Restricted Thermalization for Two Interacting Atoms in a Multimode Harmonic Waveguide

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In this article, we study the thermalizability of a system consisting of two atoms in a circular, transversely harmonic waveguide in the multimode regime. While showing some signatures of the quantum-chaotic behavior, the system fails to reach a thermal equilibrium in a relaxation from an initial state, even when the interaction between the atoms is infinitely strong. We relate this phenomenon to the previously addressed unattainability of a complete quantum chaos in the Šeba billiard [P. Šeba, Phys. Rev. Lett., 64, 1855 (1990)], and we conjecture the absence of a complete thermalization to be a generic property of integrable quantum systems perturbed by a non-integrable but well localized perturbation.

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Introduction.-- The ultracold quantum gases have been long proven to be an ideal testbench for studying the fundamental properties of quantum systems. One of the most interesting and frequently addressed topics is the behavior of quantum systems in the vicinity of an integrable point. Experimental results already include the suppression of relaxation of the momentum distribution [1] and the modified decay of coherence [2]. Note that the fully developed quantum chaos with ultracold atoms has been investigated in experiments [3].

Traditionally, the underlying integrable system is represented by the Lieb-Liniger gas [4] that is well suited to describe the dynamics of Van-der-Waals interacting bosons in a monomode atomic guide (see [5] for a review). The nontrivial integrals of motion there are intimately related to both the one-dimensional character of the atomic motion and to the effectively zero value of the two-body interaction range. The causes for lifting integrability include the virtual excitation of the transverse modes during the collision [6] and the coupling between two parallel weakly interacting Lieb-Liniger gases [2].

One would expect that in the multimode regime, when the motion becomes substantially multidimensional, no remnants of the former integrals of motion will survive. However, in this article we show that for the case of only two interacting atoms a strong separation between the transverse and longitudinal degrees of freedom remains, even in the case of the infinitely strong interaction between the atoms. We attribute this effect to the short-range nature of the interaction.

For our system we study both the degree of the eigenstate thermalization and the actual thermalization in an expansion from a class of realistic initial states. The eigenstate thermalization [2, 3] – the suppression of the eigenstate-by-eigenstate variance of quantum expectation values of simple observables – provides an ultimate upper bound for a possible deviation of the relaxed value of an observable from its thermodynamical expectation, for any initial state in principle. However, recently a new direction of research has emerged: quantum quench in many-body interacting systems [1, 2, 9, 10]. In this class of problems, the initial state is inevitably decomposed into a large superposition of the eigenstates of the Hamiltonian governing the dynamics, and the discrepancy between the result of the relaxation and thermal values is expected to be diminished. In our article we show that in the case of two short-range-interacting atoms in a harmonic waveguide, a complete thermalization can never be reached under either scenario.

We relate the absence of thermalization in our system to the previously addressed unattainability of a complete quantum chaos in the Šeba billiard – flat two-dimensional rectangular billiard with a zero-range scatterer in the middle [11]. Similarly to our system, the Šeba billiard does show some signatures of the quantum-chaotic behavior, although both the level statistics [12, 14] and the momentum distributions in individual eigenstates [15] show substantial deviations from the quantum chaos predictions. Both the Šeba billiard (first suggested and solved in Ref. [11]) and our system allow for an exact analytic solution, in spite of the absence of a complete set of integrals of motion.

The system.-- Consider two short-range-interacting atoms in a circular, transversally harmonic waveguide. In this case the center-of-mass and the relative motion can be separated. Note that the harmonic approximation for the transverse confinement has been proven to model real life atom waveguides with high accuracy. Predictions of the analogous model involving an infinite waveguide [16, 17] has been confirmed by a direct experiment-theory comparison of the energies of the quasi-one-dimensional dimers [18] and numerical calculations involving anhar-
monic potentials (see review [3] for references).

The unperturbed Hamiltonian of the relative motion is given by the sum of the longitudinal and transverse kinetic energies and the transverse trapping energy $\hat{U} = \mu \omega_{\perp}^2 \rho^2 / 2$,

$$\hat{H}_0 = -\frac{h^2}{2\mu} \frac{\partial^2}{\partial z^2} - \frac{h^2}{2\mu} \Delta_{\rho} + \hat{U} - \hbar \omega_{\perp},$$

(1)

where $\omega_{\perp}$ is the transverse frequency, $\Delta_{\rho}$ is the transverse two-dimensional Laplacian, and $\mu$ is the reduced mass. In our model, the transverse and longitudinal degrees of freedom are coupled by a potential of a Fermi-Huang type [3]:

$$\hat{V} = \frac{2\pi \hbar^2 a_s}{\mu} \delta_3(r)(\partial / \partial r)(r \cdot r),$$

(2)

were, $a_s$ is the three-dimensional $s$-wave scattering length. This approximation is valid at low collision energies (e.g., below 300 mK for Li, see a recent review [10], while the ultracold atom energies lie well below 1 µK). The model (2) stands in a excellent agreement with the experimentally measured equation of state of the waveguide-trapped Bose gas [20] and with numerical calculations with finite-range potentials [17, 21].

The ring geometry of the waveguide imposes period-$L$ boundary conditions along $z$-direction. In what follows, we will restrict the Hilbert space to the states that have zero $z$-component of the angular momentum and that are even under the $z \leftrightarrow -z$ reflection; the interaction has no effect on the rest of the Hilbert space. The unperturbed spectrum is given by (see [22]) $E_{nl} = 2\hbar \omega_{\perp} n + h^2 (2\pi l/L)^2 / (2\mu)$, where $n \geq 0$ and $l \geq 0$ are the transverse and longitudinal quantum numbers, respectively.

The interacting eigenfunctions with the eigenenergy $E_{\alpha}$ can be expressed as (see [22]):

$$\langle \rho, z | \alpha \rangle = C_{\alpha} \sum_{n=0}^{\infty} \frac{\cos(2\sqrt{\epsilon_{\alpha} - \lambda n})}{\sqrt{\epsilon_{\alpha} - \lambda} \sin \sqrt{\epsilon_{\alpha} - \lambda}} e^{-\frac{1}{2} L_n^0(\xi)}(3)$$

where the rescaled energy $\epsilon_{\alpha}$ is given by $\epsilon_{\alpha} \equiv \lambda E_{\alpha} / (2\hbar \omega_{\perp})$, $\lambda \equiv (L/a_{\perp})^2$ is the aspect ratio, $\xi \equiv z / L - 1 / 2$, $L_n^0(\xi)$ are the Legendre polynomials, $a_{\perp} = (\hbar / \mu \omega_{\perp})^{1/2}$ is the size of the transverse ground state, and $C_{\alpha}$ is the normalization constant. The eigenenergies are solutions of the following transcendental equation (see [22]):

$$\sqrt{\lambda} \sum_{n=0}^{\infty} \cot \sqrt{\epsilon_{\alpha} - \lambda n} + i \sqrt{\epsilon_{\alpha} - \lambda} - \zeta \left( \frac{1}{2} - \frac{\epsilon_{\alpha}}{\lambda} \right) = \frac{a_{\perp}}{a_s},$$

(4)

where $\zeta (\nu, x)$ is the Hurwitz $\zeta$-function (see [8]). Similar solutions were obtained for two atoms with a zero-range interaction in a cylindrically-symmetric harmonic potential [23] (that system was analysed numerically in Ref. [24]). Higher partial wave scatterers were analyzed in the Ref. [25].

At rational values of $\lambda / \pi^2$, the unperturbed energy spectrum shows degeneracies that are not fully lifted in the full [deduced from (4)] spectrum. To minimize the effect of the degeneracies, we, following Ref. [11], fix the length of the guide to $L/a_{\perp} \equiv \lambda = 2\phi_{gr} \pi^2 \approx 9774$, where $\phi_{gr} = (1 + \sqrt{5})/2$ is the golden ratio.

**Standard quantum-chaotic tests.** The results of the study of the level spacing distribution in our system are fully consistent with the analogous results for the Šeba billiard [12, 13]. For the energy range $E \gtrsim 100 \hbar \omega_{\perp}$ and the aspect ratio $(L/a_{\perp})^2 = 2\phi_{gr} \pi^2$, the distribution quickly converges to the Šeba distribution [12] at $a_s \gtrsim 10^{-1} a_{\perp}$. This distribution does show a gap at small level spacings but fails to reproduce the Gaussian tail predicted by the Gaussian Orthogonal Ensemble. At small $a_s$ the level spacing distribution tends to the Poisson one. We have also verified that in the unitary regime, $a_s \gg a_{\perp}$, the statistics of the point-by-point variations of the eigenstate wavefunction in the spatial representation is close to the Gaussian one, according to the general prediction [26] and a particular observation in the case of the Šeba billiard [11].

**Eigenstate thermalization.** According to the eigenstate thermalization hypothesis [7,8], the ability of an isolated quantum system (with few or many degrees of freedom regardless) to thermalize follows from the suppression of the eigenstate-by-eigenstate fluctuations of the quantum expectation values of relevant observables. Scattered dots at the Fig. 1 show the quantum expectation values of relevant observables. Both distributions are heavily dominated by only a few states (Fig. 1). The variation of $\langle \alpha | U | \alpha \rangle$ remains (in contrast to the quantum-chaotic billiards [27]) of the order of the mean, even for the energies much larger than any conceivable energy scale of the system. Here and below, we work in the regime of the infinitely strong interactions, $a_s = 10^6 a_{\perp}$.

For a given eigenstate, quantum expectation values of the occupation probabilities for the transverse (Fig. 2a) and longitudinal (Fig. 2b) modes show no convergence to their microcanonical expectation values, $P(n) \propto \int d\delta(E_{nl} - E)$ and $P(l) \propto \int d\delta(E_{nl} - E)$ respectively. Both distributions are heavily dominated by only a few peaks (cf. scars in the momentum space for Šeba billiards [15]).

**Relaxation from an initial state.** Now we are going to address directly the ability of our system to thermalize from an initial state $|\psi(t = 0)\rangle$. In this case, the infinite time average of the quantum expectation value of an observable $A$ will be given by $A_{\text{relax.}} \equiv \lim_{t_{\text{max}} \to \infty} \langle 1 / t_{\text{max}} \rangle \int_0^{t_{\text{max}}} \langle \psi(t) | A | \psi(t) \rangle = \sum_{|\alpha\rangle} \langle \alpha | A | \alpha \rangle$, where $|\alpha\rangle$ are the eigenstates of the system (see [8]). For a quantum-chaotic system, it is expected that the above infinite time average coincides with the
approximately a 40% deviation of the relaxed value of the first two sequences of the initial states of the type (5). The thermal prediction.

Consider the following initial state:

\[
\langle z | \psi(t = 0) \rangle \propto \cos \frac{\pi \epsilon}{\delta} \left\{ \frac{\delta}{2} - |\epsilon| \right\} \cos (2 \pi l_0 |z|) |n_0\rangle.
\]

Longitudinally, the state is represented by the ground state of a length \( L \delta \) hard-wall box split initially by an ideal beamsplitter with momenta \( \pm 2 \pi l_0 / L \); the box is centered at the maximal interatomic distance. The state is distributed among approximately \( \pi \delta / \delta \) axial modes localized about \( l = \pm l_0 \). The initial transverse state is limited to a single mode \( n_0 \). Note that for \( n_0 = 0 \) and \( \delta \approx 1 \) the state is conceptually similar to the initial state used in the equilibration experiments [1].

After relaxation, both transverse (Fig. 2a) and longitudinal (Fig. 2b) distributions remain very far from the equilibrium predictions. Fig. 1 shows the equilibrium value of the transverse trapping energy \( U \) (see [1]) for three sequences of the initial states of the type (5). The first two, with low transverse energy, show an approximately -40% deviation of the relaxed value of \( U \) from the thermal prediction, thus being seemingly correlated with its initial, negative value. Note that the correlation between the final and initial values of observables in quantum systems is addressed in Ref. [28]. Also, note that the initial states of the second sequence have a much greater spread over the longitudinal modes than the first sequence. The energy of the initial state is \( E \equiv (2/\lambda) \hbar \omega_\perp \epsilon_0 \approx 173.2 \hbar \omega_\perp \). The short-dashed (blue) line corresponds to the 17096’s eigenstate (closest in energy to \( E \) from the above, with a relative discrepancy of 10^-3) of the interacting Hamiltonian. The dotted (purple) line shows the microcanonical prediction. The rest of the parameters is the same as at the Fig. 1.

FIG. 1. The time average of the transverse trapping energy \( U_{\text{relax}} \equiv \lim_{\Delta t \to \infty} \langle U(t) \rangle / \Delta t \) after relaxation from an initial state as a function of the energy of the initial state \( E \) [see Hamiltonian (1)]. Four families of the initial states are considered. Long-dashed (green) line: state (5) with \( n_0 = 0, \delta = 0.99, \) and the energy being controlled via scanning \( l_0 \); short-dashed (blue) line: the same as the previous one, except for \( \delta = 1 \); dotted (purple) line: the state (5) with \( \delta = 0.1 \) and \( l_0 = 0 \) and the energy control via \( n_0 \); solid (red) line: state (6) with \( \delta = 2 \), \( \delta = 0.99, l_0 = 0 \) and the energy control via \( \kappa_1 \). Legends schematically show the distribution of the initial states over the quantum numbers; arrows indicate the direction in which the parameters controlling the energy are scanned. The asterisk (*) corresponds to the set of parameters used to produce the Fig. 2. Grey dots show the quantum expectation value of the trapping energy \( U \) for every hundreds eigenstate of the full Hamiltonian (11). The values of the trapping energy are shown with respect to its microcanonical expectation value \( U_{\text{therm.}} \approx E/3 \). For all the points, \( \langle L / a_\perp \rangle^2 = 2 \phi \pi \approx 9774 \) and \( a_\perp = 10^6 a_\perp \).

FIG. 2. Distribution of the mean occupation numbers for the transverse (a) and longitudinal (b) modes of the unperturbed Hamiltonian. The long-dashed (green) and solid (red) lines show the initial and time-averaged distributions for an initial state (5) with \( n_0 = 0, \delta = 0.99, \) and \( l_0 = 292.8 \). Energy of the initial state is \( E \equiv (2/\lambda) \hbar \omega_\perp \epsilon_0 \approx 173.2 \hbar \omega_\perp \). The short-dashed (blue) line corresponds to the 17096’s eigenstate (closest in energy to \( E \) from the above, with a relative discrepancy of 10^-3) of the interacting Hamiltonian. The dotted (purple) line shows the microcanonical prediction. The rest of the parameters is the same as at the Fig. 1.
Another type of the initial state
\[
\langle \rho, z|\psi(t=0)\rangle \propto \cos \frac{\pi \zeta}{\delta} \left( \frac{\delta}{2} - |\zeta| \right) \cos (2\pi l_0 \zeta) \\
\times (e^{-\kappa_1 \xi} - e^{-\kappa_2 \xi})
\]
allows for an additional spread over the transverse modes. The transverse wavefunction vanishes at the waveguide axis. The mode occupation has a minimum at \( n = 0 \), and the occupation of the ground transverse mode tends to zero for \( \kappa_1 < \kappa_2 \ll 1 \). The results for a sequence similar to the third sequence described above are shown at Fig. 4 as well. In spite of the significant initial spread over both transverse and longitudinal modes, the deviations from the equilibrium are close to the ones for the third sequence, while the energy-to-energy variations for the former are indeed less than for the latter.

Note that we have also successfully tested the convergence of the instantaneous quantum expectation values of the observables to their infinite-time averages.

**Summary and interpretation of results.** In this article, we solve analytically the problem of two short-range-interacting atoms in a circular, transversely harmonic multimode waveguide. We assess the ability of the system to thermalize from an initially excited state; a broad class of initial states has been analyzed. We find a substantial suppression of thermalization, even for the infinitely strong interactions. We associate this effect with the previously demonstrated unattainability of complete quantum chaos in the Šeba-type billiards [11–13].

We conjecture that the effect of suppression of thermalization is generic for the integrable systems perturbed, no matter how strong, by a well localized perturbation. The following reasoning applies. In a quantum chaotic system, a given eigenstate \(|\alpha\rangle\) consists of a large superposition of the eigenstates \(|\tilde{\alpha}\rangle\) of the underlying integrable system, which are drawn indiscriminately from the microcanonical shell. Number of principal components in such a superposition is a sensitive measure of the approach to a complete chaos and the subsequent thermalizability (see, for example [29]). The zero-point-localized perturbation, being a particular case of a separable perturbation, generates the eigenstates of a form \(|\tilde{\alpha}\rangle = 1/(E_\alpha - E_{\tilde{\alpha}})|\alpha\rangle\) (see [22]). There is always one and only one perturbed energy \(E_{\tilde{\alpha}}\) in between any two unperturbed energies \(E_{\alpha}\) (see [13]). In addition, for the case of the infinitely strong perturbation (where the approach to chaos is expected to be the closest) \(E_\alpha\) tends to the middle position between the two \(E_{\tilde{\alpha}}\)'s. In this case, the only energy scale that remains is the distance between the unperturbed levels, and, as a result, the number of principal components a given eigenstate \(|\alpha\rangle\) consists of is always of the order of unity. This property extends to the case of finite-range interactions, whenever the interaction range is much less than the de Broglie wavelength of the colliding atoms. Our study is the first attempt to address thermalizability of a quantum system with separable interactions.
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The waveguide system [1], as well as the Šeba billiard [2], belongs to the class of problems where an integrable system of Hamiltonian $\hat{H}_0$ is perturbed by a separable rank I interaction $V|\mathcal{L}\rangle\langle\mathcal{R}|$ (see e.g. [3]). Eigenstates $|\alpha\rangle$ of the interacting system are solutions of the Schrödinger equation

$$[\hat{H}_0 + V|\mathcal{L}\rangle\langle\mathcal{R}|]|\alpha\rangle = E_\alpha|\alpha\rangle,$$  

(1)

where $E_\alpha$ are the corresponding eigenenergies. Let us expand the eigenstate $|\alpha\rangle$ over the eigenstates $|\vec{n}\rangle$ (of energy $E_\vec{n}$) of the non-interacting Hamiltonian $\hat{H}_0$. The Schrödinger equation leads to the following equations for the expansion coefficients

$$(E_\alpha - E_{\vec{n}})|\vec{n}\rangle\langle\vec{n}|\alpha\rangle = \langle\vec{n}|\mathcal{L}\rangle\langle\mathcal{R}|\alpha\rangle \propto \langle\vec{n}|\mathcal{L}\rangle,$$  

(2)

where the omitted factor in the second equality is independent of $\vec{n}$.

As a result, any eigenfunction $|\alpha\rangle$ functionally coincides with the Green function of the non-interacting Hamiltonian taken at the energy of the eigenstate $E_\alpha$,

$$|\alpha\rangle \propto \sum_{\vec{n}}\frac{|\vec{n}\rangle\langle\vec{n}|\mathcal{L}|\alpha\rangle}{E_\alpha - E_{\vec{n}}}.$$  

(3)

The omitted factor is determined by the normalization conditions.

Substitution of this expression to the Schrödinger equation (1) leads to the following eigenenergy equation:

$$\sum_{\vec{n}}\frac{\langle\mathcal{R}|\vec{n}\rangle\langle\vec{n}|\mathcal{L}\rangle}{E_\alpha - E_{\vec{n}}} = \frac{1}{V}.$$  

(4)

Similar expressions were obtained in Refs. [2, 4] for the case of the Šeba billiard and its generalizations.

In the case of the relative motion of two short-range-interacting atoms in a circular, transversely harmonic waveguide, the derivation uses ideas of the analogous model involving an infinite waveguide [2, 4]. The unperturbed Hamiltonian here is given by Eq. (1) in [1] and the Fermi-Huang interaction (see Eq. (2) in [1]) can be written in the separable form [3] with the interaction strength and formfactors given by

$$V = \frac{2\pi a_s^2}{\mu}, \quad |\mathcal{L}| = \delta_3(r), \quad \langle\mathcal{R}| = \delta_3(r)\frac{\partial}{\partial r}(r\cdot).$$  

(5)

In what follows, we will restrict the Hilbert space to the states of zero $z$-component of the angular momentum and even under the $z \leftrightarrow -z$ reflection; the interaction has no effect on the rest of the Hilbert space. The non-interacting eigenstates are products of the transverse and longitudinal wavefunctions.

The transverse two-dimensional zero-angular-momentum harmonic wavefunctions, labeled by the quantum number $n \geq 0$, are expressed in terms of the Legendre polynomials, $L_n^0(\xi)$, where $\xi = (\rho/a_\perp)^2$ and $a_\perp = (\hbar/\mu \omega_\perp)^{1/2}$ is the transverse oscillator range. The longitudinal wavefunctions, labeled by $l \geq 0$, are the symmetric plane waves satisfying periodic conditions with the period $L$:

$$\langle z|k\rangle = (2/L)^{1/2}\cos 2\pi k\zeta, \quad \langle z|0\rangle = L^{-1/2},$$  

(7)

where $\zeta \equiv z/L - 1/2$. The unperturbed spectrum is therefore given by

$$E_{nl} = 2\hbar \omega_\perp n + \hbar^2(2\pi l/L)^2/(2\mu)$$  

(8)

Substituting the above non-interacting eigenstates and eigenenergies to Eq. (3) and using Eq. (1.445.8) in [8] for summation over $l$, one obtains Eq. (3) in [1] for the interacting eigenstates. The normalization factor $C_\alpha$ is determined by the condition

$$2\pi \int_0^L dz \int_0^\infty r^2 \rho^2 d\rho (\alpha\rho, z\zeta)\langle \rho, z |\alpha\rangle = \delta_{\alpha\alpha}$$  

(9)
Using orthogonality of the Legendre polynomials it can be expressed as

\[
C_\alpha = \frac{2}{a_\perp \sqrt{\pi L}} \left[ \sum_{n=0}^{\infty} \left( \cot \sqrt{\epsilon_\alpha - \lambda n} \right) \right]^{1/2},
\]

(10)

where the rescaled energy \( \epsilon_\alpha \) is given by \( \epsilon_\alpha \equiv \lambda E_\alpha / (2\hbar \omega_\perp) \) and \( \lambda \equiv (L/a_\perp)^2 \) is the aspect ratio.

For the Fermi-Huang interaction the eigenenergy equation (4) attains the form

\[
\frac{\partial}{\partial r} \left[ r \sum_{n,l} \langle \rho | n \rangle \langle z | l \rangle \langle n | 0 \rangle \langle 0 | 0 \rangle \right] = \frac{1}{V} \]

= 1

\[
V (11)
\]

In the limit \( r \to 0 \), the eigenstate is spherically symmetric. This allows us to deal with the \( z \)-axis only (see [6]). Substitution of the noninteracting wavefunctions (6) and (7) and energies (8) with the subsequent summation over \( l \) leads to

\[
\sqrt{\lambda} \frac{\partial}{\partial z} \left[ \sum_{n=0}^{\infty} \frac{\cos \left( 2\sqrt{\epsilon_\alpha - \lambda n} (z/L - 1/2) \right)}{\sqrt{\epsilon_\alpha - \lambda n} \sin \sqrt{\epsilon_\alpha - \lambda n}} \right] = \frac{a_s}{a_\perp}.
\]

(12)

This sum contains both the regular part and the irregular one, the latter being proportional to \( z^{-1} \). The regular part can be extracted using the identity

\[
\lim_{z \to 0} \left[ \sum_{n=0}^{\infty} (\lambda n - \epsilon)^{-1/2} \exp(-2\sqrt{\lambda n - \epsilon z} / L) \right] = \frac{L}{\lambda z}
\]

(see [6]) where \( \zeta (\nu, \alpha) \) is the Hurwitz zeta function (see, e.g., [7, 8]. Finally we arrive at the transcendental equation for the eigenenergies (4) in [1]. The summands in the sums Eqs. (3) and (4) in [1] and in Eq. (10) decay exponentially with \( n \), leading to the fast converging series. Note that the imaginary parts of the two terms in the left hand side of Eq. (4) in [1] cancel each other automatically.

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