Level rearrangement in three-body systems

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We study systems of three bosons bound by a long-range interaction supplemented by a short-range potential of variable strength. This generalizes the usual two-body exotic atoms where the Coulomb interaction is modified by nuclear forces at short distances. The energy shift due to the short-range part of the interaction combines two-body terms similar to the ones entering the Trueman-Deser formula, and three-body contributions. A phenomenon of level rearrangement is observed, similar to the Zel’ dovich effect, by the onset of an additional stable level which is eventually absorbed by the two-body threshold energy, and can be interpreted as an Efimov-like state of the short-range potential.

\section{I. INTRODUCTION}

Exotic atoms have a long history, and have stimulated interesting developments in quantum dynamics of systems involving both long-range and short-range forces. For the exploratory studies presented here, the refinements of effective theories \textsuperscript{11} are not required, and we shall restrict ourselves to the Schrödinger framework, as reviewed, e.g., in \textsuperscript{2} for the three-dimensional case, and extended in \textsuperscript{3} for the two-dimensional one.

In units simplifying the treatment of the pure Coulomb case, an exotic atom can be modeled as

\[
-\Delta \psi + V \psi = E \psi \ , \quad V = -\frac{1}{r} + \lambda v(r) ,
\]

(1)

where \( r \) is the inter-particle distance and \( \lambda v(r) \) the short-range correction, with a variable strength for the ease of the discussion.

When the above spectral problem is solved, the most striking observations are:

1. The energy shift \( \delta E = E - E_n \) as compared to the pure-Coulomb energies \( E_n = -1/(4 \mu^2) \), is often rather small, but is usually not given by ordinary perturbation theory: for instance, an infinite hard-core of small radius corresponds to a small energy shift but to an infinite first order correction.

2. Each energy \( E(\lambda) \), as a function of the strength parameter \( \lambda \), is almost flat in a wide interval of \( \lambda \), with a value close to some \( E_n \), one of the pure Coulomb energies. Then \( \delta E \) is well approximated by a formula by Deser et al., and Trueman \textsuperscript{4},

\[
\delta E \simeq \frac{a}{2 \pi \mu} ,
\]

(2)

where \( a \) is the scattering length in the short-range interaction \( \lambda v(r) \) alone.

3. If \( v(r) \) is attractive, when the strength \( \lambda \) approaches one of the positive critical values at which a first or a new bound state appears in the spectrum of \( \lambda v \) alone, the energy \( E(\lambda) \) quits its plateau and drops dramatically from the region of atomic energies to the one of deep nuclear energy. It is rapidly replaced in the plateau by the next level. This is known as level rearrangement \textsuperscript{5}.

4. The above patterns are more general, and hold for for any combination of a long-range and a short-range interaction, say \( V = V_0 + \lambda v(r) \). The Deser-Trueman formula is generalized as

\[
\delta E \simeq 4\pi |\Phi_0(0)|^2 a ,
\]

(3)

where \( \Phi_0 \) is the normalized wave-function in the external potential \( V_0 \). If \( V_0 \) supports only one bound state, then the rearrangement “extracts” states from the continuum, instead of shifting bound radial excitations. An illustration is given in Fig. \textsuperscript{1} with a superposition of two exponential potentials of range parameters \( \mu = 1 \) and \( \mu = 100 \), namely

\[
V(r) = 2 v_c(1, r) + g v_c(100, r) ,
\]

(4)

where \( v_c(\mu, r) \) is tuned to start binding at unit strength, for a reduced mass 1/2.

\begin{center}
\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{1}
\caption{Level rearrangement for a two-body system bound by the potential (4). The wrong behavior of the excited levels near \( E = 0 \) is due to the variational approximation. The dashed line indicates the approximation corresponding to the Deser-Trueman formula (5). The dotted vertical lines show the coupling thresholds for the short-range part of the interaction.}
\end{figure}
\end{center}

4. There are several possible improvements and alternative formulations of (3). For instance, \( a_r \), the bare scattering length in \( \lambda v(r) \) can be replaced by the “long-range

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corrected” scattering length where the solutions of the radial equation for $\lambda v(r)$ are matched to the eigenfunctions of the external potential. See, e.g., [6], and refs. there. In the physics of cold atoms, one is more familiar with the approach by Busch et al. [7]. It deals with the case of an harmonic oscillator modified at short distances, but the derivation can be generalized as follows. Let $u(E, r)$ the s-wave reduced radial wavefunction for $V_0(r)$ that is regular at large $r$, and energy $E < 0$, with some normalization, e.g., $u(E, r) \exp(-r\sqrt{-E}) \to 1$ for $r \to \infty$. The levels in $V_0$ correspond to the quantization condition $\int_0^\infty u(E_0, r)^2 dr = 0$, where $E_0$ is an eigenenergy of $V_0$, for instance the ground state. When a point-like interaction of scattering length $a$ is added, then the boundary condition is modified into

$$u(E, 0) + a \partial_r u(E, 0) = 0 ,$$

which can be expanded near $E_0$ to give

$$\delta E = E - E_0 \simeq -a \partial_r u(E_0, 0) \partial_E u(E_0, 0) .$$

Now, the equivalence of (5) and (3), rewritten as

$$\delta E \simeq a \left[ \partial_r u_N(E_0, 0) \right]^2 ,$$

where $u_N$ is the normalized version of $u$, comes from the relation

$$\partial_r u(E_0, 0) \partial_E u(E_0, 0) = -\int_0^\infty u(E_0, r)^2 dr ,$$

which is easily derived from the Wronskian identity, widely used in some textbooks [8], here applied to energies $E$ and $E_0$.

The generalization to a number of dimension $d \neq 3$ is straightforward for $d > 3$. For $d = 1$, the first plateau is avoided, as the short-range potential, if attractive, develops its own discrete spectrum for any $\lambda > 0$. The case of $d = 2$ is more delicate: see, e.g., [9][10].

Our aim here is to present a first investigation of the three-body analog of exotic atoms. We consider three identical bosons, though we have in mind some less simple systems for future work. We address the following questions: is there a pattern similar to the level rearrangement? is there a generalization of the Deser-Trueman formula? what are the similarities with the case where the long-range interaction is replaced by an overall harmonic confinement?

The paper is organized as follows. In Sec. II we give some basic reminders about the spectrum of a three-boson systems from the Borromean limit of a single bound state to the regime of stronger binding, with a word about the numerical techniques The results corresponding to a superposition $V_0(r) + \lambda v(r)$ are displayed in Sec. III An interpretation is attempted in Sec. IV with the a three-body version of the Deser-Trueman formula. Section V is devoted to our conclusions.

II. THE THREE-BOSON SPECTRUM WITH A SIMPLE POTENTIAL

If two bosons interact through an attractive potential, or a potential with attractive parts, $\lambda v(r)$, a minimal strength is required to achieve binding, say $\lambda > \lambda_c^2$. A collection of values of $\lambda_c^2$ can be found, e.g., in the classic paper by Blatt and Jackson [11]. In the following, we shall normalize $v_0$ so that $\lambda_c^2 = 1$.

If one assumes that $v_0(r)$ is attractive everywhere, once two bosons are bound, the 3-boson system is also bound. (The case of potentials with a strong inner repulsion would require a more detailed analysis which is beyond the scope of this preliminary investigation.) This means that for a single monotonic potential

$$V_0 = \lambda [v_0(r_{12}) + v_0(r_{23}) + v_0(r_{31})] ,$$

where $r_{ij} = |r_j - r_i|$, the minimal coupling to achieve three-body binding, $\lambda = \lambda_c^3$, is less than 1, in our units. This is implicit in the seminal paper by Thomas [12]. The inequality $\lambda_c^3 < \lambda_c^2$ is now referred to as “Borromean binding”, after the study of neutron halos in nuclear physics [13]. One gets typically $\lambda_c^3 \simeq 0.8$, i.e., about 20% of Borromean window [14].

In short, the three-boson spectrum has the following patterns:

- For $\lambda < \lambda_c^3$, no binding
- For $\lambda_c^3 < \lambda < 1$, a single Borromean bound state, and, for $\lambda$ close to 1, a second three-body bound state just below the two-body energy,
- For $1 < \lambda$, two bound states below the $2 + 1$ breakup.
- In addition, very near $\lambda = 1$, the very weakly bound Efimov states.

The excited state can be considered as the first member of the sequence of the Efimov states occurring near $g = 1$. However, it differs from the other Efimov states in the sense that when the coupling is varied, it remains below the two-body break-up threshold, at least for the simple monotonic potentials we consider here.

This is schematically illustrated in Fig. 1. The two-body energy is known analytically for a single exponential potential. The three-body energies have been calculated with variational method based on either exponential or Gaussian wavefunctions, say

$$\Psi = \sum_i \gamma_i \exp[-a_i r_{23}^n - b_i r_{31}^{n_1} - c_i r_{12}^{n_2} + \cdots] ,$$

where the dots stand for terms deduced by permutation. For $n = 1$, we wrote our own code: the range parameters

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1 We thank Pascal Naidon for a correspondence on this point.
are chosen in a geometric progression \( \{ \alpha, \alpha r, \alpha r^2, \ldots \} \). The lowest term can be linked to the energy \( E \) by the relation \( \alpha^2 = 14E/15 \) suggested by the Feshbach-Rubinow equation \([15]\). For \( n = 2 \), we used the code made available by Suzuki and Varga \([16]\). We also did some checks based on the hyperspherical expansion.

III. THE THREE-BODY ENERGIES WITH LONG- AND SHORT-RANGE FORCES

We now replace (8) by a superposition

\[
V_0 + \lambda V, \quad V = \sum_{i<j} v(r_{ij}), \quad (10)
\]

where \( v(r) \) is significantly shorter ranged than the pair potential entering \( V_0 \). In practice, we will choose the long-range part as \( V_0 = \lambda_0 \sum_{i<j} v_e(1, r_{ij}) \) of unit range, and \( v(r) = v_e(\mu r) \), with \( \mu \) ranging from 20 to 100. Note that the computations become rather delicate for \( \mu = 100 \), and would require dedicated techniques for larger \( \mu \).

In Fig. 3 are shown the spectra for \( \lambda_0 = 2 \), i.e., twice the two-body critical coupling, and \( \mu = 20, 50 \) and 100, with a magnification of the rearrangement region in the latter cases. The unit of energy is irrelevant, as it can be modified by an overall rescaling of the distances. Comments are in order:

- As in Fig. 1, a convex behavior as a function of \( \lambda \) is observed for the excited energy-levels, i.e., \( E_n(\lambda) \) with \( n > 1 \). This is permitted, provided that the sum of the first energies remains concave \([17]\).
- As in the two-body case, the transition is sharper when the range of the additional potential becomes shorter.
- There is a clear rearrangement, in the sense that for \( \lambda \to \lambda_2^0 \simeq 0.8 \), the excited state falls suddenly near the unperturbed ground-state energy.
- However, there is no second plateau for the excited state, just somewhat a smoothing of the fall-off for \( \lambda \gtrsim \lambda_2^0 \).

IV. INTERPRETATION

Let us first concentrate on the region of small \( \lambda \). One can estimate the energy shifts \( \delta_{ij} = \delta E \) corresponding to a collection of external potentials \( V_{0,i} \) and short-range potentials \( V_j \), and study empirically the properties of the matrix \( \{ \delta_{ij} \} \).

In the two-body case, one finds that the \( 2 \times 2 \) sub-determinants vanish almost exactly. This is compatible with a factorization

\[
\delta E^{(2)} \simeq A_{LR} B_{SR}, \quad (11)
\]

as a product of a long-range term depending only on \( v_0 \) and a short-range term depending only on \( \lambda v \). This is achieved by the Deser-Trueman formula, with \( A_{LR} \) be-
ing the square of the wave function at \( r = 0 \) (times 4\( \pi \)) and \( B_{SR} \) the scattering length.

In the three-body case, it is observed that the 2 \( \times \) 2 sub-determinants still nearly vanish, especially for the smaller values of the short-range strength \( \lambda \), but that the 3 \( \times \) 3 sub-determinants vanish even better (of course we compared the determinants divided by the typical values of a product of 2 or 3 \( \delta E \)). This is compatible with \( \delta E \) being a sum of two factorized contributions,

\[
\delta E^{(3)} = A_{LR} B_{SR} + A'_{LR} B'_{SR},
\]

that we conjecture as the generalization of the Deser-Trueman formula.

It is now rather natural to guess that the first contribution is a simple extension of \( \delta \) and reads

\[
A_{LR} B_{SR} = 12 \pi |\Phi_{12}(0)|^2 a, \tag{13}
\]

where \( |\Phi_{12}(0)|^2 \) is a short-hand notation for the two-body correlation factor \( \langle \Phi|\delta^{(3)}(r_2 - r_1)|\Phi\rangle/\langle\Phi|\Phi\rangle \). It is checked that this term dominates for small shifts, i.e., for small \( \lambda \), see Fig. 4. However, this term, if alone, would induce a fall-off of the atomic energies toward the nuclear region only for \( |a| \to \infty \), i.e., for \( \lambda \to 1 \), the coupling threshold for two-binding.

\[\begin{figure}[h]
    \centering
    \includegraphics[width=\textwidth]{fig4}
    \caption{Calculated energy (thick blue line, dashed for the excited state) vs. the estimate using the first term in Eq. (12) (thin black line). The calculation is done for a superposition of two exponentials, one with unit range and strength \( \lambda_0 = 2 \), and another of range parameter \( \mu = 50 \) and strength \( \lambda \).}
\end{figure}\]

The second contribution in Eq. (13) should thus account for the genuine three-body effects. So \( B'_{SR} \) is a kind of generalized scattering length that blows up when \( \lambda \) approaches the coupling threshold \( \lambda_0^2 \) for three-body binding. As the theory of three-body scattering is a little intricate, we postpone the precise definition of \( B'_{SR} \) to some further study. As for the long-range factor \( A'_{LR} \) of this second term, the simplest guess is to assume that it is proportional to the square of the wavefunction at \( r_1 = r_2 = r_3 \), or in terms of the Jacobi variables \( x \) and \( y \) describing the relative motion, \( A'_{LR} \propto \langle \Phi|\delta^{(3)}(x)|\delta^{(3)}(y)|\Phi\rangle \), but this is seemingly not the case.

Our study of generalized exotic atoms is related to the Efimov physics, \( si parva licet componere magnis \). In particular, the authors of refs. [18, 19], and probably some others, have studied how the Efimov effect is modified if each atom is submitted to an individual harmonic confinement. They also found that near a point where the two-body scattering length becomes infinite, there is a finite number of three-body bound states, instead of an infinite number in absence of confinement. The third three-body bound state in the last two plots of Fig. 3 can be interpreted as an Efimov state of the short-range potential, modified by the long-range potential.

V. CONCLUSIONS

The lowest states of three-bosons have been calculated with a superposition of long-range and short-range attractive potentials. When the strength \( \lambda \) of the latter is increased, starting from \( \lambda = 0 \), the 3-body energies decreases very slowly, and can be well approximated by a straightforward generalization of the Deser-Trueman formula involving only the 2-body scattering length. However, when \( \lambda \) approaches 0.8 (in units where \( \lambda = 1 \) is the coupling threshold for binding in the short-range potential alone), there is a departure for the Deser-Trueman formula, which can be empirically accounted for by the product of a short-range and a long-range factor. The short-range factor is the three-body analog of the scattering length and becomes very large when \( \lambda \simeq 0.8 \) which corresponds to the occurrence of a Born-\( \text{orange} \) bound state in the short-range potential alone.

Many developments are required. What is the precise definition of the three-body short-range factor? What is the corresponding long-range factor? What is the minimal ratio of range parameters required for the occurrence of the third stable three-body state? When does a fourth state show up? What are the analogs for \( N \geq 4 \) bosons? We also aim at studying some asymmetric systems. For instance, a prototype of \( (K^-pp) \) could be built, with a Coulomb interaction, that is known to produce a stable ion, below the threshold for breakup into a \( (K^-p) \) atom and an isolated proton \( \text{[20]} \). Then the strong interaction between the two protons and the strange meson \( K^- \) could be mimicked by a simple potential of range about 1 fm, to study how the existence of a nuclear bound state \( (K^-pp) \) modifies the atomic spectrum.

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