The size of two-body weakly bound objects : short versus long range potentials

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The study of the properties of weakly bound systems has found a renewed interest after the discovery of halo nuclei in nuclear physics\textsuperscript{[1,2]} as well as loosely bound dimers in molecular physics\textsuperscript{[3,5]}. These systems have very large mean square radii and small separation energies. They can be treated as two (or three)-body systems interacting through a potential. In fact, the separation energy of the one or two nucleons forming the halo is so small that their degrees of freedom can be separated from those of the nucleons constituents of the core. In the case of diffuse diatomic molecules, the situation is even better, the separation energy being several orders of magnitude less than the ionization potential of each constituent.

In this Letter, we want to discuss in very general terms the size of two-body weakly bound objects. Short and long range repulsive forces have been studied up to now in the context of nuclear and molecular physics. In particular, the variation of the size of these quantum systems as the energy approaches zero (asymptotic laws) has been actively investigated\textsuperscript{4,5}.

There is one more class of potentials which can give rise to very extended systems in the zero energy limit, namely long-range potentials for which this limit is attained when the deepness of the potential goes to zero. It is the purpose of this paper to discuss these long-range potentials and show that they predict a variation of the size of these quantum systems in the zero energy limit, different from short-range potentials. We will compare the two behaviours and discuss the transition between the short and long range regime.

Concerning short range potentials, we will discuss short range potentials presenting a repulsive core. The presence of a repulsive core in the interacting potential should actually be included to modelize the Pauli exclusion principle. We will show how the presence of the core modifies the asymptotic laws found for short range potentials, discussed up to now, which are defined by only two parameters, namely the deepness of the potential and the range.

The Letter is structured as follows. We will first show that asymptotic laws for states of any angular momentum \(l\) can be derived starting from the Schrödinger equation, without making any specific reference to the potential. Then we will discuss how we can derive these laws by using the asymptotic behaviour of the wave functions both for short and long range potentials. Finally we will use the Kratzer potential to illustrate the energy dependence of the mean square radius for long range potentials, the influence of the core in the case of short range potentials (obtained from the Kratzer potential by cutting it at some distance) and the transition from the short to the long range regime. We will use the results obtained for a square well for a comparison with short range potentials defined by only two parameters.

In this work, we will consider only spherical symmetric potentials. The spin degrees of freedom are ignored. In this case, the radial Schrödinger equation (\(\hbar = 2m = 1\)) is given by

\[-\frac{\partial^2}{\partial r^2} - \frac{2}{r} \frac{\partial}{\partial r} + \frac{\ell(\ell + 1)}{r^2} + \lambda w(r)\psi_{\ell}(r) = E_{\ell}\psi_{\ell}(r).\] (1)

where \(\lambda\) scales the deepness of the potential \(w(r)\). Since we consider only the lowest states of each angular momentum (the wavefunction has no node), they are simply labelled by \(\ell\).

The first very general result obtained from eq.\(\textsuperscript{1}\) is that long range potentials can also give rise to very extended systems. The asymptotic laws derived in molecular physics\textsuperscript{[4,5]} as well as loosely bound dimers in nuclear physics\textsuperscript{[1–3]} ensure that the rms radius is diverging with \(1/E_{\ell}\) for all \(\alpha\) as \(E_{\ell} \to 0\), which means \(\lambda \to 0\).
No such a general prediction can be made in the case of short range potentials, because in this case the zero energy limit is obtained when the coupling \( \lambda \) tends to a critical finite value \( \lambda_0 \).

In the case \( \ell = 0 \), another prediction is given by the Bertlmann-Martin inequality [10] which concerns the ground state radius and yields

\[
<r^2> \leq \frac{3}{E_1 - E_0}.
\]

(4)

where \( E_0 \) and \( E_1 \) are the energies of the ground and first excited states, respectively. Noting that \( E_1 - E_0 > 0 \), we can write \( E_1 = \varphi E_0 \) and get

\[
<r^2> \leq \frac{3}{(\varphi - 1)E_0}, \quad \varphi - 1 > 0.
\]

(5)

Consequently, for \( \ell = 0 \) the asymptotic behaviour of the rms radius as the energy tends to zero is given by this expression for all, short or long range, potentials.

In order to specify the value of \( \varphi \) and obtain predictions for \( \ell \neq 0 \), it is necessary to introduce assumptions concerning the wavefunctions.

Let’s first discuss short range potentials, characterized by a finite range \( R_0 \). Since the potential becomes negligible beyond \( R_0 \), the asymptotic form of the wavefunctions is related to the spherical Hankel functions

\[
\Psi_\ell(r) \approx e^{-\mu r}/r^\ell.
\]

(6)

As \( \mu \to 0 \) the energy tends to zero. Therefore, as long as the contribution from the inner part of the wavefunction is negligible, the rms radius is given by

\[
<r^2> \approx \int_{R_0}^\infty e^{-2\mu r}r^2e^{-2\ell f}dr/\int_{R_0}^\infty e^{-2\mu r}r^{-2\ell}dr.
\]

(7)

With this approximation, we get the relations derived by Rüisager, Jensen and Möller [11] :

\[
<r^2> \approx \frac{c_0}{|E_0|} ; \quad <r^2> \approx \frac{c_1 R_0}{\sqrt{|E_1|}} ; \quad <r^2> \approx c_2 R_0^2 ,
\]

(8)

Intuitively, the above assumptions imply the constants \( c_\ell \) to be independent of the potential. However this statement is not exact and in general \( c_\ell = c_\ell(w) \) is as expected. For \( \ell = 2 \) the rms radius behaves in the same way as for \( \ell = 2 \), namely it tends to a constant as the energy approaches zero.

Coming back to the inequality [12], in the case the \( \ell = 1 \) state is in the continuum, \( E_1 \) is set to zero (or \( \varphi = 0 \)). (Note that this procedure is not valid for confining potentials, for which \( E_\ell > 0 \).) Using the asymptotic properties of the s-state wavefunction leads to an absolute lower bound [12]

\[
<r^2> \geq \frac{1}{2|E_0|}.
\]

(9)

The equality is reached as \(-E_0 \to 0\), independently on the potential. As a consequence, in eq.(8), \( c_0 = 1/2 \) is a firm prediction, independently of the shape of the short range potential.

To get a practical insight on how much \( c_\ell \) depends on \( w \), the asymptotic laws [8] have also been studied numerically for potentials depending only on two parameters, the deepness and a typical length \( R_0 \). In particular, the square well and the gaussian potentials have been used [11]. Their typical lengths are the square well radius and the range of the gaussian, respectively. In [11] it is shown that the coefficients \( c_\ell \) seem to be not very sensitive to the particular shape of the potential.

In general, \(<r^2>_\ell = f(E, R_0, w)\), that is the mean square radii depend on the energy of the state, the typical length \( R_0 \) and the shape of the potential. Eq.(8) explicitly give the dependence of \(<r^2>_\ell \) on \( R_0 \) for short range potentials defined by two parameters. This can be seen directly from the Schrödinger equation, by means of the change of variable \( x = r/R_0 \).

As a result, \(<x^2>_\ell = f'(\epsilon, w)\) where \( \epsilon = E_\ell R_0^2 \). As soon as the potential contains more than two parameters, the scaling cannot be exact, although it may constitute a good approximation under some circumstances. As a consequence of this quasi-scaling, the \(<r^2>_\ell \) may depend on the length of the potential in a way similar to (8). Such a situation may occur in particular when the potential has a short range repulsive component.

Let us now discuss the asymptotic laws for long range potentials, using the behaviour of the wave functions. Contrary to short range potentials, the wavefunction is in this case confined inside the potential. Use can be made of the spherical Bessel function of the first kind \( j_\ell(kr) \), with \( k \to 0 \), cutting the integrals at the first zero. This procedure yields right away

\[
<r^2>_\ell \approx \frac{c_\ell(w)}{|E_\ell|} .
\]

(10)

The derivation is very crude, and merely confirms the above statement of eqs.(8) and (8–10).

Relations [8], (8) and (10) show that both short and long range potentials may predict very diffuse systems in the zero energy limit. The asymptotic laws obtained present similarities as well as differences. In fact, in the case of long range potentials, the rms diverges as \( 1/E_\ell \) not only for \( \ell = 0 \), as it has been found for short range potentials, but for any \( \ell \). Besides, the constants \( c_\ell \) are sensitive to the potential \( w \).

A question one may ask about systems with halos is how to define them. In the case of short range potentials, a natural definition arises as it has been extensively discussed in the literature [7]. A reference scale is needed to compare it to the mean square radius of the system in
order to quantify the size of the halo. This reference scale can be taken equal to the range of the short range potential which in some cases can be related to a physical scale of the system, for example the size of the core in a halo nucleus and is identified with the outer classical turning point. An ideal halo is then defined as a system for which the single halo particle has a very large probability to be inside the classically forbidden region. Its properties are therefore determined by the tail of the wavefunction and are almost independent of the potential.

For the s-state, the above discussion refers to \( E_0 \rightarrow 0 \). However, it is interesting to note that for the shell-delta potential, \( w(r) = \delta(r - R_0) \) which possesses a single bound s-level, the particle is always in the classically forbidden region for any finite \( E_0 \).

In the case of long range potentials, the definition of a halo seems less straightforward. If the potential presents a repulsive core, a natural reference scale is given by the size of this core which can be related again to some physical size as, for example, that of the core in a halo nucleus or the sum to the two atomic radii, in the case of a diffuse molecule. So, the mean square radius of the system can be compared to the range of the potential core in order to quantify the extension of the halo. Contrary to the case of short range potentials, the wavefunction of the single halo particle will always be confined in the classically allowed region and the probability of finding the particle in the potential will always be one. Finally, in the case of short range potentials, an ideal halo is only possible if the halo particle is in an s-state. In fact, for \( p \)- a d-states the centrifugal barrier plays an important role, confining the wavefunction. This is not the case for long range potentials, where the barrier plays no role and therefore wavefunctions of any angular momentum can be extended.

Let us now discuss the asymptotic laws for long and short range potentials as well as the transition between the two in a particular case, namely the Kratzer potential [13]:

\[
w(r) = -2\lambda\left(\frac{a}{r} - \frac{a^2}{2r^2}\right)
\]

(11)

where \( a \) is just a scaling parameter which gives the distance at which the potential changes from attractive to repulsive. This potential has a long range and a repulsive core. The short range case is obtained by putting the potential to zero at a variable distance \( R_{\text{cut}} \):

\[
w_{\text{cut}}(r) = -2\lambda\left(\frac{a}{r} - \frac{a^2}{2r^2}\right)\Theta(R_{\text{cut}} - r)
\]

(12)

This cut Kratzer potential has the peculiarity of being defined by three parameters, namely the size of the core, the deepness of the potential \( \lambda \) and the range \( R_{\text{cut}} \).

By solving the Schrödinger equation [10] with (11), we obtain the mean square radius for any \( \ell \):

\[
\langle r^2 \rangle_{\ell} = \frac{1}{2E_1} \left[ 3 + 5\sqrt{\gamma^2 + (\ell + \frac{1}{2})^2} + 2(\gamma^2 + (\ell + \frac{1}{2})^2) \right]
\]

(13)

where \( \gamma^2 = (a^2\lambda) \). This gives, when \( E_1 \rightarrow 0 \),

\[
\langle r^2 \rangle_0 \approx \frac{3}{E_0}, \quad \langle r^2 \rangle_1 \approx \frac{7.5}{E_1}, \quad \langle r^2 \rangle_2 \approx \frac{14}{E_2}
\]

(14)

As expected, \( \langle r^2 \rangle \) have the same dependence on the energy as predicted by (8) and (10). For the sake of comparison, note that the values of \( c_\ell \) are the same in the case of a pure Coulomb force. For the harmonic oscillator, \( c_0 \) and \( c_1 \) take the same values whereas \( c_2 = 10.5 \).

We have solved (10) with the cut Kratzer potential (12) for different values of \( R_{\text{cut}} \) in order to see explicitly how the asymptotic laws vary when we use a three instead of a two parameter potential. Particular attention has been devoted to the asymptotic region, working down to energies of the order of \( 10^{-10} \). Note that such an achievement is only possible for potentials admitting analytical solutions for which the continuity conditions can be easily solved with high accuracy, whereas solving numerically the Schrödinger equation is very uncertain at low energies. The calculations we present are performed for \( a = 1 \). The features we emphasize in this work are not qualitatively affected by this parameter. From the numerical results, we get the following approximate asymptotic laws :

\[
\langle r^2 \rangle_0 \approx \frac{c_0}{|E_0|}, \quad \langle r^2 \rangle_1 \approx \frac{c_1R_{\text{cut}}}{\sqrt{|E_1|}}, \quad \langle r^2 \rangle_2 \approx c_2R_{\text{cut}}^5.
\]

(15)

Here \( c_1 \) and \( c_2 \) slightly depend on \( R_{\text{cut}} \), whereas \( c_0 = 1/2 \) as expected (9).

Relations (13) show that, for any \( \ell \), the dependence of the mean square radii on the energy of the state is not modified even in presence of a core. This is in agreement with what the arguments based on the asymptotic behaviour of the wave functions would suggest (8).

Concerning the dependence of the mean square radii on \( R_{\text{cut}} \), we see from (15) that the cut Kratzer potential present a quasi-scaling, the dependence on the range of the potential \( R_{\text{cut}} \) being very similar to that of (8).

In order to show the dependence of the \( c_\ell \) on \( R_{\text{cut}} \) and the shape of the potential, these coefficients are shown, as a function of the energy, in figure 1 (up \( \ell = 0 \), middle \( \ell = 1 \), bottom \( \ell = 2 \), for \( R_{\text{cut}} = 3 \) (line), 6 (short-dashed line) and 12 (long-dashed line) . For comparison we show the \( c_\ell \) obtained for a short range potential defined by two parameters (dotted line). We take the square well as an example.

We see that, apart from the \( \ell = 0 \) case, as the energy tends to zero, the asymptotic values of \( c_\ell \) depend indeed on the potential. This dependence increases with \( \ell \), as one should expect if the centrifugal barrier has a
confining effect and the wavefunctions become more sensitive to the particular shape of the potential. We also see that for \( \ell = 1, 2 \) the spreading among the three cut Kratzer potential results is only of a few percents (legitimating the \textit{quasi}-scaling), much less than the differences with the square well potential results. This qualitatively underlines the differences in the inner part of the wavefunctions.

It is interesting to ask if specific physical systems are in the low-energy limit where the asymptotic laws directly give the size of the system once the separation energy is known. We have looked at the case of halo nuclei and molecular dimers, by using experimental values of the separation energy and radius to calculate the corresponding \( c_0 \). For \(^{11}\text{Be} \) the experimental separation energy is \( 5.5 \text{ MeV} \) and the rms radius is about \( 7 \text{ fm} \), which leads to \( c_0 \approx 1.1 \). The \(^4\text{He} - ^4\text{He} \) dimer has a separation energy of \( 10^{-1} \text{eV} \) and a radius of \( 70 \text{ Å} \); it yields \( c_0 = 0.52 \).

The calculated \(^3\text{He} - ^6\text{Li} \), with a separation energy of \( 10^{-2} \text{eV} \) and a radius of \( 210 \text{ Å} \), reaches \( c_0 = 0.5 \). These estimates show that the loosely bound dimers are situated in the asymptotic region, whereas the halo nuclei merely remain at its threshold, in a range sensitive to the potential. A similar conclusion has been drawn by studying the Bertlmann-Martin inequality \( [14] \).

Outside the asymptotic region, it becomes even difficult to decide between a short and a long range potential, if the only observables are the separation energy and the rms radius. The key point in this respect is obviously given by the spectrum. In both dimers and halo nuclei, the number of states is rather limited, and thus a description by a short range potential is quite natural.

Let us now come to the transition between the short and long range regime. The example of the Kratzer potential provides us with a way of studying this transition by looking at evolution of \( c_\ell \) as a function of the range \( R_{cut} \). A priori, the transition depends on the energy, but numerical results show that this dependence is simple in our case. In figure 2 we present \( c_0 \) against \( \sqrt{|E_0|} R_{cut} \). The half-point between the short range (\( c_0 = 1/2 \)) and long range regime (\( c_0 = 3 \)) lies at around \( \sqrt{|E_0|} R_{cut} = 2 \).

For higher angular momenta, the problem is more complicated because going from the short (\([14]\)) to the long range (\([15]\)) regime modifies both \( c_\ell \) and the energy dependence of the asymptotic laws.

Note that the scaling and \textit{quasi}-scaling present in eqs.\((3)\) and \((5)\) cannot be used to study the transition between short and long range regime. For example, for \( \ell = 0 \), the transition does not occur if we take the square well potential at any finite radius \( R_0 \). This is due to the fact that according to eq.\((3)\) \( c_0 = 1/2 \) independently on \( R_0 \). Nevertheless, it is clear that for a fixed energy, the required potential deepness \( \lambda \) is decreasing as \( R_0 \) increases, so that the limit \( R_0 \to \infty \) implies \( \lambda \to 0 \). It means that the square well potential only reaches the long range limit for infinite \( R_0 \).

Let us finally remark that up to now the weakly bound objects found experimentally are interpreted in the two-body description as \( s \)-states. It remains a challenging problem to observe halo states that would be interpreted, in this context, as higher angular momentum states. To the extent that a two-body description yields the basic description, they should occur as excited levels. In the nuclear case, this situation is hardly possible, because the many-body degrees of freedom will strongly affect the first \( s \)-state, and destroy the simple two-body picture. From this point of view, the dimers are better candidates.

In conclusion, we have discussed the size of two-body weakly bound objects using both long range potentials and short range potentials having a repulsive core. We have shown that not only short range but also long range potentials give rise, in the zero energy limit, to very extended systems. The asymptotic laws obtained in this case show a different energy dependence from those of short range potentials already for \( p \)- and \( d \)-states. The dependence of the asymptotic laws on the particular shape and typical length of short range potentials, defined by both two and three parameters, has also been studied. All these ideas as well as the transition of the asymptotic laws from the short to the long range regime for \( \ell = 0 \) are illustrated in the particular case of the Kratzer potential.

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FIG. 1. cut Kratzer potential : the values of $c_\ell$ are plotted against $E_\ell$ for $\ell = 0$ (up), 1 (middle) and 2 (bottom). The line corresponds to $R_{cut} = 3$; the short-dashed and long-dashed lines correspond to $R_{cut} = 6$ and 12, respectively. For comparison, the dotted line shows the results obtained with a short range potential without the repulsive core. As an example, the square well is taken. As far as $c_0$ is concerned, the arrows indicate the range of the lowest energies corresponding to halo nuclei (arrow on the right) and dimers (arrow on the left).

FIG. 2. Evolution of $c_0$ from the short to the long range regime for the cut Kratzer potential. For comparison, the dashed line shows the value of 1/2 valid when $E_0 \to 0$ for any short range potential.