Traces of integrability in scattering of one-dimensional dimers on a barrier

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Abstract

We consider molecules made of two one-dimensional short-range-interacting bosonic atoms. We show that in the process of scattering of these molecules off a narrow barrier, odd incident waves produce no unbound atoms, even when the incident energy exceeds the dissociation threshold. We demonstrate that such a feature originates from the fact that our system shares a part of its spectrum, namely its odd eigenstates, with a Bethe Ansatz integrable model, a \(\delta\)-interaction Hamiltonian with local and non-local terms, associated with a reflection group \(C_2\)—a full symmetry of a square. This partial integrability induces prohibition of chemical reactions, allowing us to make predictions about scattering processes. We suggest several experimental implementations of the effect. We also propose to use the monomer production as an alternative read-out channel in an atom interferometer: unlike in the standard interferometric schemes, no spatial separation of the output channels will be required. Our approach offers an example of use of integrable problems beyond the realm of fully integrable models.

1. Introduction

The last two decades are marked by a revival of interest in Bethe Ansatz integrable particle systems\([1–7]\), inspired by the emerged experimental relevance of the former in both many-body\([8–11]\) and few-body\([12, 13]\) cold-atom systems (see [14] for a review). Integrability, besides providing a way to produce theoretical predictions, also induces new empirically observable integrals of motion. Traditionally, the conservation of the momentum distribution is emphasised\([8, 15]\). However, another experimentally sound set of conserved quantities is derived from the conservation of the chemical composition\([16]\), i.e. the decomposition of the system onto unbound atoms, dimers\([12]\), trimers, all the way to the long polymers, the latter manifesting themselves as bosonic solitons\([17, 18]\).

Below we show that an integrability-related chemical stability also appears in a system that consists of two one-dimensional attractive short-range-interacting bosons and a narrow barrier. While generally not integrable, our system shares some of its eigenstates with a lesser studied integrable model based on a reflection group \(C_2\)\([19]\) (see also\([20–22]\) for the naming convention), a symmetry group of a square. As a result, an odd incident wave of dimers shows a strictly vanishing rate of a monomer production, no matter how far above the dissociation threshold the incident energy is.

1.1. Model

In this work, we investigate the scattering states of a bosonic dimer on a potential barrier by modeling the system as two one-dimensional \(\delta\)-interacting bosons in presence of a \(\delta\)-potential barrier located at the center of the system. The Hamiltonian reads:
\[
\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2} + g_{ab} \delta(x_1) + g_{ab} \delta(x_2) + g\delta(x_1 - x_2),
\]

with \( g_{ab} > 0 \) being the strength of the potential barrier, \( g = -\hbar^2/\mu \) \( < 0 \) the strength of the attractive interatomic interactions and where \( a \) is the one-dimensional even-wave scattering length \([23]\), \( \mu = m/2 \) the reduced mass and \( m \) the mass of the atoms.

Prior to an encounter with the barrier, the energy of the dimer reads:

\[
E = \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2 k^2}{2m} - \frac{\hbar^2}{2\mu a^2},
\]

where \( \hbar k \) is the momentum of either particle in the dimer; the latter is related to the center-of-mass incident momentum, \( \hbar K \), as \( \hbar k \equiv h K/2 \). The dissociation condition, \( k > 1/a \), can be readily inferred from the relationship (2); it ensures that the system has enough kinetic energy to invest towards dissociation [4].

The presence of the barrier in (1) breaks the integrability of the model. However, we show below that the spatially odd scattering states of the system described by (1) coincide with the ones of the integrable model described by the following Hamiltonian:

\[
\hat{H}_{C_2} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2} + g_{ab} \delta(x_1) + g_{ab} \delta(x_2) + g\delta(x_1 - x_2) + g\delta(x_1 + x_2).
\]

The above Hamiltonian can be shown to be integrable—in all symmetry sectors—using a Bethe Ansatz based on a symmetry group of a square, \( C_2 \). This model, as well as all its multidimensional and affine generalizations, was first analyzed by Gaudin [4, 19], albeit with a conjecture that there exists a single integrability-supporting value of the ratio between the coupling constants \( g_{ab} \) and \( g \). The works [24, 25] show that integrability persists for any ratio between the constants, but restrict the treatment to the ’identity’ representation of the group. The paper [26] can be used to construct other representations of the corresponding reflection groups, in particular the one we are using in this article. In the affine case, it can be shown that the model supports three independent coupling constants [27]. Note that, the same rich choice of parameters is paralleled in the Calogero–Sutherland–Moser models [7].

Let us now show that the spatially odd sector of eigenstates of the Hamiltonians given in equations (1) and (3) indeed coincide. We introduce the permutation, \( \hat{P}\psi(x_1, x_2) = \psi(x_2, x_1) \), and the spatial reflection, \( \hat{P}^r\psi(x_1, x_2) = \psi(-x_1, -x_2) \), transformations. They allow us to introduce a subspace of bosonic, spatially odd states, \( \psi_{+, \ldots} \):

\[
\hat{P}\psi_{+, \ldots}(x_1, x_2) = +\psi_{+, \ldots}(x_1, x_2),
\]

\[
\hat{P}\psi_{+, \ldots}(x_1, x_2) = -\psi_{+, \ldots}(x_1, x_2).
\]

Note that \( [\hat{P}, \hat{H}] = [\hat{P}^r, \hat{H}] = 0 \) and \( [\hat{P}, \hat{P}^r] = 0 \). The reflection symmetry with respect to the \( x_2 = -x_1 \) line—one of the four symmetry axes of the \( C_2 \) model—can be written as \( \hat{R} = \hat{P}\hat{P}^r \); it commutes with the transformations \( \hat{P} \) and \( \hat{P}^r \) and with the Hamiltonian (3). As a result, the \( \psi_{+, \ldots} \) eigenstates of the \( \hat{R} \), i.e. \( \hat{R}\psi_{+, \ldots}(x_1, x_2) = -\psi_{+, \ldots}(x_1, x_2) \), vanish for \( x_2 = -x_1 \), i.e. on the line where the (unphysical) integrability-restoring term \( g\delta(x_1 + x_2) \) in (3) acts. Hence, the spatially odd states \( \psi_{+, \ldots} \) are simultaneously eigenstates of equations (1) and (3), allowing us to connect the eigenstates of an integrable system, with all the corresponding conservation quantities associated to them, with the ones of a generally non-integrable one. Notice that this property holds only for \( N = 2 \) bosons, since in this case the unphysical non-local \( \delta(x_1 + x_2) \) interactions can be rendered unaccessible, by a node in the spatially odd sector of the Hilbert space. For more than two particles, no symmetry can generate enough nodes to hide such non-local terms. It is worth noticing that for hard-core interactions the whole area of the many-body coordinate space—not only the nodal surfaces—can be hidden. As a result, approximately half of the known reflection groups allow for a two-body hard-core empirical realization. The list includes both affine [28] and finite groups, including the non-crystallographic ones [29].

Among all the eigenstates of equation (1), we shall now focus on those corresponding to scattering states, i.e. non-normalizable states satisfying plane-wave incoming boundary conditions. Since our scattering potential conserves the spatial parity, we will be considering the even and the odd partial waves separately, along with the even and odd scattering solutions. We will show below that for the odd states, the hidden partial integrability revealed above leads to tangible consequences.

The most general form of an even scattering solution of (1) with respect to the spatial reflection symmetry \( \hat{P}^r \) reads

\[
\psi_{\text{even}}(x_1, x_2) \propto e^{-i|\varphi|/a} \cos(K X) + f_{\text{even}}(K)e^{iK|x|} + F_{\text{even}}(\varphi)e^{i\varphi},
\]

With center-of-mass coordinate \( X \equiv (x_1 + x_2)/2 \), relative coordinates \( x \equiv x_1 - x_2 \) and incoming center-of-mass momentum \( \pm K \), and where we use cylindrical coordinates \((r, \varphi)\), with \( x_1 = r \cos(\varphi) \) and \( x_2 = r \sin(\varphi) \), for the
part of the wavefunction corresponding to unbound monomers. The even monomer scattering amplitude satisfies \( F_{\text{even}}(\pi + \varphi) = F_{\text{even}}(\varphi) \). Likewise, the odd scattering solution reads:
\[
\psi_{\text{odd}}(x_1, x_2) \propto a^{-1/2} e^{-|x|a/\hbar} \sin(Kx_1) - i F_{\text{odd}}(K) \sin(Kx_2)
\]
where \( F_{\text{odd}}(\pi + \varphi) = -F_{\text{odd}}(\varphi) \). Here and below, \( \kappa = \sqrt{2((ka)^2 - 1)/a} \). Note also that due to the bosonic symmetry of the incident wave, the monomer scattering amplitudes obey \( F_{\text{even/odd}}(\pi/2 - \varphi) = F_{\text{even/odd}}(\varphi) \).

2. Preservation of chemical composition

Be the Ansatz integrable systems are known to preserve the chemical composition \[16\]. In particular, in the \( C_2 \)-integrable model \[3\], any purely dimeric incident wave will not produce unbound monomers after a collision with the barrier, even at energies higher than the dimer dissociation threshold\(^3\). This preservation of the chemical composition can be demonstrated by considering the available rapidities produced by a dimeric incident wave, all of which being substantially complex and as such, supporting no monomers. Indeed, the underlying reflection group, induced by four mirrors with a 45° angle between them can only permute and change sign of the incident rapidities, but it is not capable of altering their imaginary parts. In particular, the above conclusion is valid for a spatially odd linear combination of the incident dimeric waves. The scattering solution induced by it will also be spatially odd. But as we have shown above, odd eigenstates of the Hamiltonian \((3)\) are, at the same time, the eigenstates of the empirically relevant Hamiltonian \((1)\). This brings us to the central result of this article: \( F_{\text{odd}}(\varphi) \) is identically zero at all incident energies.

Hence, for both Hamiltonians, the corresponding odd scattering solution can be written as
\[
\psi(x_1, x_2) \propto a^{-1/2} e^{-|x|a/\hbar} \sin(Kx_2) + \delta_{\text{odd}}(K).
\]
The scattering phase \( \delta_{\text{odd}}(K) \) can be obtained after a long but straightforward calculation that mirrors the one for the \( A_2 \) reflection group \[3\] (scattering of a dimer on a monomer for three distinguishable particles of the same mass, interacting with the same strength):
\[
\delta_{\text{odd}}(K) = \frac{1}{2} \arctan \left( \frac{2a^2k(a(aa_{ab}k^2 - 1) + a_{ab})(aak(a_{ab}k^2 - 1) + a_{ab})}{a(ak(a_{ab}k^2 - 1) - 1) + a_{ab}} \right),
\]
where \( a_{ab} = -\frac{\hbar^2}{mk_{ab}} \) is the scattering length associated with the interaction of a single particle with the barrier. This result also allows to define the dimer-barrier odd scattering length as
\[
a_{ab,\text{odd}} = -\frac{d}{dK} \delta_{\text{odd}}(K = 0) = \frac{a^2}{2(a - a_{ab})}.
\]

3. Single incident dimeric wavepacket and its dissociation

By numerical solution of the time-dependent many-body Schrödinger equation associated to \((1)\), we investigate the scattering of an incident (from the left) dimer, of the form
\[
\psi_{\text{in}}(x_1, x_2, t = 0) \propto e^{-|x|a/\hbar} e^{-(x + x_0)^2/4\sigma^2 + iKx},
\]
where \( x = -x_0 \) is the position of the center of mass of the dimer at initial time.

Figure 1 shows the particle density, \( |\psi(x_1, x_2)|^2 \), at long times after the initial dimer has collided against the barrier. If the kinetic energy of the incoming dimer is smaller than the threshold of monomer formation, we observe that the dimer is partially reflected and partially transmitted. However, a ‘deflection’ via formation of monomers is clearly visible above threshold (see also figure A4 in the appendix).

For each region \( S \) of the \((x_1, x_2)\) plane, the probability \( P(S) = \int \int |\psi(x_1, x_2)|^2 \) with \( S \) being the four sectors defined as \( R \equiv \{ x_1 < 0, x_2 < 0 \}, T \equiv \{ x_1 < 0, x_2 > 0 \}, M \equiv \{ x_1 > 0, x_2 < 0 \} \cup \{ x_1 > 0, x_2 > 0 \} \) yields the transmission and reflection coefficients, \( P(T) \) and \( P(R) \), respectively, along with the monomer formation probability, \( P(M) \). Our results for the three coefficients as a function of the initial wavevector of the dimer are summarized in figure 2. We notice that the non-vanishing monomer production indeed requires \( k > 1/a \).

\(^3\) In both cases, the normalization is chosen in such a way that number of atoms falling on the barrier per unit time is the same as in unidirectional atomic beam of atoms with a velocity \( V = \hbar k / 4m \) and a unit atomic number density.

\(^4\) Note that the unphysical delocalized dimers centered about the \( x_2 = -x_1 \) axis are not generally disallowed, but they are independently forbidden in the spatially odd states.
4. Two counterpropagating dimeric wavepackets

We consider next the solution of the two-body Schrödinger equation when the following initial condition is taken:

\[ \psi(x_1, x_2, t = 0) = e^{-i\phi/2}\psi_\uparrow_\downarrow(x_1, x_2, t = 0) + e^{i\phi/2}\psi_\uparrow_\downarrow(x_1, x_2, t = 0), \]

where \( \psi_\uparrow_\downarrow(x_1, x_2, 0) \propto e^{-|x_1|^2/\sigma^2}e^{-|x_2|^2/\sigma^2}e^{-i\phi} \).

In figure 3 we show the probability density when the input state is represented by a spatially even and a spatially odd linear combinations of dimeric wavepackets, thus corresponding to the choices \( \phi = 0 \) and \( \phi = \pi \) respectively. The figure corresponds to the case where \( ka = 4 \), i.e. the input kinetic energy of each dimeric wavepacket is above the threshold for monomer formation. The figure clearly shows that, while monomers are created in the spatially even configuration, a complete suppression of output monomers is achieved when choosing a spatially odd configuration, in full agreement with the predictions obtained by the spatial odd sector of the integrable \( C_2 \) model. We stress that for interacting particles this behavior cannot only be viewed as a single-particle interference effect. For a complete discussion and comparison of results of the interacting and non-interacting case please refer to the appendix.

The monomer formation probability as a function of the phase difference \( \phi \) between the incident dimeric wavepackets is shown at figure 4. In the same figure we also show a measure proportional to the density–density correlation function \( \rho_2(x, y) \), taken at zero distance and averaged over the sample, i.e. \( \int dx \rho_2(x, x) \). Notice that the local second-order correlation \( g_2(0) \) has been already made experimentally accessible in a one-dimensional setting [30].

5. Potential experimental realizations

One-dimensional dimers appear in several areas of physics of ultracold atoms. The best possible realization for our scheme is the bosonic sector of the Hilbert space of a spin-up spin-down pair of spin-\( \frac{1}{2} \) fermions [12]. At the
one dimer level, the problem is identical to two spin-0 bosons. At the many dimer level, spin-1 fermions do not form any polymers longer than dimers, thus making possible using continuous dimer beams in the interferometric applications. In this case, the $\delta$-interaction model is well justified in the regime where the size of the ground transverse vibrational state in the guide greatly exceeds the three-dimensional scattering length $[23]$. Other implementations of one-dimensional dimers are also possible. For instance, for repulsively interacting bosons, dimeric bound states have been implemented in photonic lattices $[31, 32]$, and shown to model the two-particle extended Bose–Hubbard Hamiltonian.

A priori, the one-dimensional dimers described in this article can be constructed using any type of one-dimensional bosonic particles provided that the corresponding interaction potential is sufficiently shallow; quantitatively, it will be required that the width of the interaction potential $w$ exceeds its scattering length $a$ $[33]$. A remarkable example is offered by the recently realized dimers of Rydberg polaritons $[34]$, where the $w$ is greater than $a$ by at least an order of magnitude. In both cases considered above, a narrowly focussed sheet of light can be used to generate a fixed one-particle barrier. A similar requirement, $w_{ab} \gg |a_{ab}|$, must be applied to the sheet waist $w_{ab}$ (see appendix for more details about finite width barriers).

### 6. Potential applications

One may regard the process of a collision between two dimeric wavepackets and the barrier as a recombination process in an atom interferometer. Indeed, the intensity of all three output channels of the scattering event—right moving dimers, let moving dimer, and the monomer production—are expected to depend periodically on the relative phase between the input packets (see figure 4 for the latter). Unlike the first two, the dimer production is a new possibility.

Recall that in a chip-based atom accelerometer $[35]$, the interferometer arms need not be spatially separated: however the readout still requires the separation between the channels thus expanding the minimal size of the

![Figure 3. Probability density after the collision of the barrier as a function of the dimensionless coordinates $x_1/L$ and $x_2/L$ for a linear superposition of two motional states of the dimer with input kinetic energies higher than the dissociation energy ($ka = 4$) and an initial relative phase between dimers $\phi = 0$ (a) and $\phi = \pi$ (b). In (a) we observe how monomers are produced while in (b) they probability density is completely suppressed. The other parameters are the same as in figure 1. On top of each figure we show a schematic representation of the initial state.](image)

![Figure 4. Total monomer production after the collision of a linear superposition of two motional states of the dimer against the barrier as a function of the relative phase between the two contrapropagating dimeric wavepackets. The integral shown on the right axis is proportional to the empirically relevant (see $[30]$) two-body correlation function $g_2$. The input kinetic energy is set to two times the dissociation energy ($ka = 4$). The other parameters are the same as in figure 1.](image)
device. We suggest that in a dimer-based interferometer, the read-out stage of the process can also be made compact if the total dimer population, accessible through the two-body correlation function [30] is used as an output.

Monomer formation affect the kinetic energy of the system. The possibility of an accurate detection of velocities or kinetic energies would yield a novel type of inelastic interferometer, where variation of thermodynamic quantities allow to infer a phase shift (see appendix for details).

7. Conclusions

In this article we have shown that for short-range-attractive-interacting one-dimensional bosonic atoms, scattering of a spatially odd motional state of a dimer off a barrier produces—even above the dissociation threshold—no unbound atoms. This prohibition originates from a map—valid in the bosonic, spatially odd sector of the Hilbert space—between the Hamiltonian of the system and a known, generally unphysical, Bethe Ansatz integrable Hamiltonian associated with the symmetries of a square. Potential experimental realizations include the waveguide confined atomic dimers and bound states of two Rydberg polarons. We also suggest that in the context of chip-based atom accelerometers, using the monomer production—accessible through the second-order local correlation function $g_2(0)$ right after recombination—as an output channel may allow to further miniaturize the readout.

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Appendix. Non-interacting versus interacting bosons

In this appendix we compare the scattering of two non-interacting particles and two attractively interacting bosons against a potential barrier, i.e. we integrate the Schrödinger equation following from (1) with $g = 0$ and $g = \pi$ respectively and study the dynamics of the system.

Figure A1 shows the two-dimensional probability density $|\psi(x_1, x_2)|^2$ of the outcomes of the collision against a delta barrier of two non-interacting particles in a superposition state with relative phase $\phi = 0$ (a)–(c) and $\phi = \pi$ (b)–(d) (i.e. in the same conditions as in figure 4 of the main text). We prepare the system with two different kinetic energies that correspond to values below (a), (b) and above (c), (d) the critical $k$ for which monomers would be created in the interacting case if $g_{a,b}/|g| = 1$.

The behaviour shown in figure A1 is readily understood by analyzing the possible outcomes of the collisional process among two wavepackets $\psi_{L/R}$ incoming on the barrier from left or right respectively, with relative phase $\phi$ (see figure A2). The reflection and transmission coefficients for each particle are denoted by $t_{r,t}$ and $r_{r,t}$. Using the fact that the scattering of a single quantum particle from a delta potential barrier leads to an $\pi/2$ relative phase between transmitted and reflected waves we represent in figure A2 the final outputs of the collision using the following notation: black colors indicate the final probability density due to the left incoming wave, while red is used for the right one, with its imprinted phase $\phi$. The final probability density in each sector is obtained by taking the square modulus of the wavefunction.

As an example, figures A1(c), (d) can be understood as follows. Since for large incoming momenta $k\Delta_{a,b} = 2$ one has $t_{r} = r_{a} = 1/2$ for $\phi = 1, 2$ and we have taken two incoming wavepackets of equal amplitude, $|\psi_{a,b}| = |\psi_{b,a}|$, then for $\phi = 0 (\phi = \pi)$ the wavepackets in diagonal panels add up destructively (constructively) while the antidiagonal panels have the opposite behaviour, thus explaining the opposite behaviors of figures A1(c) and (d). The case of figures A1(a), (b) is similarly derived, taken into account that for small incoming momenta $t_{r} \ll r_{a}$: in this case for relative phase $\phi = 0$ there is almost no destructive interference in the diagonal panels since the two amplitudes are very different, while this can occur in the antidiagonal panels, where the two amplitudes have the same magnitude.

The picture changes considerably in the case of attractive interactions, as shown in figure A3. For small incoming wavevector (figures A3(a), (b)), the bound states cannot be broken, hence, there is never population of the antidiagonal panels for any choice of $\phi$ and $G$. For large incoming wavevector however, bound states can in principle be broken. The population of the antidiagonal panels corresponds to the population of monomers, i.e.
when on particle is on the right and one on the left of the barrier. For relative phase $\phi = 0$ they are visible in figure A3(c), while they are absent for $\phi = \pi$ figure A3(d). Following the above discussion for non-interacting case, the absence of monomer formation for $\phi = \pi$ could be interpreted as a destructive interference phenomenon. More deeply, as discussed in the main text, its origin is due to the conservation of chemical composition in integrable systems.

The consequences of this is that we have a inelastic signature of the phase shift among the two incoming wavepackets: when monomers are created, the potential energy of the system decreases while the kinetic energy increases due to conservation of energy. This energy exchange cannot be observed in the non-interacting case, as no binding energy exists. In figure A4(a) we compare the change of kinetic energy and potential energy (that includes both barrier and attractive interactions) for a single incoming wave after the collision with the barrier has occurred. Here we can clearly see that indeed in the interacting case there is an exchange of kinetic and...
potential energy, as we can see in figure A4(a) where the two curves separate as monomers start to be produced for \( k \alpha > 1 \). Alongside the energy, also the momenta of each wave after the collisional process are affected by the process of monomer creation and the generated monomer wavepackets propagate at a lower velocity than dimers (see figure A4(b)).

Figure A3. Dimers created in a superposition state such that their relative phase is \( \phi = 0 \) (a)–(c) and \( \phi = \pi \) (b)–(d). Interactions are set as \( g_{ab}/|\psi| = 1 \), and the input momentum towards the center is \( k \alpha = 3/4 \) (a), (b) and \( k \alpha = 2 \) (c), (d).

The conclusion of this analysis is that for both non-interacting and interacting particles one could use the measure of ‘deflection’ probability amplitude (i.e. the intensity in the antidiagonal panels) for interferometric applications, i.e. to infer the phase shift among the two wavepackets. However, in the interacting case, monomer counting, measurement of velocity or kinetic energy yield an additional channel for phase readout.

Finally, it is important to remark that our method does not require dense monochromatic monomer beams otherwise needed to see the two- or more-body interference. The method presented in this work is based not on a generic few-body interference but on a specific property given by Bethe Ansatz integrable systems chemical selection rules. Thus, we do not need to wait for the spatial separation of the beams to detect the relative phase between the interferometer arms.
A.1. Effect of a barrier of finite width

We also explore the effects on the monomer production for a finite-width barrier. In figure A5 we show the equivalent of figure 3(b), i.e. the probability density of dimers with initial relative phase $\phi = \pi$, calculated in the case where the scattering potential is not a delta barrier but a Gaussian barrier $f(x, \sigma) = \frac{8\sigma}{\sqrt{\pi\sigma}} e^{-\frac{x^2}{4\sigma^2}}$. We find that, as long as the wavelength $\lambda$ of the propagating dimers is much larger than the barrier width, barely no monomer production occurs. In the opposite case, when the barrier width becomes comparable to $\lambda$, a weak monomer production signal starts to appear, indicating the breakdown of the integrability in the model.

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