

We find that the combination of two effects, (i) finite time delay in wave packet propagation associated with a 1D collision and (ii) longitudinal trapping lift the integrability of a system of identical bosons in 1D with contact interactions. To quantify the effect of non-integrability for a non-degenerate gas, we derive a set of kinetic equations and apply them to the analysis of the monopole mode of a 1D gas. We find this decrement to be small enough to be neglected in experiment and state therefore that the main source of non-integrability and thermalization in cold atomic Bose-gases in elongated traps in the 1D regime is virtual excitation of transversal degrees of freedom that gives rise to effective velocity-changing 3-body elastic collisions [22–24].

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