The three-body pseudo-potential for atoms confined in one dimension

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I. INTRODUCTION

At sufficiently low temperature, ultracold atoms in very elongated harmonic traps can be considered as in a one-dimensional (1D) geometry. For bosons, the idealization of the trap in terms a 1D harmonic waveguide permits one to achieve a mapping with the Lieb-Liniger model [1, 2]. In this context, few-body systems in 1D attracted recent interest [3, 4]. As a consequence of the Yang-Baxter criterion [4], the three-body problem occupies also a central place in studying the breakdown of integrability in these systems [5–11]. Interestingly, virtual excitations of pairs of atoms in the transverse modes of the waveguide led to the introduction of a 1D zero-range three-body force [6, 7]. This force has important consequences in the prediction of a 1D dilute liquid state [12, 13]. Moreover, it permits one to predict the existence of an excited trimer state in the vicinity of the dimer threshold [14, 15]. This prediction coincides exactly with the one derived directly from the dimensional reduction of the 3D Schrödinger equation in the presence of a 1D waveguide [16].

In Ref. [15] a renormalization procedure is used to cure the divergencies coming from the bare zero-range three-body force. In Ref. [13] a three-body contact condition is used instead, to implement the zero-range model. These two last studies lead to exactly the same reduced equation of the three-body problem, referred hereafter as the 1D Skorniakov Ter-Martirosian (STM) equation. Nevertheless the 1D STM equation in Ref. [16] differs from the later even though, the same prediction for the excited trimer state is obtained near the dimer threshold.

In this work, a three-body zero-range pseudo-potential leading to a mathematically well-behaved problem is derived both in configuration (section II) and in momentum space (section III). The pseudo-potential has the same form than the two-body A-potential in the two-dimensional (2D) space [17]. In section IV the STM equation for three-bosons interacting via the two- and the three-body zero-range forces is derived. This STM equation is identical to the one obtained in Refs. [14, 15]. The A parameter of the pseudo-potential can be any positive real. However the first order Born approximation breaks this A-freedom and a specific value of A permits to recover the renormalized strength of the zero-range force in section V. Finally in section VI the equivalence between the zero-range 1D model and the dimensional reduction method is obtained in the vicinity of the dimer threshold where the Born approximation is accurate.

II. REGULARIZED ZERO-RANGE THREE-BODY FORCE

In this section the 1D three-body contact potential is introduced in complete analogy with the 2D two-body problem. Let us consider three particles of same mass m labeled by the index i ∈ {1, 2, 3}. The positions of the three particles are given by the coordinates zi. The center of mass of the system is C = (z1 + z2 + z3)/3 and the two other Jacobi coordinates are

\[ z_{ij} = z_i - z_j ; \quad Z_{ij} = \frac{2}{\sqrt{3}} \left( z_k - \frac{z_i + z_j}{2} \right), \quad (1) \]

where all the index i, j, k are distinct and are a cyclic permutation of the triplet (1, 2, 3). The general form of the zero-range three-body potential can be written as

\[ V_{3pp}^3\Psi(z_1, z_2, z_3) = \frac{\hbar^2}{m} \delta(z_{12})\delta(z_{23})\psi_3(C). \quad (2) \]

the function \( \langle C|\psi_3 \rangle \), is denoted hereafter as the three-body contact. It will will be shown later that it characterizes the singular behavior of the wavefunction at the contact of the three particles. For a given pair \( (ij) \), one introduces the hyper-radius \( R = \sqrt{Z_{ij}^2 + z_{ij}^2} \) and the hyper-coordinates \( \mathbf{R} = z_{ij}\hat{e}_z + Z_{ij}\hat{e}_Z \), where \( (\hat{e}_z, \hat{e}_Z) \) is an orthonormal basis. The potential in Eq. (2) can be expressed as

\[ V_{3pp}^3\Psi(z_1, z_2, z_3) = \frac{2\hbar^2}{m\sqrt{3}} \delta^2(\mathbf{R})\psi_3(C). \quad (3) \]

Due to its s-wave character, the expression of the zero-range potential in Eq. (3) does not depend on the choice of a specific pair of particles in the definition of the hyper-coordinate \( \mathbf{R} \). For the bare three-body zero-range potential used for example in Ref. [13], the
three-body contact $\psi_3(C)$ is just the value of the wavefunction at the contact of the three particles. However, similarly to the two-dimensional Green’s function, for a given value of the three-body contact, the two-dimensional delta distribution in Eq. (3) gives rise to a logarithmic singularity of the wavefunction at $R = 0$: $\Psi(z_1, z_2, z_3) \sim \ln (R/\ell) \pi \psi_3(C)/\sqrt{3} + \ldots$ where $\ell$ is a characteristic length of the system. The bare zero-range potential leads thus to a mathematically not well-behaved model. In practice, the bare potential can be used in the Born approximation, where the wavefunction at first order is regular at the contact \cite{13}. When the bare potential is used non perturbatively as in Ref. \cite{13}, a renormalizing procedure of the strength is necessary.

In order to construct a zero-range pseudo-potential, one has to introduce a regularizing operator such that when applied to the wavefunction considered, it gives a finite value of the three-body contact. For this purpose, one fixes the later characteristics length $l$ by imposing a boundary condition at the contact of the three particles as $R \to 0$ for all the wavefunctions solution of the Schrödinger equation:

$$\Psi(z_1, z_2, z_3) = \frac{\psi_3(C)}{\pi \sqrt{3}} \ln \left( \frac{R}{a_3} \right) + \ldots \quad (4)$$

where $a_3$ is the 1D three-body scattering length. This boundary condition has been already introduced for the three-body problem in 1D in Ref. \cite{14}. Equations (3) and (4) are formally equivalent to the definition of a zero-range force in the 2D two-body problem \cite{17} \cite{18}. For instance, in the free 1D space and in absence of two-body force, one finds from the contact condition in Eq. (4) one trimer at energy $E_3 = -\frac{4e^{-z_1}k^2}{m a_3^2}$, analogous to the dimer in 2D for a zero-range potential.

It is then straightforward to use for the three-body zero-range force, the known expression of the 2D $\Lambda$-potential that encapsulates the contact condition of Eq. (4):

$$V_3^{\Lambda \mathrm{pp}}(z_1, z_2, z_3) = -\frac{\pi \sqrt{3} \hbar^2}{m \ln (e^f \Lambda \sigma_3/2)} \delta(z_{12}) \delta(z_{13})$$

$$\lim_{R \to 0} \left[ 1 - \ln \left( \frac{e^f \Lambda R}{2} \right) R \frac{\partial}{\partial R} \right] \Psi(z_1, z_2, z_3). \quad (5)$$

The parameter $\Lambda$ in the pseudo-potential of Eq. (5) is any positive number, i.e. for any value of $\Lambda$, the pseudo-potential imposes the contact condition of Eq. (4). In Eq. (5), one identifies the $\Lambda$-dependent strength

$$g_3(\Lambda) = -\frac{\pi \sqrt{3} \hbar^2}{m \ln (e^f \Lambda \sigma_3/2)} \quad (6)$$

and the regularizing operator

$$\langle C|R_A|\Psi \rangle = \lim_{R \to 0} \left[ 1 - \ln \left( \frac{e^f \Lambda R}{2} \right) R \frac{\partial}{\partial R} \right] \Psi(z_1, z_2, z_3). \quad (7)$$

One can verify that for a state satisfying the contact condition in Eq. (4), one recovers as expected the strength of the zero-range force with $g_3(\Lambda)\langle C|R_A|\Psi \rangle = \frac{\hbar^2}{m} \psi_3(C)$.

### III. THREE-BODY PSEUDO-POTENTIAL IN THE MOMENTUM REPRESENTATION

In what follows, the three-body zero-range pseudo-potential is derived in the momentum representation. The momentum of the three particles are denoted by $k_i$. To avoid any ambiguities with the equations in configuration space, the bra-ket notation will be used below. The analogy with the two-body problem in 2D can be pursued and the derivation follows along the same lines as in Refs. \cite{12} \cite{21}. For this purpose, one defines the Jacobi coordinates in the momentum space. The momentum of the center of mass is $k_C = k_1 + k_2 + k_3$. The two other Jacobi coordinates are defined by

$$k_{ij} = \frac{k_i - k_j}{2}; \quad K_{ij} = \frac{2k_i - (k_i + k_j)}{3}. \quad (8)$$

In what follows, the notations $k = k_{12}$ and $K = K_{12}$ are used. Similarly to what has been done in the previous section, one introduces the hyper-momentum

$$Q = k_u + \frac{\sqrt{3}}{2} K u_z. \quad (9)$$

The stationary Schrödinger equation at energy $E$, for a system with only one interaction term given by the three-body force of Eq. (2) is in the momentum space

$$\langle Q^2 + k_C^2/6 + mE/\hbar^2 \rangle |Q, k_C|\Psi \rangle = -(k_C|\psi_3). \quad (10)$$

Equation (10) gives the high momentum behavior of the wavefunction for all energies and also in the possible presence of other non singular three-body potential. The three-body contact can be thus defined in the momentum representation by

$$\langle k_C|\psi_3 \rangle = -\lim_{Q \to \infty} Q^2 \langle Q, k_C|\Psi \rangle. \quad (11)$$

Let us consider the Green’s function at the negative energy $-\hbar^2\Lambda^2/m$ in the center of mass frame, for a vanishing hyper-radius ($R \to 0$):

$$\int \frac{d^2Q \exp iQ \cdot R}{(2\pi)^2} \times \frac{1}{Q^2 + \Lambda^2} = -\frac{1}{2\pi} \ln \left( \frac{e^f \Lambda R}{2} \right) + \ldots \quad (12)$$

Equation (12) can be used for any positive value of the parameter $\Lambda$ and permits one to express the three-body contact condition in Eq. (4) as

$$\frac{2}{\sqrt{3}} \int \frac{d^2Q}{(2\pi)^2} \left[ \langle Q, k_C|\Psi \rangle + \frac{(k_C|\psi_3)}{Q^2 + \Lambda^2} \right] = \frac{\hbar^2(k_C|\psi_3)}{mg_3(\Lambda)}. \quad (13)$$

From Eqs. (2) and (13), one can deduce the three-body pseudo-potential in the momentum representation

$$\langle k_1, k_2, k_3|V_3^{\Lambda \mathrm{pp}}|\Psi \rangle = g_3(\Lambda)\langle k_C|R_A|\Psi \rangle. \quad (14)$$
where
\[ \langle k_C|\mathcal{R}_\Lambda|\Psi \rangle = \frac{2}{\sqrt{3}} \int \frac{d^2 Q}{(2\pi)^2} \left[ \langle Q, k_C|\Psi \rangle + \frac{\langle k_C|\Psi_3 \rangle}{Q^2 + \Lambda^2} \right]. \tag{15} \]

IV. STM EQUATION

In this section the bound states made of three identical bosons are considered. The three particles interact via the three-body pseudo-potential of Eq. (14). Moreover, each pair of particles \((ij)\) interact via the zero-range potential of the Lieb-Liniger model:
\[ V(z_{ij}) = -\frac{2\hbar^2}{m a_2} \delta(z_{ij}), \tag{16} \]

where \(a_2\) is the 1D two-body scattering length. One introduces the two-body contact, which corresponds to the value of the wavefunction at the contact of two particles considered. For the contact of the pair (12), one has in the momentum representation:
\[ \langle K, k_C|\psi_2 \rangle = \int \frac{dk}{2\pi} \langle k, K, k_C|\Psi \rangle. \tag{17} \]

In the center of mass frame the wavefunction can be factorized as \(\langle k, K, k_C|\Psi \rangle = (2\pi)^3\delta(k_C)\langle k, K|\phi \rangle\). The two- and three-body contact are also factorized as \(\langle K, k_C|\psi_2 \rangle = (2\pi)^3\delta(k_C)\langle K|S_2 \rangle\) and \(\langle k_C|\psi_3 \rangle = (2\pi)^3\delta(k_C)S_3\). The three-body Schrödinger equation for a bound state of energy \(E = -\frac{\hbar^2 q^2}{m}\) is thus
\[ \left( k^2 + \frac{3}{4}K^2 + q^2 \right) \langle K|S_2 \rangle = -S_3 + \frac{2a_2}{a_2} \langle K|S_2 \rangle \]
\[ -\langle -k - K/2|S_2 \rangle + \langle -k - K/2|S_2 \rangle. \tag{18} \]

The STM equation follows from Eq. (18) after integration over the relative momentum \(k\):
\[ \left( a_2 - \frac{1}{\sqrt{q^2 + 3K^2}} \right) \langle K|S_2 \rangle + \frac{a_2 S_3}{\sqrt{4q^2 + 3K^2}} \]
\[ = 4 \int \frac{dK'}{2\pi} \frac{\langle K'|S_2 \rangle}{K^2 + K'^2 + 2KK'} \tag{19} \]

Injection of Eq. (18) in the contact condition (13) gives
\[ \frac{3}{a_2} \int \frac{dK}{2\pi} \frac{\langle K|S_2 \rangle}{\sqrt{4K^2 + q^2}} = -\frac{S_3 \ln(qa_3 e^{\gamma}/2)}{\pi \sqrt{3}}. \tag{20} \]

This last relation permits to close Eq. (13) and to recover the set of equations for the two-body contact obtained in Refs. 13, 15. Remarkably, an exact implicit equation on the binding wavenumber \(q\) has been derived from Eqs. (19) and (20) in Ref. 13.

V. \(\Lambda\)-DEPENDENT AND RENORMALIZED STRENGTHS

In Ref. 13, a renormalization of the bare three-body interaction is used for the derivation of the trimer spectrum as a function of the ratio between the two scattering length \(a_3\) and \(a_2\). Interestingly, the renormalized strength introduced in Ref. 13 for a bound state of binding wavenumber \(q\) coincides with \(g_3(q)\). In the point of view of the pseudo-potential, this corresponds also to the value \(\Lambda = q\) in the regularizing operator. For this choice, the explicit dependence on the three-body contact in Eq. (13) is exactly canceled. In the following lines, it is shown that this choice is relevant for the first Born approximation of the zero-range pseudo-potential.

Let us consider a regime where the three-body pseudo-potential gives a small contribution in the eigenergies. In the center of mass frame, the eigenstate can be decomposed in two parts:
\[ |\phi\rangle = |\phi^{(0)}\rangle + |\delta\phi\rangle, \tag{21} \]

where \(|\phi^{(0)}\rangle\) is an eigenstate of the three-body problem without the three-body pseudo-potential. The wavefunction \(\phi^{(0)}(z_1, z_2, z_3)\) is thus regular at the contact of the three-particles and the singular behavior is solely included in the perturbation \(|\delta\phi\rangle\). In the momentum space, the perturbation \(Q|\delta\phi\rangle\) is much smaller than \(Q|\phi^{(0)}\rangle\) except in the high momentum limit where
\[ (Q|\delta\phi\rangle \sim -\frac{S_3}{Q^2 + q^2}. \tag{22} \]

Equation (22) is valid above a given \(Q_0\) i.e. for \(Q > Q_0 \gg q\). However, for \(\Lambda = q\), the contribution in Eq. (22) is exactly canceled in the regularization and
\[ R_{\Lambda=q}|\phi\rangle \sim \frac{2}{\sqrt{3}} \int \frac{d^2 Q}{(2\pi)^2} (Q|\phi^{(0)}\rangle = \phi^{(0)}(R = 0). \tag{23} \]

Thus, in this perturbative regime the choice \(\Lambda = q\) permits one to recover the Born approximation of the bare zero-range potential where \(1/|\ln(qa_3)|\) is the small parameter.

VI. THREE-BODY PROBLEM NEAR THE DIMER THRESHOLD IN A 1D WAVEGUIDE

In the case of a 1D harmonic atomic waveguide, the effect of virtual excitations of pairs of particles in the direction transverse to the free motion breaks the integrability in the many-body quasi-1D problem. For taking this effect into account, it is necessary to introduce a perturbation to the Lieb-Liniger model. It has been shown that this perturbation can be modeled at the first order Born approximation by a zero-range bare three-body potential with the strength \(\tilde{g}^\text{Born}_3\):
\[ \tilde{g}^\text{Born}_3 = -\frac{6\hbar^2 a_3^2}{ma_2^2} \ln \left( \frac{4}{3} \right). \tag{24} \]
where $a_\perp = \sqrt{2\hbar/(m\omega)}$ is the characteristic length of the waveguide.

When the 2-body scattering length $a_2$ is large and positive, i.e. at the threshold of the dimer of binding wavevumber $1/a_2$, the Lieb-Liniger model predicts a shallow trimers (the McGuire trimer) in the 1D waveguide. Virtual excitations of pairs of particles induce a perturbation of this trimer of binding wavevumber $q = 2/a_2$. This last wavevumber gives the momentum space of the parameter $\Lambda$ chosen when the Born approximation is achieved on the pseudo-potential. At the leading order of logarithmic accuracy, one can then identify the bare strength in Eq. (24) with $g_3(\Lambda)$ and $\Lambda = 1/a_2$. One finds $\ln(a_3/a_2) \sim \frac{\pi a_2^2}{4\sqrt{3m(4/3)\lambda}}$ for $a_2 \to \infty$. In this regime, in presence of the three-body potential, in addition to the perturbed McGuire state, another trimer is found near the atom-dimer continuum. Importantly, the asymptotic law near the threshold for the two trimers coincide exactly with the ones found from the dimensional reduction of the 3D Schrödinger equation in presence of an harmonic waveguide [14]:

$$q_0 \sim \frac{2}{a_2} + \frac{4a_2^2}{a_1^2} \ln \left( \frac{4}{3} \right), \quad q_1 \sim \frac{1}{a_2} + \frac{2a_4^2}{3a_2^2} \ln^2 \left( \frac{4}{3} \right), \quad (25)$$

where $q_0$ and $q_1$ are the binding wavevumbers.

In the dimensional reduction method of Ref. [16], there is no three-body force in the Hamiltonian and the quasi-1D character of the system is revealed by a summation over the transverse mode in the STM equation:

$$\left( \frac{1}{\sqrt{4K^2 + q^2}} - a_2 \right) \langle K|S_2 \rangle = -2 \int \frac{dK'}{\pi} \sum_{n=0}^{\infty} \frac{1}{4^n} \frac{1}{a_2^2 + q^2 + K^2 + K'^2 + KK'} \langle K'|S_2 \rangle. \quad (26)$$

The momentum $1/a_\perp$ plays the role of a cut-off in the integral term of Eq. (26). In the limit where the momentum $K, K'$ and $q$ are much smaller that $1/a_\perp$, one has

$$\sum_{n=1}^{\infty} \frac{1}{4^n} \frac{1}{a_2^2 + q^2 + K^2 + K'^2 + KK'} \sim \ln \left( \frac{4}{3} \right) a_\perp^2. \quad (27)$$

The approximation in Eq. (27) was the one used for the derivation of the asymptotic law for the two trimers in Eq. (25). In what follows it is shown that this approximation is equivalent to the Born approximation of Eq. (24) performed with the zero-range pseudo-potential.

For that purpose, one considers formally the effective three-body potential $V_3$ which gives Eq. (24). The Hamiltonian is

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^{3} \frac{\partial^2}{\partial z_i^2} - \frac{2\hbar^2}{ma_2} \sum_{i<j<3} \delta(z_{ij}) + V_3. \quad (28)$$

The absence of singular behavior of the eigenstates of Eq. (28), shows that necessarily the potential $V_3$ is non-local in the configuration space. One can remark that the regime where the two-body contact $\langle K|S_2 \rangle$ is negligible for a momentum $K$ of the order of $1/a_\perp$, corresponds to the regime where the zero-range three-body force can be treated in the Born approximation. Then using the approximation Eq. (27), one finds an energy dependent potential valid in the Born approximation. For an hypermomentum $Q \lesssim 1/a_\perp$, one can write in the center of mass frame

$$\langle k, K|V_3|\phi \rangle = -\frac{\hbar^2}{m} \pi \ln(4/3) (k^2 + \frac{3}{4} K^2 + q^2) a_3^3 \frac{a_1}{a_2}$$

$$\times \int \frac{dK'dK'}{(2\pi)^2} \langle k', K'|\phi \rangle. \quad (29)$$

and $\langle k, K|V_3|\phi \rangle \sim 0$ for $Q \gtrsim 1/a_\perp$. In Eq. (29), $\int_\subset$ means an integration in the domain where the hyper-momentum $Q' = \sqrt{k'^2 + \frac{3}{4} K'^2}$ is smaller than $1/a_\perp$. Multiplying Eq. (29) by $\langle \phi|k, K \rangle$ and assuming that $V_3$ is a small perturbation, one can use the relation

$$\langle \phi|\hat{H}_0 - E|k, K \rangle \sim \frac{2\hbar^2}{ma_2} \langle (S_2|K)$$

$$+ \langle S_2| - k - K/2 \rangle + \langle S_2|k - K/2 \rangle \rangle. \quad (30)$$

The integration of the resulting equation on the hypermomentum in the domain $Q < 1/a_\perp$ gives the expectation value of the effective three-body potential in the center of mass frame:

$$\langle \phi|V_3|\phi \rangle \sim -\frac{6\hbar^2 a_3^4}{ma_2} \ln \left( \frac{4}{3} \right) |\phi(R = 0)|^2. \quad (31)$$

One thus recovers the same strength of the three-body potential as the one of the zero-range model in the Born approximation in Eq. (24).

VII. CONCLUSION

The three-body $\Lambda$-potential introduced in this paper leads to a mathematically well-behaved Schrödinger equation, avoiding thus a renormalization procedure of a bare zero-range force. This pseudo-potential is used in the context of atoms in a 1D waveguide where the virtual excitations in the transverse modes give rise to an effective zero-range three-body force in addition to the usual two-body force of the Lieb-Liniger model. For the three-body problem, in the limiting case of a large two-body scattering length, a three-body potential is obtained from the STM equation derived directly from the 3D Schrödinger equation in the presence of a 1D waveguide. This potential treated at the Born approximation explains the equivalence found near the dimer threshold, between the zero-range potential approach and the direct method of Ref. [14].
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