One-dimensional Bose chemistry: effects of non-integrability

V. A. Yurovsky and A. Ben-Reuven

School of Chemistry, Tel Aviv University, 69978 Tel Aviv, Israel

M. Olshanii

Department of Physics & Astronomy, University of Southern California, Los Angeles, CA 90089-0484, USA

(Dated: February 9, 2020)

Three-body collisions of ultracold identical Bose atoms under tight cylindrical confinement are analyzed. A Feshbach resonance in two-body collisions is described by a two-channel zero-range interaction. Elimination of the closed channel in the three-body problem reduces the interaction to a one-channel zero-range one with an energy dependent strength. The related problem with an energy independent strength (the Lieb-Liniger-McGuire model) has an exact solution and forbids all chemical processes, such as three-atom association and diatom dissociation, as well as reflection in atom-diatom collisions. The resonant case is analyzed by a numerical solution of the Faddeev-Lovelace equations. The results demonstrate that as the internal symmetry of the Lieb-Liniger-McGuire model is lifted, the reflection and chemical reactions become allowed and may be observed in experiments.

PACS numbers: 03.65.Nk,32.80.Pj,03.75.Nt,34.50.-s

Ultracold atoms under tight cylindrical confinement can reach the “single-mode”, or quasi-one-dimensional (1D) regime, where only the ground state of transverse motion is significantly populated. Quasi-1D atomic quantum gases have been realized recently in elongated atomic traps (see [1, 2, 3, 4]), two-dimensional optical lattices (see [5, 6, 7]), atomic waveguides (see [8] and references therein), and atomic integrated optics devices (see [9, 10] and references therein). These systems attract increasing attention due to their possible applications to atomic interferometry, quantum measurement, and quantum computation.

Properties of quasi-1D systems are frequently analyzed using the Lieb-Liniger-McGuire (LLMG) model [16, 17] with δ function atom-atom interaction $U_a \delta (z)$, where $z$ is the interatomic distance. The interaction strength $U_a$ has been related in Ref. [11] (being denoted as $g_{1D}$) to the three-dimensional (3D) elastic scattering length $a_3D$ and the waveguide transverse frequency $\omega_\perp$. The LLMG model has an exact Bethe-ansatz solution [16, 17] expressed as the superposition of plane waves with all possible permutations of the asymptotic momenta $p_j$, one per each atom. Therefore, the atoms can exchange their momenta, but the asymptotic momentum set $\{p_j\}$ remains unchanged.

If the interatomic interaction is attractive ($U_a < 0$), the atoms can form a two-body (2B) bound state (diatom), described by complex asymptotic momenta $p \pm i \kappa$, where $\kappa = -m \pi U_a$ serves as a reciprocal diatom size and $m$ is the atomic mass. However, a three-body (3B) association is forbidden in the LLMG model, as it corresponds to a change of two real momenta in the set $\{p_1, p_2, p_3\}$ for a three-atom system by complex ones in the set $\{-p, p/2 + i \kappa, p/2 - i \kappa\}$. The dissociation and reflection in atom-diatom collisions are forbidden by the same reason (the last process corresponds to a transition $\{p, p/2 - i \kappa, -p/2 + i \kappa\} \rightarrow \{p, -p/2 + i \kappa, p/2 - i \kappa\}$). Therefore, all chemical processes, i. e., atom-diatom transitions are forbidden in the LLMG model.

The integrability of the LLMG model results from its high internal symmetry. This symmetry can be violated in real physical systems, e. g., when Feshbach resonance is used to tune the elastic scattering length. The effect of Feshbach resonance appears in 2B scattering when the collision energy of a pair of atoms in an open channel is close to the energy of a bound state (resonant molecule) in a closed channel (see Ref. [14]). Two-body Feshbach resonance collisions in atomic waveguides have been analyzed in Ref. [15]. The results demonstrate that when the collision energy is low enough compared to the trap frequency, the problem can be treated as essentially 1D, but with an energy-dependent zero-range interaction. The present work demonstrates that a Feshbach resonance leads to non-integrability of few-body problems, allowing for chemical processes (association and dissociation), and atom-diatom reflection.

The approach used in Ref. [13] for two-atom scattering leads in a 3B problem to a system of two coupled equations for the wavefunctions in the momentum representation, $\varphi_0(q_1, q_2, q_3)$ and $\varphi_1(q_1, q_m)$, associated with the three-atom and atom-molecule channels, respectively. Using a system of units in which $\hbar = 1$, the equations are

$$ E \varphi_0(q_1, q_2, q_3) = \frac{1}{2m} \sum_{j=1}^{3} q_j^2 \varphi_0(q_1, q_2, q_3) $$
$$ + \frac{1}{2\pi} U_a \sum_{j=1}^{3} \int d^3 q' \delta(q'_j - q_j) \delta(Q - Q') \varphi_0(q'_1, q'_2, q'_3) $$
\[ E \varphi_1(q_1, q_m) = \left( \frac{q_1^2}{2m} + \frac{q_m^2}{4m} + D_{1D} \right) \varphi_1(q_1, q_m) \]
\[ + \left( \frac{3}{\pi} \right)^{1/2} g \int dq_3 \varphi_0(q_1, q_m - q_3, q_3) \]
\[ \varphi_0(q_1, q_2, q_3) \]

Here \( q_j \) are the momenta of the atoms, \( q_m \) is the momentum of the resonant molecule, and \( Q = q_1 + q_2 + q_3 \) is the center-of-mass momentum. The parameters of the 1D problem — the atom-atom interaction strength \( U_a \), the atom-molecule coupling strength \( g \), and the detuning between the atomic and molecular states \( D_{1D} \) — can be expressed in terms of 3D resonance scattering parameters (see Ref. [15]). The indistinguishability of the bosonic atoms leads to the symmetry of the wavefunction \( \varphi_0(q_1, q_2, q_3) \) over permutation of the atomic momenta. The energy \( E \) is counted from the threshold of the three-atom channel.

Equation (2) neglects the interaction associated with collisions between the resonant molecule and the third atom. It allows a simple elimination of the atom-molecule channel function \( \varphi_1 \). As a result, the three-atom channel wavefunction obeys the equation
\[ E \varphi_0(q_1, q_2, q_3) = \frac{1}{2m} \sum_{j=1}^{3} q_j^2 \varphi_0(q_1, q_2, q_3) \]
\[ + \frac{1}{2\pi} \sum_{j=1}^{3} U_{eff}(q_j) \int dq' \delta(q_j' - q_j) \delta(Q - Q') \varphi_0(q_1, q_2, q_3) \]

involving an effective atom-atom interaction strength
\[ U_{eff}(q) = U_a + \frac{2|g|^2}{E + i0 - D_{1D} - 3q^2/(4m)} \]
\[ \text{(4)} \]

This strength appears to be the same function of the collision momentum as in the 2B problem (see Ref. [15]), but here the collision energy of two atoms is expressed in terms of the total energy \( E \) and the third atom momentum \( q \) due to momentum and energy conservation (letting \( Q = 0 \) in the center-of-mass system used here and below).

For a momentum dependent \( U_{eff} \) the internal symmetry of the LLMG model is broken, and a resonant case does not allow a Bethe-ansatz solution. This case is analyzed here by a numerical solution of the Faddeev-Lovelace equations. Using the conventional Faddeev reduction method (see Ref. [15]), one obtains a 1D integral equation
\[ X(p, p_0) = 2Z(p, p_0) + \frac{m^2}{2\pi^2} \int dq Z(q, q) T_{1D}(q) X(q, p_0) \]
\[ Z(q, q) = \frac{2\kappa^3}{\pi m} \frac{1}{mE + i0 - p^2 - pq - q^2} \]
\[ \text{(5)} \]

for the symmetric transition amplitude \( X(p, p_0) \). Here the 2B scattering amplitude \( T_{1D}(q) \), corresponding to the momentum-dependent \( U_{eff}(q) \), has the form (see Ref. [15])
\[ T_{1D}(q) = U_{eff}(q) \left[ 1 + \frac{i}{2} m U_{eff}(q) \left( mE - \frac{3}{4} q^2 + i0 \right)^{1/2} \right]^{-1} \]

Equations similar to Eq. (3) have been used in Refs. [15, 20] for non-resonant 1D problems.

The poles of \( T_{1D}(q) \) at \( q = \pm 2\sqrt{m(E - E_b)}/3 \) correspond to 2B bound states (diatoms) with the binding energy \( E_b = \kappa^2/m \). The reciprocal diatom size \( \kappa \) here and in Eq. (3) is a solution of the cubic equation (see Refs. [12, 21])
\[ \kappa^3 + \frac{m}{2} U_a \kappa^2 + m D_{1D} \kappa + \frac{1}{2} m^2 D_{1D} U_a - m^2 |g|^2 = 0. \]
\[ \text{(6)} \]

These states are superpositions of the closed and open channels. The probability to find the diatom in the open channel is \( W_0 = (\kappa^2 + m D_{1D}) / (3\kappa^2 + m U_a \kappa + m D_{1D}) \). This probability varies from 1 far off resonance to \( \frac{1}{4} \) in resonance for \( U_a = 0 \).

In the numerical solution of Eq. (6) the transition amplitude is expressed in terms of odd and even amplitudes \( X_+ (p, p_0) = X(p, p_0) \pm X(-p, p_0) \), \( p > 0 \), that satisfy uncoupled equations. The contributions of the poles of \( T_{1D}(q) \) are separated from the Cauchy principal-value integrals as in Ref. [20]. At \( E > 0 \), when chemical processes are allowed, the function \( Z(q, p) \) has singularities on the real axis too. Unlike the 3D case with logarithmic singularities, in the 1D case the singularities are simple poles and are treated in a similar way as the poles of \( T_{1D}(q) \).

The reflection, transmission, and dissociation probabilities in the collision of an atom with momentum \( p_0 \) and a diatom with momentum \( -p_0 \) can be expressed in terms of the amplitude \( X(p, p_0) \) as, respectively,
\[ P_{\text{ref}}(p_0) = \left| \frac{4\pi m}{3p_0} W_0 X(-p_0, p_0) \right|^2 \]
\[ P_{\text{tran}}(p_0) = \left| 1 + i \frac{4\pi m}{3p_0} W_0 X(p_0, p_0) \right|^2 \]
\[ P_{\text{diss}} = 1 - P_{\text{ref}} - P_{\text{tran}}. \]
\[ \text{(8)} \]

Here the factor \( W_0 \) describes the open-channel fraction in the incoming and outgoing waves. The results can be conventionally expressed in terms of dimensionless parameters: the non-resonant interaction strength \( u = m^{1/3} |g|^{-2/3} U_a \), the collision energy \( \epsilon_2 = 3p_0^2 / (4m D_0) \), and the detuning \( b = D_{1D}/D_0 \), where an energy scale \( D_0 = m^{1/3} |g|^{4/3} \) is used.

Consider an association of three atoms with momenta \( p_1, p_2, \) and \( p_3 \) (\( p_1 + p_2 + p_3 = 0 \) in the center-of-mass system). The momenta of the resulting atom and diatom
configuration (actions become small perturbations. The dependence of these processes vanish in fast collisions, when the interaction strengths. The dissociation appears above the threshold, for the conditions in Fig. 1. The 3B association rate attains its maximum at a collision energy $\epsilon_3$ ranging between 2 and 4 (depending on $u$, $b$, and $\theta$), and decreases to zero for slow collisions. These processes vanish in fast collisions, when the interactions become small perturbations. The dependence of the association rate on the energy distribution between the atoms behaves differently for various $u$ and $b$ values (see Fig. 2). No association occurs at $\theta = 0$ when two atoms have equal momenta.

Given a fixed collision energy, the reflection, dissociation, and association persist over a detuning interval (see Fig. 3). The oscillating behavior of the probabilities results from interference of the odd and even amplitudes $X_\pm (p, p_0)$, which are analogs of partial waves in 3D scattering. However, unlike the 3D case, where only the s-wave contributes to low-energy scattering due to a centrifugal barrier, in the 1D case both odd and even amplitudes have to be taken into account at all energies. All chemical processes, as well as reflection, vanish at large detunings, when the energy dependence of the interaction strength $U_{\text{eff}}$ becomes negligible [see Eq. (4)].

$$E = \frac{1}{2m} (p_1^2 + p_2^2 + p_3^2) = \frac{3}{4m} p_*^2 - E_b.$$  

The association rate coefficient is given by

$$K_3 (p_1, p_2, p_3) = \frac{2\pi^2 m^3}{2T_{3D} p_*} W_0 \left[ \sum_{j=1}^{3} |T_{1D} (p_j) X (p_j, p_*)|^2 + \sum_{j=1}^{3} |T_{1D} (p_j) X (p_j, -p_*)|^2 \right].$$

Except for the dimensionless three-atom collision energy $\epsilon_3 = E/D_0$, the rate coefficient depends on the energy distribution between the three atoms. This distribution can be parameterized by an angle $0 \leq \theta \leq \pi/6$, such that $p_1 = \sqrt{3mE/4} \cos \theta$, $p_2, p_3 = \sqrt{3mE/4} \cos (\theta \pm 2\pi/3)$. At $\theta = 0$ one of the momenta attains the maximal possible value $p_1 = \sqrt{3mE/4}$, while $p_2, p_3 = -p_1/2$. A symmetric configuration ($p_1 = -p_2 = \sqrt{mE}, p_3 = 0$) corresponds to $\theta = \pi/6$. The association rate coefficient is plotted below in units of $\hbar/m$.

The calculated probabilities and rate coefficient are presented in Fig. 1 as functions of the corresponding dimensionless collision energies. The results demonstrate total reflection for slow collisions. Similar reflection behavior has been obtained in Ref. [20] for a case of non-identical atoms with energy-independent interaction strengths. The dissociation appears above the threshold, where $3p_0^2/(4m) > E_b$ (or $\epsilon_2 > 1$ for the conditions in Fig. 1). The 3B association rate attains its maximum at a collision energy $\epsilon_3$ ranging between 2 and 4 (depending on $u$, $b$, and $\theta$), and decreases to zero for slow collisions. These processes vanish in fast collisions, when the interactions become small perturbations. The dependence of the association rate on the energy distribution between the atoms behaves differently for various $u$ and $b$ values (see Fig. 2). No association occurs at $\theta = 0$ when two atoms have equal momenta.

Given a fixed collision energy, the reflection, dissociation, and association persist over a detuning interval (see Fig. 3). The oscillating behavior of the probabilities results from interference of the odd and even amplitudes $X_\pm (p, p_0)$, which are analogs of partial waves in 3D scattering. However, unlike the 3D case, where only the s-wave contributes to low-energy scattering due to a centrifugal barrier, in the 1D case both odd and even amplitudes have to be taken into account at all energies. All chemical processes, as well as reflection, vanish at large detunings, when the energy dependence of the interaction strength $U_{\text{eff}}$ becomes negligible [see Eq. (4)].
restoring integrability of LLMG model. For a repulsive non-resonant interaction \( U_a > 0 \) the bound state exists while \( D_{1D} < 2|g|^2/U_a \) [see Eq. (7)], or while \( b < 2/u \). As \( b \to 2/u \) the bound state becomes more shallow, leading to a drastic increase of the association rate. The dependence on the non-resonant interaction strength (see Fig. 4) demonstrates a similar behavior: a drastic increase of the association rate near the threshold at \( u = 2/b \), and a decrease of all the rates at large absolute values of \( u \) due to the restoration of integrability.

Thus, a substantial association rate can be observed for collision energies ranging over several units \( D_0 \), which must lie below the transverse frequency \( \omega_\perp \), in order to conserve the quasi-1D behavior of the system. This condition is satisfied for relatively weak resonances \( \mu \Delta < \omega_\perp a_{\perp}/a_{3D} \) and small detunings \( \mu (B - B_0 - \Delta) - \omega_\perp < \sqrt{\omega_\perp \mu \Delta a_{\perp}/a_{3D}} \), when the relations between the 1D and 3D scattering parameters of Ref. 15 are applicable. These relations lead to expressions for the energy unit, its resonant value \( B_0 \),

\[
D_0 = m^{1/3} (\omega_\perp a_{3D} \mu)^{2/3} \left( 1 - C \frac{a_{3D}}{a_{\perp}} \right)^{-4/3},
\]

and the dimensionless parameters

\[
\begin{align*}
&u = \left( \frac{8m\omega_\perp^2 a_{3D}^2}{\mu \Delta} \right)^{1/3} \left( 1 - C \frac{a_{3D}}{a_{\perp}} \right)^{-1/3}, \\
b = \frac{1}{D_0} \left[ \mu (B - B_0) - \omega_\perp + C \frac{a_{3D}}{a_{\perp}} \mu \Delta \left( 1 - C \frac{a_{3D}}{a_{\perp}} \right)^{-1} \right].
\end{align*}
\]

Here \( \Delta \) is the phenomenological resonance strength, \( \mu \) is the difference between the magnetic momenta of an atomic pair in the open and closed channels, \( B - B_0 \) is the detuning of the external magnetic field \( B \) from

FIG. 4: Probabilities of reflection (solid line) and dissociation (dashed line) in atom-diatom collisions calculated for fixed dimensionless collision energy \( \epsilon_2 = 3.6 \) and detuning \( b = 0 \) as functions of the dimensionless non-resonant interaction strength \( u \). The scaled rate coefficient of 3B association \( K_{3m}/h \) is presented by the dot-dashed \((b = 0, \epsilon_3 = 2.4, \theta = \pi/6)\) and dot-dot-dot-dashed \((b = 1, \epsilon_3 = 4.5, \theta = \pi/10)\) lines.
[11] M. Olshanii, Phys. Rev. Lett. 81, 938 (1998).
[12] T. Bergeman, M. Moore, and M. Olshanii, Phys. Rev. Lett. 91, 163201 (2003).
[13] M. Moore, T. Bergeman, and M. Olshanii, J. Phys. (Paris) IV 116, 69 (2004).
[14] E. Timmermans, P. Tommasini, M. Hussein, and A. Ker-man, Phys. Rep. 315, 199 (1999).
[15] V. A. Yurovsky, Phys. Rev. A 71, 012709 (2005).
[16] E. H. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963).
[17] J. B. McGuire, J. Math. Phys. 5, 622 (1964).
[18] W. Glockle, *The Quantum Mechanical Few-Body Problem* (Springer, Berlin, 1983).
[19] L. R. Dodd, J. Math. Phys. 11, 207 (1970); C. K. Majumdar, J. Math. Phys. 13, 705 (1972).
[20] L. R. Dodd, Aust. J. Phys. 25, 507 (1972).
[21] K. V. Kheruntsyan and P. D. Drummond, Phys. Rev. A 58, 2488 (1998).
[22] C. Mora, R. Egger, and A. O. Gogolin, Phys. Rev. A 71, 052705 (2005).
[23] S. Sinha, A. Yu. Cherny, D. Kovrizhin, and J. Brand, cond-mat/0506060.