

Restoring integrability in one-dimensional quantum gases by two-particle correlations

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We show that thermalization and the breakdown of integrability in the one-dimensional Lieb-Liniger model caused by local three-body elastic interactions is suppressed by pairwise quantum correlations when approaching the strongly correlated regime. If the relative momentum k is small compared to the two-body coupling constant c the three-particle scattering state is suppressed by a factor of $(k/c)^{1/2}$. This demonstrates that in one-dimensional quantum systems it is not the freeze out of two body collisions but the strong quantum correlations which ensures integrability.

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Integrable systems [1] allow for deep conceptual insight into many problems of field theory and statistical physics by providing exactly solvable models with rich properties. Thermalization is precluded in integrable models because the number of integrals of motion equals to the number of degrees of freedom and the *memory* of the initial state persists in the system forever. A strictly one-dimensional (1D) system with local (delta-functional) interactions is a prime example of an integrable model [2].

In the real world, 1D systems are realized by strong transverse confinement ($\hbar\omega_{\perp}$ being the level spacing for the radial confinement Hamiltonian), which *freezes out* the radial degrees of freedom. An example are ultracold atoms in a tight waveguide where the interval between its ground and first radially excited states exceeds both the chemical potential ($\mu \ll \hbar\omega_{\perp}$) and the temperature of the atomic system ($k_B T \ll \hbar\omega_{\perp}$). Such a system can be described by the Lieb-Liniger model [2]. Recently it has been shown in experiment that one can cool in 1D by evaporation to $k_B T < \frac{1}{5}\hbar\omega_{\perp}$ [3] and theoretically that the freeze out of two body collisions in proportional to $\exp[-2\hbar\omega_{\perp}/(k_B T)]$ does not necessarily lead to a stop of thermalization [4]. Local three-body elastic collisions, where higher radial modes are excited virtually, are only suppressed by a ratio of the mean interaction energy to $\hbar\omega_{\perp}$ and lead to thermalization and a breakdown of integrability [5].

Nevertheless the beautiful experiments by Kinoshita *et al.* [6] showed that for strongly correlated 1D systems thermalization is negligible. In this Rapid Communication we analyze how these two experiments and the theoretical model can be reconciled and show that the virtual three-body collisions described in [4] are suppressed by quantum correlations in strongly correlated 1D Bose gas.

We start by considering N identical bosons in 1D configuration with the Hamiltonian

$$\hat{H} = -\sum_{j=1}^N \frac{\partial^2}{\partial x_j^2} + 2c \sum_{j>j'} \delta(x_j - x_{j'}) + \sum_{j>j'>j''} U_{3b}(x_j - x_{j'}, x_j - x_{j''}), \quad (1)$$

thereby we use units where Planck's constant is 1 and the mass of the atom is $\frac{1}{2}$. In these units the strength of interaction of two atoms in a tight waveguide is $c = 2a_s/l_{\perp}^2$, where a_s is the three-dimensional (3D) s -wave scattering length and $l_{\perp} \gg a_s$ is the size of the transverse motion ground state of an atom in the waveguide [7].

Equation (1) differs from the Hamiltonian of the Lieb-Liniger model by including the term U_{3b} that describes three-body collisions (its value is nonzero, only if both its arguments are approximately 0, i.e., three atoms come close to each other). U_{3b} is obtained by adiabatic elimination of transverse modes virtually excited by the 3D short-range pairwise atomic interaction [4]. Note that the effective three-body interactions between polar molecules emerge in a similar way due to virtual transitions to an off-resonant internal state [8].

In a nondegenerate state, where free phase space is available for the scattered particles, U_{3b} leads to thermalization due to scattering of particles since a three-particle elastic collision in 1D, unlike a two-particle collision, allows for redistribution of the colliding particles momenta. In the ground state, this type of interactions not only changes the energy of the system but also precludes the Lieb-Liniger quasimomenta from being integrals of motion. U_{3b} is the source of thermalization and leads to a breakdown of integrability.

In what follows, we calculate this three-body scattering amplitude in the presence of the delta-functional pairwise interactions. The real part of this scattering amplitude determines the vertex for the effective three-body interaction by analogy with two-particle scattering in two dimensions [9–11]. The thermalization rate is proportional to the square of its absolute value. The stronger the *pairwise* interparticle repulsion, the smaller is the probability of a close encounter of three particles. This results in suppression of the three-body scattering amplitude, which is the main subject of the present Rapid Communication.

To analyze Hamiltonian (1) for $N=3$ we express it in hyperspherical coordinates R, α defined as [12]

$$R \sin \alpha = \frac{x_1 - x_2}{\sqrt{2}}, \quad R \cos \alpha = \sqrt{\frac{2}{3}} \left(x_3 - \frac{x_1 + x_2}{2} \right) \quad (2)$$

and the center-of-mass coordinate $X = \frac{1}{3}(x_1 + x_2 + x_3)$:

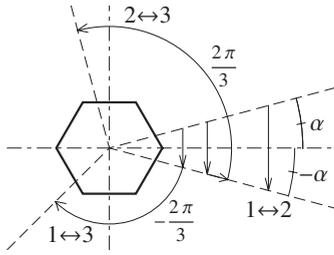


FIG. 1. Transformations of the hyperangle α corresponding to the pairwise permutations of particles $j \leftrightarrow j'$. The regular hexagon indicates the symmetry of the Hamiltonian of three pairwise-interacting identical particles. The two-body interaction potential has delta-functional singularity on straight lines (not shown in this figure) going through opposite vertices of the hexagon, cf. Eq. (3). See text for the details.

$$\hat{H} = -\frac{1}{3} \frac{\partial^2}{\partial X^2} - \frac{1}{R} \frac{\partial}{\partial R} R \frac{\partial}{\partial R} - \frac{1}{R^2} \frac{\partial^2}{\partial \alpha^2} + \frac{\sqrt{2}c}{R} \sum_{\nu=-2}^3 \delta(\alpha - \nu\pi/3) + U_{3b}(R, \alpha). \quad (3)$$

If one deals with three particles in the 3D space, the total number of degrees of freedom equals to 9. After separation of the center-of-mass motion, six degrees of freedom remain. The corresponding coordinates in the usual 3D case are R , α , and four angles characterizing the orientation of two independent differences of the particles radius vectors [12]. In our 1D case, the coordinate space reduces, after separation of the center-of-mass motion, to a plane, R and α being its polar coordinates.

For indistinguishable bosons the permutation $x_1 \leftrightarrow x_2$ corresponds to the reflection operation that changes α to $-\alpha$. The two remaining pairwise permutations, $x_3 \leftrightarrow x_2$ and $x_1 \leftrightarrow x_3$, correspond to the product of this reflection and rotation in the plane by $-2\pi/3$ and $2\pi/3$, respectively, as shown in Fig. 1. The two cyclic permutations of x_1, x_2 , and x_3 correspond to mere rotations by $\pm 2\pi/3$. The three-body interaction potential (its particular form will be specified later) must be invariant with respect to the permutation of the particles. The Hamiltonian of the three particles interacting via pairwise interactions only, i.e., Eq. (3) except of the term $U_{3b}(R, \alpha)$, possesses a richer symmetry (the symmetry group D_6 of a regular hexagon [13]; two of its six reflection-symmetry axes are shown in Fig. 1 by dash-dotted lines). Adding any reasonable effective three-body interaction does not change this symmetry.

The Schrödinger equation for the three-particle wave function is $\hat{H}\Psi(x_1, x_2, x_3) = (k_1^2 + k_2^2 + k_3^2)\Psi(x_1, x_2, x_3)$. The wave numbers k_j can be defined from the set of transcendental equations [2] provided that the periodic boundary conditions are set on the interval of the length L . By setting $L \rightarrow \infty$, we obtain a continuous spectrum of real k_j s in the repulsive case ($c > 0$). Then we separate the center-of-mass motion and describe the relative motion in hyperspherical coordinates: $\Psi(x_1, x_2, x_3) = \exp[i(k_1 + k_2 + k_3)X]\psi_r(R, \alpha)$. The kinetic energy of the relative motion is $k^2 = \frac{1}{3}[(k_1 - k_2)^2 + (k_2 - k_3)^2 + (k_3 - k_1)^2]$. We decompose the wave function of the three colliding particles in the center-of-mass frame as [12]

$$\psi_r(R, \alpha) = \sum_{n=0}^{\infty} F_n(R) \chi_n(R, \alpha), \quad (4)$$

where $\chi_n(R, \alpha)$ is an eigenfunction of the hyperangle-dependent part of the Hamiltonian

$$\left[-\frac{\partial^2}{\partial \alpha^2} + \sqrt{2}cR \sum_{\nu=-2}^3 \delta(\alpha - \nu\pi/3) \right] \chi_n(R, \alpha) = \lambda_n^2(R) \chi_n(R, \alpha). \quad (5)$$

Due to the bosonic symmetry,

$$\chi_n(R, \alpha) = \chi_n(R, \pm \alpha + 2\pi\nu'/3), \quad \nu' = -1, 0, 1. \quad (6)$$

Equation (6) defines the spectrum of eigenvalues and, hence, the adiabatic hyperspherical potentials $\lambda_n^2(R)/R^2$. The eigenfunctions are

$$\chi_n(R, \alpha) = \tilde{\chi}_n(R, \alpha) + \tilde{\chi}_n(R, \alpha - 2\pi/3) + \tilde{\chi}_n(R, \alpha + 2\pi/3), \quad (7)$$

where

$$\tilde{\chi}_n(R, \alpha) = \begin{cases} \cos[\lambda_n(R)(\pi/6 - |\alpha|) - \pi n/2], & |\alpha| \leq \pi/3 \\ 0, & \text{otherwise,} \end{cases} \quad (8)$$

and the eigenvalues are the positive roots of the equation

$$\lambda_n(R) \tan[\pi\lambda_n(R)/6 - \pi n/2] = cR/\sqrt{2}, \quad n = 0, 1, 2, \dots \quad (9)$$

After integrating out the hyperangular variable, the Schrödinger equation reduces to the set of coupled ordinary differential equations

$$-\frac{1}{R} \frac{d}{dR} R \frac{d}{dR} F_n - \sum_{n'=0}^{\infty} \left\{ \tilde{W}_{nn'}(R) \frac{d}{dR} F_{n'} + [\tilde{Y}_{nn'}(R) - \tilde{U}_{nn'}(R)] F_{n'} \right\} + \frac{\lambda_n^2(R)}{R^2} F_n = k^2 F_n, \quad (10)$$

where

$$\tilde{W}_{nn'}(R) = 2 \int_0^{\pi/3} d\alpha \frac{\tilde{\chi}_n(R, \alpha)}{B_n(R)} \frac{\partial}{\partial R} \tilde{\chi}_{n'}(R, \alpha), \quad (11)$$

$$\tilde{Y}_{nn'}(R) = \int_0^{\pi/3} d\alpha \frac{\tilde{\chi}_n(R, \alpha)}{B_n(R)R} \frac{\partial}{\partial R} R \frac{\partial}{\partial R} \tilde{\chi}_{n'}(R, \alpha), \quad (12)$$

$$\tilde{U}_{nn'}(R) = \int_0^{\pi/3} d\alpha \frac{\tilde{\chi}_n(R, \alpha) U_{3b}(R, \alpha) \tilde{\chi}_{n'}(R, \alpha)}{B_n(R)}, \quad (13)$$

$$B_n(R) = \int_0^{\pi/3} d\alpha \tilde{\chi}_n^2(R, \alpha). \quad (14)$$

Neglecting all off-diagonal (coupling) terms is termed adiabatic hyperspherical approximation [14]. However, for the sake of clarity, we neglect also diagonal terms \tilde{W}_{nn} and \tilde{Y}_{nn}

[12]. Indeed, the respective terms decrease more rapidly than others by a factor of $1/R$ as $R \rightarrow \infty$, and at $cR \lesssim 1$ the correction to the adiabatic potential $\lambda_0^2(R)/R^2$ due to $\tilde{Y}_{00}(R)$ is less than 5%. The finite value of \tilde{W}_{00} can be neglected compared to $\lambda_0^2(R)/R^2 \rightarrow \infty$ as $R \rightarrow 0$.

In what follows we assume the long-wavelength limit $k \ll c$, which holds in the regime of strong interactions [2] at temperatures of the order of or less than the chemical potential. It enables us to consider in Eqs. (4) and (10) only the lowest hyperangular mode, $n=0$, because in higher modes scattering is not efficient. We introduce the effective radius r_0 of the three-body interactions: U_{3b} rapidly vanishes for interatomic separation values exceeding r_0 . For atoms trapped in a tight waveguide, r_0 , such as the effective range of two-body collisions, is much smaller than other available length scales, in particular, $r_0 \ll c^{-1}$. We consider now, under the assumptions mentioned above, the equation

$$-\frac{1}{R} \frac{d}{dR} R \frac{d}{dR} F_0 + \left[\frac{\lambda_0^2(R)}{R^2} + \tilde{U}_{00}(R) \right] F_0 = k^2 F_0 \quad (15)$$

with the boundary conditions requiring F_0 to be finite for both $R=0$ and $R \rightarrow \infty$, for the ‘‘partial wave’’ corresponding to the lowest eigenvalue $\lambda_0(R)$, whose asymptotic expressions are

$$\lambda_0(R) \approx \begin{cases} \sqrt{\frac{3\sqrt{2}cR}{\pi}}, & cR \ll 1 \\ 3 - \frac{18\sqrt{2}}{\pi cR}, & cR \gg 1. \end{cases} \quad (16)$$

We assume that the averaged over the hyperangle three-body interaction potential $\tilde{U}_{00}(R)$ vanishes at $R > r_0$, where $r_0 \ll c^{-1}$.

First we solve Eq. (15) for $R > r_0$. For $cR \lesssim 1$ the two independent solutions are the modified Bessel functions of the zeroth order [15] $I_0(2\sqrt{\beta R})$ and $K_0(2\sqrt{\beta R})$, where $\beta = (3\sqrt{2}/\pi)c$ (we call them the inner solutions). The outer *real* solutions hold for $cR \gg 1$ and are the Bessel functions of the third order $J_3(kR)$ and $Y_3(kR)$. Now we note that in the range $c^{-1} \ll R \ll k^{-1}$ the outer solutions can be represented by their asymptotics $J_3(kR) \approx (kR)^3/48$ and $Y_3(kR) \approx (-16/\pi)/(kR)^3$. The outer and inner solutions can be tailored by quasiclassical solutions in two dimensions

$$\phi_{qc}^{\pm}(R) = \frac{C^{\pm}}{\sqrt{\lambda_0(R)}} \exp \left[\pm \int_0^R dR' \frac{\lambda_0(R')}{R'} \right]. \quad (17)$$

Note that two-dimensional quasiclassical solutions differ from one-dimensional ones [16] by a prefactor $1/\sqrt{R}$. By a proper choice of the constants C^{\pm} we match at $R \sim c^{-1}$ the quasiclassical solutions to the inner solutions: $\phi_{qc}^+(R)$ to $I_0(2\sqrt{\beta R}) \approx (4\pi\sqrt{\beta R})^{-1/2} \exp(2\sqrt{\beta R})$ and $\phi_{qc}^-(R)$ to $K_0(2\sqrt{\beta R}) \approx (4\sqrt{\beta R}/\pi)^{-1/2} \exp(-2\sqrt{\beta R})$, respectively. On the other hand, the asymptotics of the quasiclassical solutions at $cR \gg 1$ are

$$\phi_{qc}^+(R) \approx \frac{\Xi}{\sqrt{12\pi}} (cR)^3, \quad \phi_{qc}^-(R) \approx \frac{\sqrt{\pi}}{\sqrt{12\Xi}} (cR)^{-3}, \quad (18)$$

where $\Xi \approx 0.18$ is a numerical constant. This tailoring enables us to construct two independent real solutions $F^{\pm}(R)$ of Eq. (15) in the whole range $R > r_0$ with the following asymptotics:

$$F^+(R) \approx \begin{cases} I_0(2\sqrt{\beta R}), & cR \lesssim 1 \\ \frac{8\sqrt{3}\Xi}{\sqrt{\pi}} \left(\frac{c}{k}\right)^3 J_3(kR), & cR \gg 1, \end{cases} \quad (19)$$

$$F^-(R) \approx \begin{cases} K_0(2\sqrt{\beta R}), & cR \lesssim 1 \\ -\frac{\pi\sqrt{\pi}}{32\sqrt{3}\Xi} \left(\frac{k}{c}\right)^3 [Y_3(kR) + bJ_3(kR)], & cR \gg 1, \end{cases} \quad (20)$$

where b is a real number of the order of or less than 1. In other words, the term $Y_3(kR) \propto R^{-3}$ is only the leading term of the expansion of $F^-(R)$ in the intermediate range of R ; the solution $J_3(kR)$ vanishing for small $kR \ll 1$ is contained, in a general case, in terms beyond the accuracy of the quasiclassical approximation [16]. The upper limit to the magnitude of b follows from the fact that quasiclassical expression (18) for $\phi_{qc}^-(R)$ holds up to $R \sim k^{-1}$.

The general solution of Eq. (15) for $R > r_0$ is then

$$F_0(R) = C_1 F^+(R) + C_2 F^-(R). \quad (21)$$

The particular ratio between the coefficients C_1 and C_2 is found from matching the logarithmic derivatives of the solution given by Eq. (21) and its solution at $R < r_0$.

As a concrete example, illustrating the basic physics through simple analytic expressions, we take the three-body interaction potential in the form of the sum of a rectangular potential well and a term compensating the adiabatic hyperspherical potential at $R < r_0$:

$$\tilde{U}_{00}(R) = -q^2 - \beta/R, \quad R < r_0. \quad (22)$$

Without loss of generality, we assume further that $k \ll q$. In this case the regular solution at $R < r_0$ is $J_0(qR)$. Matching the logarithmic derivatives of the solutions at $R > r_0$ and $R < r_0$, recalling that $r_0 \ll c^{-1}$, and using the asymptotics $I_0(z) \approx 1$ and $K_0(z) \approx -\ln z$ at $z \rightarrow 0$, we obtain

$$\frac{C_1}{C_2} = \ln(2\sqrt{\beta r_0}) + \frac{J_0(qr_0)}{2qr_0 J_1(qr_0)}. \quad (23)$$

Then we calculate the partial scattering amplitude \tilde{f}_0 (corresponding to the scattering channel with $n=0$) introduced by expressing Eq. (21) at $R \rightarrow \infty$ in the form

$$F_0(R) \approx \text{const} [J_3(kR) - i\tilde{f}_0 H_3^{(1)}(kR)], \quad (24)$$

where $H_3^{(1)}(z) = J_3(z) + iY_3(z)$ is the Hankel function of the first kind, corresponding to the outgoing (scattered) wave. Note that there are various definition of the scattering amplitude in 2D, differing by a complex prefactor [10,17,18]. The rate of three-body collisions is proportional to $|\tilde{f}_0|^2$.

Using Eqs. (19) and (20), we obtain

$$\tilde{f}_0 = \frac{1}{-\Omega\left(\frac{c}{k}\right)^6[\ln(4\beta r_0) + \mathcal{J}] + b + i}, \quad (25)$$

where $\Omega = 384(\Xi/\pi)^2 \approx 1.26$ and $\mathcal{J} = J_0(qr_0)/[qr_0J_1(qr_0)]$. Other choice of $\tilde{U}_{00}(R)$ rather than Eq. (22) gives different value for \mathcal{J} , but does not change the general structure of Eq. (25). Although the exact value of b cannot be obtained from the quasiclassical matching of solutions, it is relatively small ($|b| \lesssim 1$) and thus b can be neglected in Eq. (25).

From Eq. (25) we conclude that the three-body scattering amplitude decreases in proportion to $(k/c)^6$ as $c \rightarrow \infty$, and the three-body scattering rate in a 1D system of bosons in the case of strong pairwise interaction is suppressed by a factor $\sim (k/c)^{12}$. This suppression is the main result of the present Rapid Communication. Averaging over collision momenta in a moderately excited strongly interacting state we obtain the scattering rate suppression factor $\sim \gamma^{-12}$, where $\gamma = c/n_{1D}$ is the Lieb-Liniger parameter [2] and $n_{1D} = \langle \hat{\Psi}^\dagger(x)\hat{\Psi}(x) \rangle$ is the 1D density of particles, $\hat{\Psi}(x)$ being the bosonic field annihilation operator.

We can now compare our result with the zero-distance three-particle correlation function $g_3(0) = \langle \hat{\Psi}^{\dagger 3}(x)\hat{\Psi}^3(x) \rangle / n_{1D}^3$. In the strong interaction limit $\gamma \gg 1$, we have $g_3(0) \propto \gamma^{-6}$

[19,20]. This thus proves the conjecture [4] that the pairwise interactions and the quantum correlations induced by them in a strongly interacting 1D bosonic system suppress the three-body elastic scattering rate and, hence, thermalization by a factor $\propto g_3^2(0)$. In other words, strong quantum correlations restore integrability as a 1D system approaches the Tonks-Girardeau regime. This observation is in agreement with the experimental results [6].

In conclusion we remark that integrability in tightly confined 1D systems is not, as suggested by quasiclassical arguments, caused by the freeze out of two-body collisions but is ensured by the quantum correlations in a strongly interacting 1D system. The genuinely quantum effect of virtual excitations to higher radial states opens a way to thermalization by three-body collisions and breaks integrability in the quantum description of a 1D system. These three-body collisions can be suppressed by quantum correlations caused by strong pairwise repulsions. If they dominate, as in a strongly correlated 1D Tonks-Girardeau gas, they restore the integrability of the system. This points to an interesting difference between classical and quantum systems.

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- [1] H. B. Thacker, *Rev. Mod. Phys.* **53**, 253 (1981).
 [2] E. H. Lieb and W. Liniger, *Phys. Rev.* **130**, 1605 (1963).
 [3] S. Hofferberth *et al.*, *Nat. Phys.* **4**, 489 (2008).
 [4] I. E. Mazets, T. Schumm, and J. Schmiedmayer, *Phys. Rev. Lett.* **100**, 210403 (2008).
 [5] Another possibility to violate integrability in 1D is to place (by means of Feshbach resonance) a weakly bound molecular state very close to the dissociation limit, thus making the effective atom-atom interaction energy dependent and therefore not describable by a delta-functional pseudopotential; see V. A. Yurovsky, A. Ben-Reuven, and M. Olshanii, *Phys. Rev. Lett.* **96**, 163201 (2006).
 [6] T. Kinoshita, T. Wenger, and D. S. Weiss, *Nature (London)* **440**, 900 (2006).
 [7] M. Olshanii, *Phys. Rev. Lett.* **81**, 938 (1998).
 [8] H. P. Büchler, A. Micheli, and P. Zoller, *Nat. Phys.* **3**, 726 (2007).
 [9] M. Schick, *Phys. Rev. A* **3**, 1067 (1971).
 [10] D. S. Petrov and G. V. Shlyapnikov, *Phys. Rev. A* **64**, 012706 (2001).
 [11] A simple way to prove it is to use the lowest order constrained variational approach as in S. Cowell *et al.*, *Phys. Rev. Lett.* **88**, 210403 (2002).
 [12] E. Braaten and H.-W. Hammer, *Phys. Rep.* **428**, 259 (2006).
 [13] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Butterworth-Heinemann, Oxford, 2003), Chap. XII.
 [14] J. Macek, *Z. Phys. D* **3**, 31 (1986).
 [15] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, Washington, DC, 1964), Chap. 9.
 [16] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Butterworth-Heinemann, Oxford, 2003), Chap. VII.
 [17] I. R. Lapidus, *Am. J. Phys.* **50**, 45 (1982).
 [18] S. K. Adhikari, *Am. J. Phys.* **54**, 362 (1986).
 [19] D. M. Gangardt and G. V. Shlyapnikov, *Phys. Rev. Lett.* **90**, 010401 (2003).
 [20] V. V. Cheianov, H. Smith, and M. B. Zvonarev, *Phys. Rev. A* **73**, 051604(R) (2006).