Binding three or four bosons without bound subsystems

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We estimate the ratio $R = g_3/g_2$ of the critical coupling constants g_2 and g_3 that are required to achieve binding of two or three bosons, respectively, with a short-range interaction, and examine how this ratio depends on the shape of the potential. Simple monotonous potentials give $R \simeq 0.8$. A wide repulsive core pushes this ratio close to $R = 1$. On the other hand, for an attractive well protected by an external repulsive barrier, the ratio approaches the rigorous lower bound $R = 2/3$. We also present results for $N = 4$ bosons, sketch the extension to $N > 4$, and discuss various consequences.

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I. INTRODUCTION

The phenomenon of ''Borromean'' binding is well known [1,2]. In our world with three dimensions, a short-range potential $gv(r)$ does not always achieve binding of two bodies, even if v is attractive or contains attractive parts. A minimal strength is needed. More precisely, if one defines g_2 as the minimal strength to bind two particles of unit mass in the potential v, then the strength g required to bind two particles of mass m in the same potential must be such that $mg \geqslant g_2$. Similarly, binding three identical bosons of mass m requires $mg \geqslant g_3$ for the pairwise interaction $g\Sigma v(r_{ij})$, where r_{ij} denotes the distance between particles i and j. The crucial observation is that $g_3 < g_2$, implying that for a mass m and a coupling g such that $g_3 < mg < g_2$, the three-body system is bound while none of its subsystems is bound.

Borromean binding is implicit to understand the Thomas collapse [3]. When the range of the potential v is reduced, or equivalently, when $g \to g_2$ from above, the three-body binding energy $E_3(g)$ becomes very large compared to the two-body energy E_2. Also the Efimov effect [4], i.e., the proliferation of loosely bound excited states in the three-body spectrum near $g = g_2$ implies that the three-body ground-state already exists at this point.

An example of three-body bound state without bound subsystem is the ^{6}He nucleus, considered schematically as a (α,n,n) system. It is stable against spontaneous dissociation, while neither the $(\alpha,n) = {}^5$He nor the (n,n) systems are bound. The name ''Borromean'' was given to such nuclei [1,2] after the Borromean rings, which are interlaced in such a subtle topological way, that when one removes one of them, the two others become unlocked.

Borromean or nearly Borromean bound states also exist in molecular physics, as seen, for instance, from Ref. [5] and references therein. In both the nuclear and the molecular case, the basic potential includes a hard core at short distances. This motivates the present study of Borromean binding with potentials whose shape differs from the purely attractive models considered in some earlier investigations [6,7].

Let $R = g_3/g_2$ be the ratio of critical coupling constants. For simple monotonous potentials, such as Yukawa, Gaussian, or exponential, it is found [6] that R is very close to 0.8. This is in agreement with the rigorous lower bound $R \geqslant 2/3$ [6]. The fact that all simple potentials give almost the same $R \simeq 0.8$ is understood as follows: at vanishing energy, the wave function extends very far outside the potential well, and thus does not probe very accurately the details of the short-range interaction, which is just seen as a contact attraction.

There are, however, reasons to believe that R can appreciably differ from 0.8. The aim of the present paper is precisely to study how R evolves when one starts from a simple monotonous potential and adds either an inner core or an external barrier.

When an external barrier of growing size is added to the potential, R evolves from $R \simeq 0.8$ to $R \to 2/3$. An example is provided by $v \propto r^2 \exp(-2\mu r) - \exp(-\mu r)$ when μ varies, or, similarly, by combinations of Gaussians.

When an inner core is implemented, a transition is observed from $R \simeq 0.8$ to $R \to 1$. This will be seen for the Morse and the Pöschl-Teller potentials when an appropriate parameter is varied. An extreme case consists of a hard core of radius c and an attractive delta shell $-\delta(r-d)$ located at $d > c$. The critical strength g_2 can be calculated exactly. One can also calculate exactly the strength g_∞ that makes the two-body scattering length vanish and hence is sufficient to bind the infinite boson matter [8], with the result g_∞/g_2

$=c/d$. Thus, as $d\to c$, g_∞/g_2 approaches 1 and so does any g_N/g_2 ratio with N finite.

Note that the ratio R cannot exceed $R=1$ for the additive potential $V=g\Sigma v(r_{ij})$, provided v is purely attractive. This means that one cannot conceive a situation where two-body systems are bound while a three-boson system is unbound. The following proof is due to Basdevant [9]. For $g<g_2$, let $\varphi(r)$ be the ground-state wavefunction of the two-body system, with energy E_2. The trial wavefunction $\Psi=\varphi(r_{12})\varphi(r_{13})$ can be used for the three-body Hamiltonian written as

$$H=\frac{\mathbf{p}_2^2}{2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)+\frac{\mathbf{p}_3^2}{2}\left(\frac{1}{m_1}+\frac{1}{m_3}\right)+\frac{\mathbf{p}_2\cdot\mathbf{p}_3}{m_1}+v(r_{12})+v(r_{23})+v(r_{31}), \tag{1}$$

leading to an expectation value $2E_2$ if the interaction $v(r_{23})$ is neglected. So $E_3\leqslant 2E_2<0$ if $v\leqslant 0$ Q.E.D. The proof holds for an asymmetric interaction $V=\Sigma v_{ij}$ with v_{12} binding $(1,2)$ and v_{13} binding $(1,3)$, and v_{23} only weakly attractive or even vanishing. We believe that this result remains true if v is not purely attractive, but we have not been able to prove this generalization.

This paper is organized as follows. In Sec. II, we discuss how to compute accurately the critical couplings g_N. In Sec. III, we present the results obtained for the Morse model and a few other potentials: the three-body binding energy obtained at $g=g_2$, at the edge of binding for the two-body systems; the critical coupling g_3 for three-body systems; an estimate of g_4, the minimal strength necessary to bind four bosons. It is expected that $g_4<g_3$, with, however, the constraints $g_4/g_3\geqslant 3/4$ and $g_4/g_3\geqslant 1/2$ established in Ref. [6]. The numerical estimate of g_4 requires delicate variational calculations, especially when the potential displays both attractive and repulsive parts. A simple extrapolation to g_∞, i.e., the infinite boson matter, will be presented in Sec. IV. Some conclusions and a list of open problems are presented in Sec. V.

II. VARIATIONAL METHODS

There are well-known techniques, in particular variational methods [10], to compute with very high precision the binding energy $E_N(g)$ of a system of N particles in a regime $g>g_N$ where binding is established. It is a slightly different art, however, to estimate the value g_N corresponding to the border of the stability domain. Even in the simple case of $N=2$ constituents, this is not completely obvious, as seen, e.g., from the discussion in Refs. [11,12] for the Yukawa potential.

A first strategy consists in computing accurately the binding energy $E_N(g)$ in a domain where binding occurs and letting g decrease. As a behavior

$$E_N\propto-(g-g_N)^2 \tag{2}$$

is expected, one better looks at $(-E_N)^{1/2}$ as a function of g and checks a straight behavior as $E_N\to 0$. As in Ref. [13], a Padé-type of approximation is found adequate to extrapolate toward g_N. In a typical variational method, the Schrödinger equation $(T+V)\Psi=E_N\Psi$ is solved by expanding the wave function on a basis of functions

$$\Psi=\sum_i C_i\varphi_i. \tag{3}$$

In a given set of φ_i, the weights C_i (represented by a vector $\mathbf{C}$) and the variational energy E are obtained from a generalized eigenvalue equation

$$(\tilde{T}+g\tilde{V})\mathbf{C}=E\tilde{N}\mathbf{C}, \tag{4}$$

involving the restrictions of the kinetic-energy operator T and potential energy V to the space spanned by the φ_i, and a definite-positive matrix $\tilde{N}$, which does not reduce to the unit matrix when the φ_i are not orthogonal.

An alternative (though not strictly legal) method for estimating the critical coupling g_N consists of looking directly at the point $E=0$ and rewriting the eigenvalue equation as

$$\tilde{V}\mathbf{C}=-\frac{1}{g}\tilde{T}\mathbf{C}, \tag{5}$$

involving, again, a Hermitian matrix on the left, and a definite-positive matrix on the right. In principle, the wavefunction need not be normalizable at $E=0$, but in practice, one can use a basis of normalizable functions, provided one allows for components with very long range.

The results presented below have been checked using both the extrapolation method and the direct estimate of the critical coupling.

When the number of terms in Eq. (3) is incremented, there is a dramatic increase of the number of nonlinear parameters entering the basis functions (the coefficients a_{ij} in the examples below). The minimization of the variational energy by varying these parameters becomes (i) ambiguous, as neighboring sets of values give comparable energies, and (ii) intractable, even with sophisticated minimization routines. A simple trick [14] is inspired by the work of Kamimura [15]. It consists of imposing all a_{ij} parameters to be chosen in a single geometric series. Then only the lowest and the largest values have to be optimized numerically. The minimization is much faster. The slight loss in accuracy is more than compensated by the possibility of increasing easily the number of terms. This works rather well for achieving a reasonable accuracy. When one aims at very precise results, more sophisticated techniques are required, such as the well-documented and powerful stochastic variational method (SVM) [10,16].

It remains to choose the basis functions in Eq. (3). We have compared the results obtained with exponential functions

$$\varphi_i=\exp\left(-\sum a_{ij}r_{ij}\right)+\cdots \tag{6}$$

and Gaussians

$$\varphi_i=\exp\left(-\sum a_{ij}r_{ij}^2\right)+\cdots, \tag{7}$$

where the parentheses can be rewritten as the most general quadratic form involving relative Jacobi coordinates. In both cases, the ellipses are meant for terms deduced by permutation, to ensure the proper symmetry properties of the trial basis.

The former basis is by far more efficient when the expansion (3) is limited to a small number of terms. For instance, a single exponential function is sufficient to demonstrate the stability of the ion $Ps^-=(e^+e^-e^-)$ in quantum chemistry, while several Gaussians are needed. However, when the number of terms increases, the exponential basis, even when associated with a stochastic search, tends to give rise to numerical instabilities similar to those described, e.g., by Spruch and Delves [17]. The problem can certainly be circumvented [18], but we found it more convenient to use SVM with Gaussians to get stable and accurate results. Anyhow, the results involving more than $N=3$ particles have been obtained with Gaussians only, since one cannot derive simple analytic expressions for the matrix elements within the exponential basis. Note that when N increases, the surface and tail of the system play a relatively less important role, so the use of Gaussian functions should become more appropriate.

III. RESULTS FOR g_3/g_2 AND g_4/g_2

In this section, we present some results on $R=g_3/g_2$ and $R_4=g_4/g_2$. We restrict ourselves to symmetric three- or four-body systems, involving identical bosons. Some results on equal-mass particles with asymmetric interaction have been given in Refs. [6,7].

To simplify the discussion on the influence of the parameters such as the constituent mass, the range and the strength, we use scaling laws. Consider, for instance, the case of two particles of mass m interacting through a Yukawa potential $-K\exp(-\mu r)/r$. A change of variable $\mu r\to r$, where the new r is dimensionless, transforms the Hamiltonian H governing the relative motion into

$$H=\frac{\hbar^2\mu^2}{m}\left[-\Delta_r-g\,\frac{\exp(-r)}{r}\right], \tag{8}$$

where $g=Km/(\mu\hbar^2)$ involves the product of the strength K and the constituent mass m, as expected. The spectral properties of the dimensionless bracket as a function of g gives access to all cases. A similar scaling transformation can be applied to all potentials we shall consider.

A. Monotonous potentials

We consider here three simple functional forms, Yukawa, exponential, and Gaussian, corresponding to

$$-v(r)=\frac{\exp(-\mu r)}{r},\quad \exp(-\mu r),\quad \exp(-\mu^2 r^2), \tag{9}$$

respectively, where, without loss of generality, the range parameter μ and the constituent mass m can be set to $\mu=m=1$ by simple rescaling.

TABLE I. Comparison of critical couplings g_N to achieve binding of $N=2$, 3, and 4 identical bosons in a Yukawa (Y), exponential (E), or Gaussian (G) potential. Also shown is g_∞, which corresponds to a vanishing of the two-body scattering length, the E_3 obtained for $g=g_2$, and the four-body energy E_4 for $g=g_3$.

Potential	g_2	$E_3(g_2)$	g_3/g_2	$E_4(g_3)$	g_4/g_3	g_∞/g_2
Y	1.68	–0.172	0.80	–0.320	0.81	0
E	1.45	–0.047	0.80	–0.093	0.80	0
G	2.68	–0.236	0.79	–0.438	0.80	0

The critical couplings are displayed in Table I. As already stressed, the most remarkable feature is the close clustering of all values of R near 0.80. This means a 20% window for Borromean three-body binding. Similarly, all values of R_4 are found around 0.64. There is no obvious meaning to the observation that $g_4/g_3\simeq g_3/g_2$. Anyhow, g_{N+1}/g_N cannot be smaller than $N/(N+1)$ [6], so it should tend to 1 as N increases.

B. Potentials with external barrier

The potential

$$v(r)=a\exp(-\mu^2r^2/2)+b\exp(-2\mu^2r^2) \tag{10}$$

has been used by Nielsen, Fedorov, and Jensen [19], to study Borromean binding in two dimensions. By rescaling, one can fix $m=\mu=1$. The cases $(a,b)=(-1,0)$ and $(a,b)=(1,-2)$ are shown in Fig. 1 for illustration. For a and b both negative, this potential reduces to a simple monotonous function, and, not surprisingly, a ratio $R\simeq0.80$ is obtained for the critical couplings g_3 and g_2. With a and b of different signs, one can build a potential that looks like an almost pure harmonic oscillator at small values of r and vanishes only at distances that are very large as compared to the size of the ground-state wave function. One then obtains $R\to2/3$.

In this limit, we are, indeed, approaching the situation where the decomposition

$$\tilde{H}_3(m,g)=\sum_{i<j}\tilde{H}_2^{(i,j)}(3m/2,g) \tag{11}$$

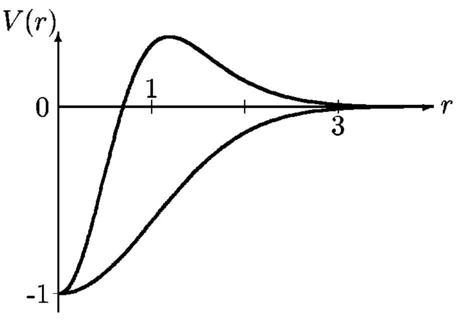

FIG. 1. Shape of the potential of Eq. (10) for $(a,b)=(1,-2)$ (with external barrier) and $(-1,0)$ (monotonous).

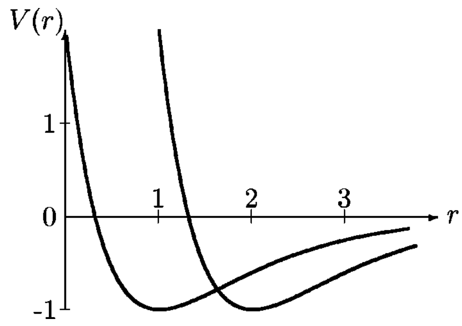

FIG. 2. Shape of the Morse potential for $r_0=1$ (left) and $r_0=2$ (right).

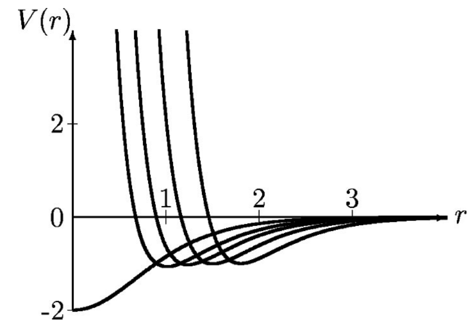

FIG. 3. Shape of the Pöschl-Teller potential for $\alpha=1$ (monotonous) and, from left to right $\alpha=2,3,5$, and 9.

corresponds to an exact factorization of the wave function [20,6], and thus the vanishing of $\tilde{H}_3(m,g)$ implies that of $\tilde{H}_2^{(i,j)}(3m/2,g)$ i.e., $g_3=2g_2/3$ [6]. Otherwise, one simply gets from Eq. (11), when saturated with the exact three-body wave function, $E_3(m,g)=\Sigma\langle\tilde{H}_2\rangle\geqslant 3E_2(3m/2,g)$, i.e., $g_3\geqslant 2g_2/3$. Here,

$$\tilde{H}_N(m,g)=\sum_k \frac{\mathbf{p}_k^2}{2m}+g\sum_{k<l} v(r_{kl})-\frac{\left(\sum_k \mathbf{p}_k\right)^2}{2Nm} \qquad (12)$$

is the translation-invariant Hamiltonian describing the relative motion of N particles.

Table I gives the values for a pure Gaussian potential, corresponding to $(a,b)=(-1,0)$: one obtains $g_2=2.680$, $g_3/g_2=0.79$ and $g_4/g_3=0.80$. For the potential $(a,b)=(1,-2)$ also shown in Fig. 1, the values become $g_2=21.20$, $g_3/g_2=0.672$, and $g_4/g_3=0.754$. We are already very close to the limit where $g_{N+1}/g_N=N/(N+1)$.

C. Morse potential

The Morse potential reads

$$v(r)=\exp[-2\mu(r-r_0)]-2\exp[-\mu(r-r_0)]. \qquad (13)$$

Again, one can set $m=\mu=1$ by rescaling. The shape is displayed in Fig. 2, for $r_0=1$ and $r_0=2$. The two-body problem with this potential can be worked out exactly [21]. In particular, the critical coupling g_2 is obtained from an equation involving the Kummer function, which can be solved easily. Our normalization is such that $g_2\to 1/4$ as r_0 increases. The critical couplings g_3 and g_4 have been estimated numerically, as well as $E_3(g_2)$, the three-body ground-state energy at the edge of binding two-body systems, and similarly $E_4(g_3)$. The results are shown in Table II.

TABLE II. Same as Table I, but for a Morse potential (13), whose characteristic radius r_0 is varied.

r_0	g_2	$E_3(g_2)$	g_3/g_2	$E_4(g_3)$	g_4/g_3	g_∞/g_2
0.	0.810	–0.0411	0.799	–0.0808	0.798	0
1.0	0.369	–0.0325	0.797	–0.0636	0.790	0
2.0	0.254	–0.0174	0.807	–0.0333	0.794	0
3.0	0.250	–0.0081	0.862	–0.0146	0.860	0.09
4.0	0.250	–0.0046	0.900	–0.0080	0.907	0.28

A warning is that the calculation becomes very difficult as r_0 becomes larger than about three. Our parametrization becomes inadequate. The vanishing of the wave function at small interparticle distance r_{ij} is obtained at the expense of huge cancellations in the expansion (3). This considerably reduces the accuracy. Specific methods can be developed for interactions with hard core, see, e.g., [22] and references therein. Our results, however, seem good enough to show unambiguously the trends of the R_N ratios as the size r_0 of the core increases.

The size of the attractive pocket is measured by the interval between r_1, where the potential vanishes, and r_0, where it reaches its minimum. Within our normalization, $\delta r=r_0-r_1=\ln 2$ is constant. As r_0 increases, $\delta r/r_0\to 0$, and the Morse potential becomes similar to the attractive delta shell with a hard core described in Sec. I in the limit $d/c\to 1$, and then a behavior $R\to 1$ is expected. This is clearly observed in Table II. The trend is, however, rather slow. For moderate values of r_0, our numerical results are well reproduced by a fit

$$R\simeq 1-c\frac{\delta r}{r_0}\simeq 1-\frac{0.43}{r_0}, \qquad (14)$$

with $c\simeq 0.62$. For larger r_0, some departure is observed, probably due to the difficulties in the variational calculation. We believe the behavior (14) is rather general.

D. Pöschl-Teller potential

The Pöschl-Teller potential reads

$$v(r)=\frac{\alpha(\alpha-1)}{\sinh^2(\mu r)}-\frac{\alpha(\alpha+1)}{\cosh^2(\mu r)}, \qquad (15)$$

with, again, $\mu=m=1$ for the range and the mass of each constituent. The strength factors of the repulsive and attractive terms are tuned to give a zero-energy two-body state, i.e., $g_2=1$ [21]. The potential is drawn in Fig. 3 for some values of α.

In the case $\alpha=1$, we have a simple monotonous potential, and, not surprisingly, a value $R\simeq 0.8$ is found, as seen in Table III.

TABLE III. Same as Table I, but for a Pöschl-Teller potential (15), for several values of its parameter α.

α	g_2	$E_3(g_2)$	g_3/g_2	$E_4(g_3)$	g_4/g_3	g_∞/g_2
1	1.	–0.135	0.797	–0.264	0.796	0
2	1.	–0.064	0.818	–0.131	0.777	0
3	1.	–0.046	0.836	–0.085	0.835	0
5	1.	–0.032	0.859	–0.060	0.856	0.12
9	1.	–0.018	0.885	–0.042	0.878	0.23

For $\alpha>1$, we can again define the size of the attractive well as $\delta r=r_0-r_1$, with $v(r_1)=0$ and $v'(r_0)=0$. The fit of R using the empirical formula (14) turns out to be quite good. This can be checked from the values displayed in Table III.

For both the Morse and Pöschl-Teller potentials, the approximate equality of g_4/g_3 and g_3/g_2 survives a strong repulsive core, unlike the case of an external barrier. There is, however, a slight difference in the patterns exhibited by these potentials. In the Morse case, the ratios g_4/g_3 and g_3/g_2 start departing from about 0.80 at the same value of the parameter r_0 for which g_∞/g_2 becomes positive, i.e., binding the infinite boson matter requires a minimal strength. In the Pöschl-Teller case, g_4/g_3 and g_3/g_2 immediately increase when the parameter α becomes larger than 1, though g_∞/g_2 still vanishes for a while.

E. More complicated potentials

In Ref. [14] the ratio R is studied for the potential

$$v(r)=\frac{r^2}{\alpha^2}\exp(-2\mu r)-\exp(-\mu r), \qquad (16)$$

which is shown in Fig. 4, for selected values of the parameters. We fix the scales such that $\mu=m=1$. For α very large, this potential is always attractive, and one thus obtains the usual $R\simeq 0.80$. On the other hand, for very small α, we have an almost pure oscillator $v(r)\simeq r^2-\alpha^2$ in the region of interest, and one gets $R\to 2/3$. For intermediate values of α, the potential exhibits both an internal pocket of attraction and an external attractive tail.

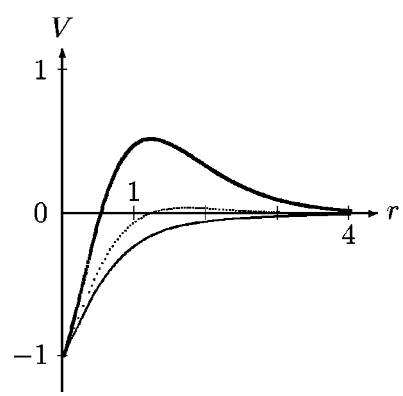

FIG. 4. Potential of Eq. (16), for $\alpha=0.4$ (thick line), $\alpha=1$ (thin line), and $\alpha=0.67$ (dotted line). The potential is always negative at large distance r.

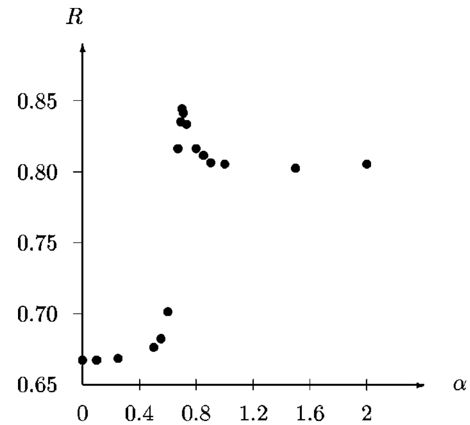

FIG. 5. Computed value of $R=g_3/g_2$ for the potential of Eq. (16), for various values of the parameter α.

The numerical results are shown in Fig. 5. The expected behavior $R=2/3$ for $\alpha\to 0$ and $R\simeq 0.80$ for $\alpha\to\infty$ are verified. Near $\alpha=0.70$, there is an interesting tunnelling between the internal and the external pockets of attraction. The barrier is seen as an internal core by the latter, and this pushes R toward 1, as for a Morse potential of large radius.

IV. LARGER SYSTEMS

The case of an infinite boson matter sheds some light on our discussion. For a purely attractive potential, a system containing many bosons is bound, however weak the strength g: we will thus set $g_\infty=0$. Now, if the potential contains a large repulsive part, it is conceivable that binding requires a minimal strength of the potential, say $g>g_\infty>0$ to pull the wave function in the attractive parts of the potentials. A result that looks *a posteriori* reasonable is that g_∞ is the value of the coupling for which the scattering length vanishes [8]. Indeed, the optimal state of the infinite boson matter is a compromise between the large-density limit, for which the kinetic energy is too large, and the extreme dilution. The latter case, dominated by two-body collisions at zero energy, should exhibit a tendency toward binding, i.e., a negative scattering length.

The scattering length can be calculated analytically or numerically for the potentials considered previously. Then it is rather straightforward to determine the value g_∞ of the strength that makes it vanish. Of course, for a potential whose integral is negative, the scattering length is already negative in the weak coupling limit, and remains negative until $g=g_2$. This corresponds to $g_\infty=0$.

In Tables I, II, and III, we display the value g_∞ for which the scattering length vanishes. This is simply $g_\infty=0$ for the monotonous potentials of Table I and the limiting cases $r_0=0$ of the Morse potential and $\alpha=1$ of Pöschl-Teller. As r_0 or α increases, one observes almost simultaneously g_∞ becoming finite and $R=g_3/g_2$ departing from about 0.80 and approaching $R=1$. This is the limit between, say, simple potentials that are purely attractive or contain a small repulsion, and nontrivial potentials with a strong core.

V. DISCUSSION AND OUTLOOK

In this paper, we have studied some aspects of the phenomenon of Borromean binding in three dimensions by comparing the critical couplings g_N required for binding $N=2$, 3, or more bosons interacting with various types of potentials.

All monotonous, short-range potentials give almost the same ratios $g_3/g_2 \simeq 0.80$ and $g_4/g_2 \simeq 0.64$.

We then considered potentials with a short-range attraction and an external repulsive barrier, which behave very much like an oscillator, and, not surprisingly, give ratios of critical couplings close to the lower bound $g_{N+1}/g_N = N/(N+1)$. These potentials with an external barrier are not very often encountered in physical systems. They are, however, interesting, since, according to Ref. [19], they are the only ones to give rise to Borromean binding in two dimensions.

We then studied the more physical case of potentials with a strong repulsive core at short distances. The window for Borromean binding turns out to be much narrower than for purely attractive potentials.

The present investigation could be extended to excited states. In particular, as long as $g_3 < g_2$, the Efimov effect should remain as g approaches g_2. It would be interesting to study how the onset and disappearance of Efimov states change when the strength of the core is varied.

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