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One-dimensional ultracold atomic gases: impact of the effective range on integrability

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The one-dimensional one-component Bose and Fermi gases are considered in a regime of large effective range. We focus our study on the three-body problem, which is at the heart of the integrability issue. For fermions, the vicinity of the integrability is characterized by large deviations with respect to the predictions of the Bethe ansatz. For the consistency of the contact model, it appears essential to take into account the contact of three particles.

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The one-dimensional (1D) Bose and Fermi gases with zero-range interactions are celebrated examples of exactly solvable many-body problems $^{1-4}$. Ultracold atoms offer the stupendous possibility to achieve these systems in the degenerate regime by using highly elongated cigar traps $^{5-7}$. Moreover, using magnetic Feshbach resonances and/or tuning the trap parameters make it possible to study 1D systems in strongly correlated regimes. This way, the Tonks-Girardeau and the super Tonks-Girardeau phases have been achieved $^{8-12}$. In addition, the existence of confinement induced resonances and resonances shifts have been confirmed $^{12}$. In this letter we consider the three-body problem, which is at the heart of the integrability issue. For fermions, the vicinity of the integrability is characterized by large deviations with respect to the predictions of the Bethe ansatz. For the consistency of the contact model, it appears essential to take into account the contact of three particles.

One-dimensional ultracold atomic gases: impact of the effective range on integrability

In this letter we consider the three-body problem, which is intimately related to the integrability issue $^{4}$. To this end we use a Hamiltonian two-channel model (HTCM), which encapsulates the Feshbach mechanism. Whereas the CM and the HTCM are strictly equivalent at the two-body level, in the three-body problem the HTCM gives large deviations with respect to the predictions based on the BA. We show that in the limit of the contact of three particles, all the solutions of the HTCM have the same type of singularity not satisfied by the BA. The behavior of the wave function in the limit where the three particles fall ones on the others appears then as a key ingredient in the violation of the integrability. We show that equivalence of the CM and of the HTCM can be achieved at the three-body level by imposing continuity conditions on the wave function.

Our modeling is based on a parameterization of the two-body 1D asymptotic scattering state including the effective range term. For an incoming wave of relative wave number $k_{0}$ and relative coordinate $z$, we write it as

$$
\langle z | \psi_{k_{0}} \rangle = e^{ik_{0}z} + [f_{0}(k_{0}) + \text{sgn}(z)f_{1}(k_{0})]e^{ik_{0}|z|}.
$$

In Eq. (1), $f_{0}$ (respectively $f_{1}$) is the scattering amplitude in the even (respectively odd) sector, parameterized as

$$
f_{\eta}(k_{0}) = \frac{-(ik_{0}a_{\eta})^{\eta}}{1 + ik_{0}a_{\eta} + b_{\eta}(ik_{0})^{1-\eta}(-a_{\eta})^{\eta}}.
$$

For ultracold atoms in a 1D waveguide, the scattering lengths $a_{\eta}$ and the effective range parameters $b_{\eta}$ in Eq. (2) can be expressed as a function of 3D scattering parameters in the homogeneous space $^{23,30}$. In what follows, we consider only positive values of the effective range parameter $b_{\eta} > 0$, an assumption justified in the limit of narrow resonances $^{20,21}$. The existence of a dimer in the system is particularly relevant in the context of the integrability. From the analyticity of the scattering amplitude, one finds a single bound state i.e., a dimer $|\phi_{\eta}\rangle$ of energy $-\hbar^{2}\kappa_{\eta}^{2}/m$ in the even sector for all values of $a_{0}$ and in the odd sector only for positive values of $a_{1}$

$$
\langle z | \phi_{\eta} \rangle = \sqrt{\kappa_{\eta}}(1 + 2b_{\eta}\kappa_{\eta}^{3-2\eta})^{-1/2}[1 - 2\eta\theta(z)]e^{-\kappa_{\eta}|z|}
$$

where $\theta(z)$ is the Heaviside function and in the odd sector ($\eta = 1$), one recognizes the sign function $\text{sgn}(z) = 2\theta(z) - 1$. The dimer binding wave number $\kappa_{\eta}$ in Eq. (3) is the positive root of

$$
1 - a_{0}\kappa_{\eta} - b_{\eta}(a_{\eta})^{\eta}\kappa_{\eta}^{3-\eta} = 0.
$$

We now come to the integrability issue for a system of $N$ one-component bosons (respectively fermions) where the two-body scattering occurs only in the even (respectively in the odd) sector $^{31}$. Integrability means that the eigenstates are given by the BA and there is thus no diffractive scattering i.e., the wave numbers of

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the particles are globally conserved after multiple collisions in the system [34]. The expressions of the transmission and reflection (corresponding to the exchange of momentum between the particles) coefficients in the scattering of two particles are thus particularly relevant. From Eq. (1), considering a pair of particles \((i, j)\) of wave numbers \((k_i, k_j)\), they are related to the scattering amplitudes by \(t^{ij}_0 = 1 + f_0((k_i - k_j)/2)\) and \(r^{ij}_0 = (-1)^j f_0((k_i - k_j)/2)\). A necessary condition for integrability is given by the Mc Guire-Yang-Baxter criterion, which follows from the absence of diffractive scattering in the three-body integrable problem \[22\]:

\[
\begin{align*}
\eta^{12} \eta^{13} \eta^{23} + t^{ij}_0 \eta^{ij} \eta^{jk} = t^{jk}_0 \eta^{jk} \eta^{ij}.
\end{align*}
\]

For \(\eta = 0\) this last equality is verified iff \(b_0 = 0\) (Lieb Liniger model) and for \(\eta = 1\) iff \(|a_1| = \infty\) i.e., in the Fermi Tonks-Girardeau (FTG) regime \[34\] \[35\]. This is in strong contradiction with the results of Refs. \[18\] \[19\] where the BA was used as an eigenstate of contact models in regimes where Eq. (5) is not satisfied \[36\]. To understand this discrepancy, in the rest of this letter we focus on the three-body problem which has the advantage of the simplicity while being a cornerstone of the integrability.

We first use a CM which includes the effective range as a straightforward generalization of the Lieb Liniger model \[20\] \[21\]. It is analogous to the one used in the context of narrow Feshbach resonances for atoms in the three-dimensional space \[15\] \[38\] \[39\]. For convenience we introduce the shorthand notation \((z)_N \equiv (z_1, z_2, \ldots, z_N)\) for the \(N\) coordinates of the system and \(z_{ij} = z_i - z_j\) for the relative coordinate of the pair of particles \((ij)\). The CM is defined as follows: firstly, for all the configurations where \(i \neq j\), \(z_{ij} \neq z_{ij}\), the wave function \((\langle z_N|\Psi\rangle)\) verifies the Schrödinger equation without any interaction between particles; secondly, for each pair of interacting particles \((ij)\) the wave function verifies the contact condition

\[
\lim_{z_{ij} \to 0^+} \left(1 + a_0 \partial_{z_{ij}} + (-a_0)^2 b_0 \partial_{z_{ij}}^2\right) \langle (z_N|\hat{\Pi}^{ij}_0|\Psi\rangle = 0
\]

where for \(\eta = 0\) (respectively for \(\eta = 1\)) the operator \(\hat{\Pi}^{ij}_0\) symmetrizes (respectively antisymmetrizes) the state \(|\Psi\rangle\) in the exchange of the particles \(i\) and \(j\). In Eq. (6), the positions \(z_{ij} = (z_i + z_j)/2\) and \(z_k\) \((k \neq i, j)\) are kept fixed \[40\]. One can verify that the exact expressions of the scattering amplitudes in Eq. (2) are deduced from the contact conditions of Eq. (6) by using the wave-function of Eq. (1). If a dimer exists and the system is integrable, then the ground state for three particles is a trimer of energy \(-4\hbar^2 \kappa^2/m\) given by the BA \[2\]:

\[
\langle z_1, z_2, z_3|\psi^{BA}_0| \rangle = e^{-\kappa \sum_i z_{ij}} \prod_{i<j} \left[1 - 2\eta \theta(z_{ij})\right].
\]

Following the standard method in Refs \[11\] \[11\], one considers the contact condition in Eq. (6) for each pair \((ij)\) in domains where the third particle \(k\) is distinct from the center of mass \(Z_{ij}\) (i.e., \(z_k \neq Z_{ij}\)). Surprisingly, following this reasoning the BA appears as a solution of the contact model with \(\kappa = \eta \kappa\) and the binding wavenumber of the trimer \(q^{BA}_0 = 2\kappa\), thus in deep contradiction with the Mc Guire-Yang-Baxter criterion.

The consistency of the CM is thus puzzling and to go further we now use a HTCM which is a more conventional approach. In this model, the scattering process between two particles of mass \(m\) is only due to the coherent coupling between the pair of particles and a molecular state of mass \(2m\). For a plane wave of wave number \(k\), we choose the convention \(\langle k|\psi\rangle = \exp(ikz)\) and we denote the creation operator in the open channel \(\hat{a}_{n,k}^\dagger\), where \(n = 0\) for bosons and \(n = 1\) for fermions. The creation operator for molecules in the closed channel is denoted by \(\hat{b}_{n,k}\), where the index \(n\) permits one to distinguish the composite boson (i.e., the molecule) made of two fermions, from the molecule made of two bosons. We consider only pure systems with identical particles and for each system \((\eta = 0\) or \(\eta = 1)\), the Hamiltonian is

\[
\hat{H}_\eta = \int \frac{dk}{2\pi} \left[ \epsilon_k \hat{a}_{n,k}^\dagger \hat{a}_{n,k} + \frac{E^\eta_n}{2} \hat{b}_{n,k}^\dagger \hat{b}_{n,k} \right]
\]

\[
+ \left[ \frac{\hbar^2 \lambda^\eta_n}{m} \int \frac{dk K}{(2\pi)^2} |\langle \kappa|\delta^\eta_0\rangle \hat{a}_{\kappa+\kappa}^\dagger \hat{a}_{\kappa-k}^\dagger \hat{b}_{\kappa,k} + \text{h.c.} | \right].
\]

In Eq. (8), \(\epsilon_k = \frac{\hbar^2 k^2}{2m}\) is the single particle kinetic energy, \(\lambda^\eta_n\) is the strength of the coherent coupling between the two channels and \(E^\eta_n\) is the internal energy of the molecular state. The function \(\langle \kappa|\delta^\eta_0\rangle\) in the second line of Eq. (8) is a cut-off for the inter-channel coupling

\[
\langle k|\delta^\eta_0\rangle = (ik)^n e^{-k^2 \epsilon^2/4}.
\]

Physically, the short-range parameter \(\epsilon\) represents the length scale below which the collisional properties have a 3D character. For atoms moving in the monomode regime of a 1D harmonic waveguide of atomic frequency \(\omega_\perp\), it is typically of the order of the transverse length \(a_\perp = \sqrt{\hbar/(m \omega_\perp)}\). At this scale the 1D effective model of Eq. (8) is no more relevant. This explains the fundamental interest of considering the zero-range limit \((\epsilon \to 0)\) which permits one to capture the universal 1D properties for energies much smaller than the level spacing in the waveguide i.e., \(\hbar^2/(m \omega_\perp^2)\). In the zero-range limit, the scattering lengths and the effective range parameters of the HTCM are given by

\[
a_0 = \frac{m E^0_1}{\hbar^2 |\lambda_0|^2}; a_1 = \frac{1}{\sqrt{2 \frac{1}{\epsilon} - \frac{m E^0_1}{\hbar^2 |\lambda_0|^2}}}; b_0 = \frac{1}{|\lambda_0|^2}.
\]

The molecular energy in the odd sector \((E^0_1)\) is a bare parameter which diverges in the zero-range limit in such a way that \(a_1\) keeps a desired finite value, whereas the parameters \(E^0_0\) and \(\lambda_0\) stay finite in this limit. In the HTCM, a three-body state is the coherent superposition
of a particle state (denoted by \( |\psi_0^\eta\rangle\)) in the open channel and of a mixed channel state (denoted by \( \sqrt{3}|\psi_{00,m}^\eta\rangle/\lambda_\eta\)). In the center of mass frame, it can be written as

\[
|\Psi_\eta\rangle = \int \frac{dkdK}{(2\pi)^2} \frac{\langle k, K|\psi_0^\eta\rangle^*}{\sqrt{3}|\lambda_\eta\rangle} \hat{a}_{\eta, -K}^\dagger \hat{a}_{\eta, K}^\dagger |0\rangle + \int \frac{dK}{(2\pi)^2} \frac{\langle K|\psi_{00,m}^\eta\rangle}{\lambda_\eta} \hat{a}_{\eta, -K}^\dagger \hat{a}_{\eta, K}^\dagger |0\rangle.
\] (11)

For a positive energy \( (E > 0)\), \( |\Psi_\eta\rangle\) is a scattering state and we denote the three-particle incoming state by \( |\psi_0^\eta\rangle\). In Eq. (11), \( (k, K)|\psi_0^\eta\rangle\) is symmetric (for \( \eta = 0\)) or antisymmetric (for \( \eta = 1\)) in the exchange of two particles i.e., in the transformation \( (k \rightarrow -k)\) or \( (k \rightarrow k_\pm = \mp \frac{K}{2} \pm k)\). The projection of the Schrödinger equation at energy \( E\) onto the open channel gives

\[
(E - \frac{3\epsilon_k}{2} - 2\epsilon_k)|k, K|\psi_0^\eta\rangle = \frac{2\epsilon_k^2}{m} \left[ (k|\delta_0^\eta\rangle(K|\psi_0^\eta\rangle + \langle k_\pm|\delta_0^\eta\rangle(K_\pm|\psi_0^\eta\rangle + \langle k_\pm|\delta_0^\eta\rangle(K_\pm|\psi_0^\eta\rangle) + \text{ 'non } \delta \text{ terms' (13)}
\] (12)

Using Eq. (13), the mixed channel wave function associated with the BA in Eq. (7) is given by

\[
\langle Z|\psi_{00,m}^{\eta, \text{BA}}\rangle = -\kappa_\eta^{1-\eta} [1 - 2\eta \theta(Z)]^2 e^{-2\kappa_\eta|Z|}
\] (14)

and in the momentum representation

\[
\langle K|\psi_{00,m}^{\eta, \text{BA}}\rangle = -4\kappa_\eta^{2-\eta} (4\kappa_\eta^2 + K^2)^{-1}.
\] (15)

Importantly, for fermions the mixed channel wave function in Eq. (14) is discontinuous at the three-body contact \( \text{sgn}(0) = 0 \) and thus \( \langle Z = 0|\psi_{00,m}^{\eta, \text{BA}}\rangle = 0 \). Combining Eq. (12) with the projection of the Schrödinger equation onto the one atom plus one molecule space, one obtains in the zero-range limit a 1D STM equation (13)

\[
\frac{(ik)^{\eta}3^{2-\eta} - (K|\psi_0^\eta\rangle)}{f_0(k^2 K)} + \int \frac{dk}{2\pi} \mathcal{M}_\eta(K, k, E) \langle k|\psi_0^\eta\rangle = \int \frac{dk}{2\pi} (-ik)^{\eta}(k, K|\psi_0^\eta\rangle.
\] (16)

In Eq. (16) we have introduced the kernel

\[
\mathcal{M}_\eta(K, k, E) = \frac{4(k + K/2)^{\eta}(K + k/2)^{\eta}}{\epsilon_k^{\eta/2} (E + \epsilon_k^{\eta})} + K^2 + kK + k^2
\] (17)

and the relative momentum \( K_{rel}^\eta = \sqrt{\frac{mE}{\pi} - \frac{3}{4} K^2} \), where for a negative argument of the square root one uses the standard analytic continuation in scattering theory i.e., \( \sqrt{-q^2} = -i|q| \). For a state of negative energy \( (E < 0)\), there is no incoming three-particle state \( (|\psi_0^\eta\rangle = 0)\) and the prescription \( E \rightarrow E + i0^+ \) in Eq. (17) can be omitted. For \( b_\eta \neq 0 \), one can deduce from Eq. (16) the large momentum behavior \( (|K| \rightarrow \infty)\) of the mixed channel wave function solution of the problem as a function of its value at the contact of the three particles:

\[
\langle K|\psi_0^\eta\rangle \sim \frac{8}{3(-2)^{\eta}} \langle Z = 0^+|\psi_0^\eta\rangle + \langle Z = 0^-|\psi_0^\eta\rangle
\] (18)

We are now ready to compare the trimers obtained from Eq. (16) with the BA. It is clear that for \( b_\eta \neq 0 \), the BA in Eq. (14) and Eq. (15) does not fulfill the correct asymptotic behavior in Eq. (15) which confirms the non-integrability. For bosons, this result was found in a model including also the direct particle-particle interaction (14). The fact that for fermions, the three-body problem is ill-defined when both \( b_1 = 0 \) and the numerator of Eq. (13) is not zero, shows also that the BA in Eq. (15) can never be an exact solution of Eq. (16). (15). This can be shown as follows: firstly, for \( \eta = 1 \) and \( b_1 = 0 \) at large momentum, Eq. (16) is scale invariant and the mixed channel wave function can be searched as a power law: \( (K|\psi_0^\eta\rangle \propto K^n\); secondly, the integral in the first line of Eq. (16) is definite at least if \( s < -1\); thirdly, implementing the limit of large momentum in Eq. (16) one finds \( (K|\psi_0^\eta\rangle \propto 1/K \) unless the numerator of Eq. (18) equals zero, which completes the proof. Similarly to the integrable case, we have found numerically that whenever a dimer exists, there exists also one and only one trimer characterized by an even symmetry (i.e., \( (K|\psi_0^\eta\rangle = (K|\psi_0^\eta\rangle)\)). We denote the trimer energy

![FIG. 1: Spectrum of the trimers as a function of the wave number of the dimer in units of \( b_\eta \). Continuous line: bosons (\( \eta = 0 \)), dashed line: fermions (\( \eta = 1 \)). Inset: detail of the region where \( q_0^\eta \sim \kappa_\eta \), and \( \delta q_0^\eta = 2\sqrt{(|q_0^\eta|^2 - \kappa_\eta^2)/3} \) is plotted in units where \( b_\eta \) equals one.](image)
by \(E_0 = -(\hbar^2 q_0^2)/2m\). In Fig. 1, the wave number \(q_0\) is plotted as a function of the dimer wave number \(\kappa_\eta\).

In the limit of large scattering length \([a_\eta \gg b_1^{(3-2\eta)}}\]), the binding wave number of the trimer tends to the integrable limit \(q_0^\eta \sim 2\kappa_\eta\). For bosons, the convergence is fast and one can verify straightforwardly that for \(b_0 = 0\), Eq. 15 is the trimer solution of Eq. 16. For fermions, the convergence toward the integrable limit is very slow: one finds the approximate law \(q_0^\eta \sim 2\kappa_1[1 + 1.86/\ln(0.466 \times b_1/a_1)]\). The shape of the mixed channel wave function converges also slowly toward the BA of Eq. 15. It is plotted in Fig. 2 for a very large value of the ratio \(a_1/b_1\). The use of a logarithmic scale in the inset of Fig. 2 provides a zoom of the neighborhood of the three-body contact. In this last region, the deviation with respect to the integrable solution is large due to the discontinuity of the BA at \(Z = 0\) for \(\eta = 1\) in Eq. 14. In the opposite limit of a large dimer wave number, \(q_0^\eta \sim \kappa_\eta\) and the mixed channel wave function tends to the expected results for a shallow two-body (i.e., atom-dimer) bound state \(\langle Z|\psi_{D^1,\text{BA}}\rangle \sim \exp(-\delta q_0^\eta/|Z|)\) and \(\delta q_0^\eta = 2\sqrt{(q_0^\eta)^2 - \kappa_\eta^2}/3\).

We find numerically \(\delta q_0^\eta \sim -2.66/a_0\) for \(a_0 \to -\infty\) \((\kappa_1 \sim -\sqrt{a_0/b_0})\) and \(\delta q_1^\eta \sim 0.835 \times \sqrt{a_1/b_1}\) for \(a_1 \to 0^+\) \((\kappa_1 \sim 1/\sqrt{a_1/b_1})\).

After this study of the three-body problem with the HTCM, we point out that making the assumption that for \(b_\eta \neq 0\), \(\partial Z^{-\eta}/\partial Z|\psi_{D^1}\rangle\) is continuous at \(Z = 0\) filters out the spurious behavior in the vicinity of the three-body contact. Therefore the BA, which does not belong to the correct domain cannot be an eigenstate of the system. It is then possible to derive Eq. 16 from the CM as follows. Using a standard method in contact models, one includes in the free Schrödinger equation \(\delta\) source terms which are related to the two-body singularities of the wave function 33. In our case, one obtains Eq. 12 in the exact zero-range limit \((\epsilon = 0)\) and the particle wave function can be then expressed in terms of the mixed channel wave function. Equation 16 follows from the application of the contact condition Eq. 6 on this last expression.

To conclude, we have used the HTCM as a guide to define the correct domain for the free Hamiltonian of the CM in the three-body problem. This way, we concur these two different approaches in accordance with the Mc Guire-Yang-Baxter criterion. Exploring the phase diagram of the 1D atomic gas from small to large effective ranges is an open issue both experimentally and theoretically. Current experimental techniques make it possible to explore few- and many-body properties in regimes of large effective ranges [12,13,16,17]. One expects large deviations from the integrable dynamical properties, observable in the thermalization or in the response functions [48,50].

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In our study, the deviation from integrability is analyzed in a strictly 1D context. In Refs. [32, 33] these deviations are due to the three-dimensional character of the waveguide in quasi 1D ultracold atomic systems.