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Bertlmann–Martin inequality for a weakly bound particle

M Lassaut, M Keriaki and R J Lombard

Division de Physique théorique†, Institut de Physique Nucléaire 91406 Orsay Cedex, France

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Abstract. The Bertlmann–Martin (BM) inequality for the rms radius is checked against the exact value in the case of a particle in a weak central potential having a single bound state. A number of usual potentials are considered in one and three dimensions. The BM inequality is poorly saturated but the correction factor φ needed to recover the exact rms radius is weakly depending on the shape of the potential, except for the Hulthén potential. For potentials having a hard-core component, we found that φ, which depends on the bound-state energy, tends to a universal curve as the hard core radius increases.

1. Introduction

More than two decades ago, Bertlmann and Martin (BM) derived a number of inequalities from the Thomas–Reiche–Kuhn dipole sum rule and similar expressions [1, 2]. One of them relates the rms radius of the ground-state wavefunction $\psi_0(r)$, defined as

$$\langle r^2\rangle_0 = \left(\int r^2|\psi_0(r)|^2\,\mathrm{d}^n r\right)\Big/\left(\int |\psi_0(r)|^2\,\mathrm{d}^n r\right)$$

to the lowest dipole energy difference

$$\langle r^2\rangle_0 \leqslant \frac{n\hbar^2}{2m(E_1 - E_0)} \tag{1}$$

where n is the dimension of the space, m is the mass of the particle, E_0 and E_1 are the ground state (1s) and lowest dipole state (1p) energies, respectively. This inequality is valid in the case of a particle moving in a central potential. It has been discussed in details for Λ-hypernuclei [3, 4], a rather unique case in the strong interaction sector. The BM inequality, which turns to an equality for the harmonic oscillator potential, is saturated within a few per cent for a large class of potentials, as long as the particle is well confined [3, 4].

For a loosely bound state the situation is different. A one-dimensional example, the modified Pöschl–Teller potential [3], has shown that (1) is far from being saturated in such a case. On the other hand, the wavefunction of a weakly bound particle is not very sensitive to the shape of the potential. Consequently it suggests the possibility of establishing a dimensional relationship:

$$\langle r^2\rangle_0 = \frac{n\hbar^2}{2m(E_1 - E_0)}\varphi. \tag{2}$$

The correction factor φ will vary with the energy difference; it is not expected, however, to be strongly dependent on the shape of the potential. If this dependence ranges over a few

† Unité de Recherche des Universités Paris 11 et Paris 6 Associée au CNRS.

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per cent only, equation (2) could yield an approximate value of the rms radius. Furthermore, if the variation of φ exhibits a monotonic hierarchy among the potentials, its lowest value will provide us with a lower limit.

The purpose of this work is to check the validity of these intuitive arguments on a couple of typical examples. We shall concentrate our study on potentials admitting a single (1s) bound state. Accordingly, the lowest energy difference has to be replaced by $-E_0$. Actually the appropriate variable is $\varepsilon = E_0/E_{0\max}$, where $E_{0\max}$ is the lowest possible eigenvalue such that the considered potential admits a single bound state. The aim is to investigate the variation of $\varphi(\varepsilon)$ in the dimensional relationship

$$\langle r^2\rangle_0 = \frac{n\hbar^2}{2m(-E_0)}\varphi(\varepsilon)$$

for the set of potentials currently used.

Part of our motivations is found in the existence of the so-called halo nuclei, in which the binding energy of the last neutron is much smaller than the average binding energy per particle. Because of this peculiar situation, a two-body approximation is justified [5], and (2) could serve as a determination of the rms radius of the halo wavefunction, at least to fix a lower and an upper bound. In this case, however, it is important to take into account the Pauli principle between the loosely bound neutron and the core particles. Within a two-body framework, this can be achieved approximately by adding a hard core component to the binding potential. As we shall see, the presence of a hard core has a strong influence on φ, and brings a kind of universal behaviour. As shown in the appendix, this is given by

$$\varphi \approx \tfrac{1}{6}(1 + 2\sqrt{\varepsilon} + 2\varepsilon).$$

This situation is of particular interest since hard-core potentials are often found between molecular states. Thus, the present finding could be applied to weakly bound molecules such as He_2. Note that for applications to two-body systems, the mass m has to be replaced by the reduced mass μ.

This paper is organized as follows. Section 2 is devoted to one-dimensional cases for which analytical solutions exist. More realistic three-dimensional cases are studied in section 3. Conclusions are drawn in 4.

2. The one-dimensional case

We commence this section by considering the modified Pöschl–Teller potential:

$$V(x) = -\frac{\hbar^2}{2m}\alpha^2\frac{\lambda(\lambda-1)}{\cosh^2\alpha x}. \tag{3}$$

Although this potential depends on two parameters, we shall see in the final results that (2) is not affected by α, which plays the role of a scaling factor. More generally, we remark that the BM inequality is invariant under the scaling transformation:

$$V(x) \to \gamma^2 V(\mu x).$$

The corresponding Schrödinger equation is given by

$$\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) + \left[-k^2 + \alpha^2\frac{\lambda(\lambda-1)}{\cosh^2\alpha x}\right]\psi(x) = 0. \tag{4}$$

Here, m denotes the mass of the particle and $k^2 = -2mE/\hbar^2$. The complete solution can be found in [6]. Let us simply recall the ground-state (lowest even) wavefunction:

$$\psi_0(x) = N_0[\cosh\alpha x]^{1-\lambda} \tag{5}$$

where N_0 is the normalization factor. In the one-dimensional case, the lowest 1p state is replaced by the lowest odd parity state. Since this is at zero energy for $\lambda = 2$, when λ ranges over the interval $[1, 2]$ the potential has a single bound state; its (ground-state) energy and rms radius are respectively given by

$$E_0 = -\frac{\hbar^2}{2m}\alpha^2(\lambda - 1)^2 \tag{6}$$

$$\langle x^2\rangle_0 = \frac{1}{\alpha^2}\left(\int_0^\infty \frac{u^2\,\mathrm{d}u}{[\cosh u]^{2\lambda-2}}\right)\bigg/\left(\int_0^\infty \frac{\mathrm{d}u}{[\cosh u]^{2\lambda-2}}\right). \tag{7}$$

The rms radius can be expressed by using the generalized zeta function [7]:

$$\langle x^2\rangle_0 = \frac{1}{2\alpha^2}\zeta(2, \lambda - 1). \tag{8}$$

Accordingly, the BM inequality reads

$$\frac{1}{2}\zeta(2, \lambda - 1) \leqslant \frac{1}{(\lambda - 1)^2}. \tag{9}$$

To turn it into an equality, the necessary correction factor φ is obviously

$$\varphi = \tfrac{1}{2}(\lambda - 1)^2\zeta(2, \lambda - 1). \tag{10}$$

In order to display the variation of φ with energy over the domain of interest, namely $\lambda \in [1, 2]$, it is convenient to introduce the relative variable

$$\varepsilon = E_0/E_{0\max} = (\lambda - 1)^2 \tag{11}$$

with $E_{0\max} = E_0(\lambda = 2)$. It gives immediately

$$\varphi(\varepsilon) = \frac{\varepsilon}{2}\zeta(2, \sqrt{\varepsilon}). \tag{12}$$

Recalling that

$$\zeta(2, z) = \sum_{n=0}^{\infty}\frac{1}{(n + z)^2} \tag{13}$$

it is easily checked that at zero energy, the limiting value is $\varphi(0) = \frac{1}{2}$.

The second example is the finite square-well potential:

$$\begin{aligned} V(x) &= -V_0 \qquad |x| \leqslant a \\ &= 0 \qquad |x| > a. \end{aligned} \tag{14}$$

The solution is found in any textbook, so we just write the final results. Introducing $u_0 = \sqrt{V_0}a$ and $u^2 = u_0^2 - \frac{2mE_0}{\hbar^2}$, the eigenvalues E_0 are solutions of $u\tan u = \sqrt{u_0^2 - u^2}$. Since we restrict the spectrum to a single bound state, the maximum of the potential strength is fixed by setting the lowest odd state solution to zero energy, as in the previous example. Here the maximum acceptable value of u_0 is $\pi/2$, and we have

$$\varepsilon = E_0/E_{0\max} = 0.627(u\tan u)^2. \tag{15}$$

The BM inequality reads

$$\frac{1}{6}\left[2(u\tan u + 1)^2 - 3\tan^2 u + \frac{1}{1 + u\tan u}\right] \leqslant 1. \tag{16}$$

Consequently the correction factor $\varphi(\varepsilon)$ is given by the left-hand side of this inequality. It is easy to verify that $\varphi(0) = \frac{1}{2}$ as before. In fact, as we shall see in the next section, the

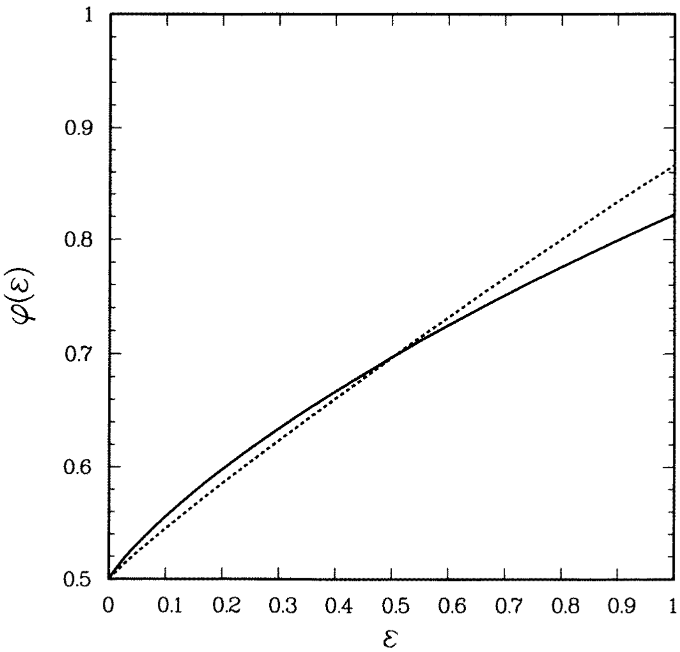

Figure 1. Separation energy dependence $\varepsilon = E_0/E_{0\max}$, equation (11), of the corrective factor φ to the one-dimensional BM inequality for: the Pöschl–Teller potential (——) and the square-well potential (- - - -).

value of $\varphi(0)$ is independent of the potential. It allows us to derive a lower bound to the rms radius.

In figure 1, we display the variation of φ with ε for the two studied potentials. The two curves have a rather similar shape, the largest deviation being found at $\varepsilon = 1$, at the threshold of the lowest odd state. It amounts to less than 8%, which is reasonably small in view of the sharp difference in the shape of the two potentials.

3. The three-dimensional case

Assuming spherical symmetry, the following set of potentials has been chosen.

(1) The shell-delta potential:

$$V(r) = -V_0 c\delta(r - c).$$

(2) The square-well potential:

$$V(r) = -V_0 \Theta(c - r).$$

(3) The Hulthén potential:

$$V(r) = -V_0 \frac{\mathrm{e}^{-r/a}}{1 - \mathrm{e}^{-r/a}}.$$

(4) The Wood–Saxon potential:

$$V(r) = -V_0 \frac{1}{1 + \mathrm{e}^{(r-c)/a}}.$$

Although not exhaustive, this choice allows us to study the behaviour of the correction factor φ over a large domain of potential shapes and curvatures. Note that the lengths are expressed in units which scale with $\hbar$, m and $-E_0$.

As in the one-dimensional case, the parameter space is restricted to the one allowing a single bound state ($\ell = 0$). The limits are obtained by setting the lowest $\ell = 1$ state at zero energy, which is achieved by a method developed in [8] for the Hulthén and Wood-Saxon potentials.

As the solutions of the corresponding Schrödinger equations are well known, we shall simply quote the final expressions for φ and $\varepsilon = E_0/E_{0\max}$, when analytical results exist. For the Wood–Saxon potential, the results are displayed on curves.

In the introduction it was remarked that it could be desirable in some cases to add a hard core component to the binding potential. It simulates the antisymmetrization between the loosely bound particle and the core particles generating the binding potential. Although not perfect, this method yields a hint towards the influence of the Pauli correlations.

In practice, we have considered the four cases defined above, introducing a hard-core component and shifting each potential by r_c. The presence of the hard core does not change the properties of the 1s state (translational invariance) but it has an influence on the energy of the 1p level. Except for the Hulthén potential, the results will be given as a function of $\chi = (c + r_c)/c$. The case $\chi = 1$ corresponds to r_c =0. They are given below.

The shell-delta potential:

$$\varphi(u) = \frac{1}{6}(1 + 2u^2\chi^2) + \frac{2}{9}\frac{u^3(3\chi - 1)}{e^{2u} - 1 - 2u} \tag{17}$$

$$\varepsilon = u^2/u_0^2 \tag{18}$$

with

$$u_0(1 + \coth u_0) = \frac{3\chi^2}{3\chi^2 - 3\chi + 1}.$$

The square-well potential:

$$\varphi = \frac{1}{18}\left[\frac{3}{2}((2\chi - 1)u\cot u - 1)^2 + \frac{1}{2}(1 - u\cot u)^2 - 3\cot^2 u - \frac{1}{u\cot u - 1}\right] \tag{19}$$

and

$$\varepsilon = \frac{u^2\cot^2 u}{u_0^2\cot^2 u_0} \tag{20}$$

with

$$u_0\cot u_0 = -\sqrt{y_0^2 - u_0^2}$$
$$\tan y_0 + y_0(\chi - 1) = 0 \qquad y_0, u_0 \in \left[\frac{\pi}{2}, \pi\right]. \tag{21}$$

The Hulthén potential (as a function of r_e):

$$\varphi = \frac{1}{6}\left[\frac{1 + 9u + 33u^2 + 48u^3 + 24u^4}{(u+1)^2(2u+1)^2} + \frac{(2ur_e)(1 + 6u + 6u^2)}{(u+1)(2u+1)} + 2r_e^2u^2\right] \tag{22}$$

where $u^2 = -2mE/\hbar^2$ and $x = u^2/u_0^2$.

Here u_0 has to be calculated numerically from the critical value of the V_0 bringing the 1p level to zero energy.

The Wood–Saxon potential requires numerical solutions. Note that because of scaling properties, ε is actually independent of the c or a parameter. We have chosen to fix c. On

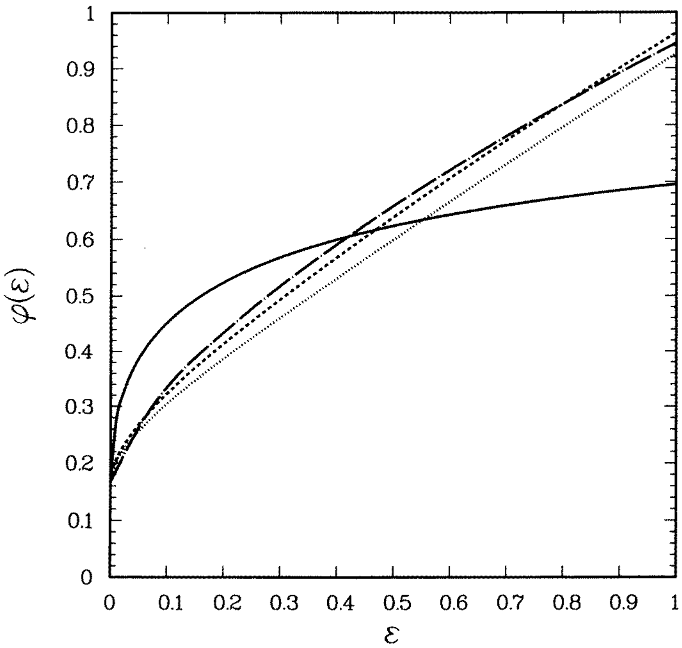

Figure 2. Separation energy dependence $\varepsilon = E_0/E_{0\max}$ of the corrective factor φ to the three-dimensional BM inequality for: the Hulthén potential (——), shell-delta potential (· · · · · ·), square-well potential (- - - -) and the Wood–Saxon potential, $c = 2.5$, $a = 0.5$, (— · —).

the other hand, by varying a between 0.4 and 0.8, the corresponding φ's describe practically indistinguishable curves. Consequently all the plotted results are taken from $a = 0.5$.

For ordinary potentials, with no hard-core component, the results are displayed in figure 2. Except for the Hulthén potential, the spreading of the correction factor φ is relatively small. Nevertheless, the Hulthén potential results clearly indicate that the assumption of a weak variation of φ against the shape of the potential can be wrong. Arguing for the lack of sensitivity of the weakly bound 1s wavefunction to details of the potetntial can be misleading.

It is particularly interesting to remark that the asymptotic value of φ, reached for $\varepsilon \to 0$ is the same for all potentials. It corresponds either to the 1s state energy approaching 0 or to cases pushing the lowest virtual 1p state at infinity. The limit is easily obtained from the asymptotic properties of the 1s wave function, and it yields an absolute lower bound

$$\langle r^2 \rangle_0 \geqslant \frac{\hbar^2}{4m} \frac{1}{(-E_0)} \tag{23}$$

where m is to be replaced by the reduced mass μ for applications to concrete examples. Indeed this lower bound corresponds to the asymptotic behaviour found for the 1s state by Fedorov *et al* [9].

Results obtained with a hard-core component are displayed in figures 3–6, for the shell-delta, square-well, Wood–Saxon and Hulthén potentials, respectively.

Generally speaking, the hard-core component reduces φ but keep unchanged the lowest limit, which can be understood simply by the translational invariance of the properties of the 1s wavefunction as its energy tends to zero. Except for the Hulthén potential, as r_c increases, φ undergoes a monotonic change up to a limit corresponding to a asymptotic

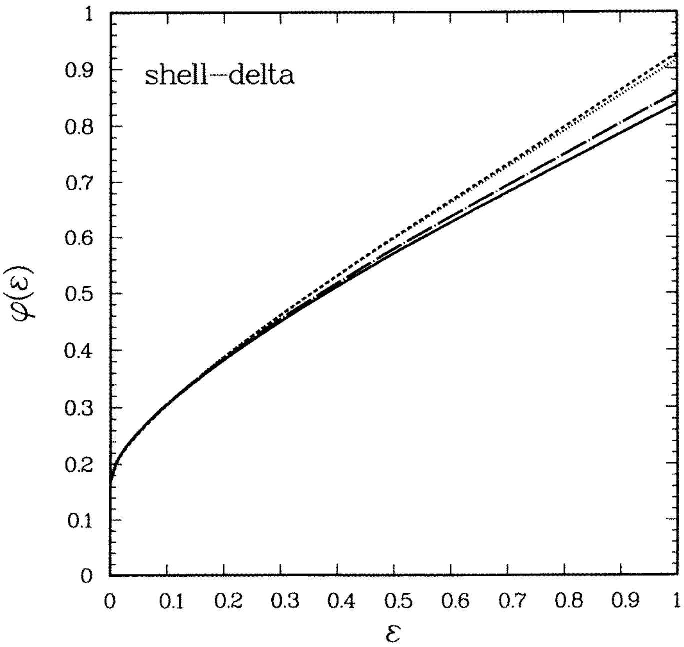

Figure 3. Hard-core dependence of the corrective factor φ as a function of ε for the shell-delta potential: $\chi = 1$ (- - - -), $\chi = 1.1$ $(\cdots\cdots)$, $\chi = 2$ (— · —) and $\chi = 5(+\infty)$ (——).

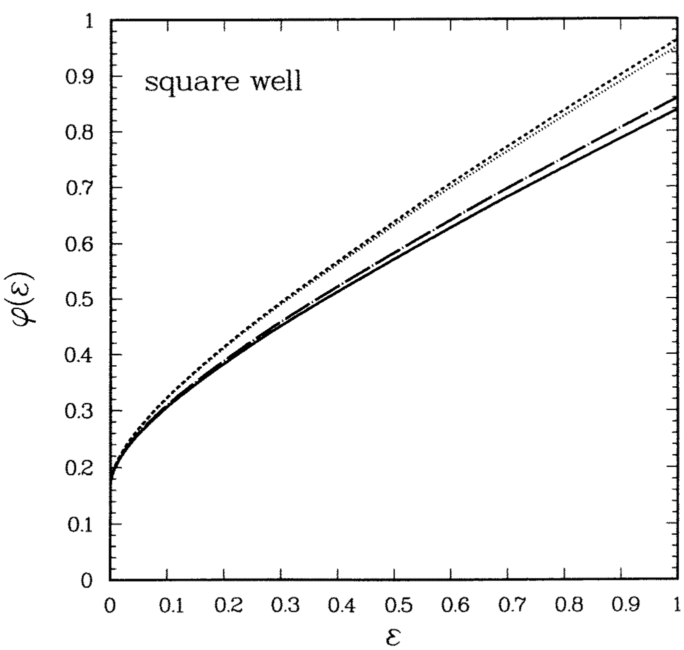

Figure 4. Same as in figure 3 but for the square-well potential: $\chi = 1$ (- - - -), $\chi = 1.1$ $(\cdots\cdots)$, $\chi = 2$ (— · —) and $\chi = 5(+\infty)$ (——).

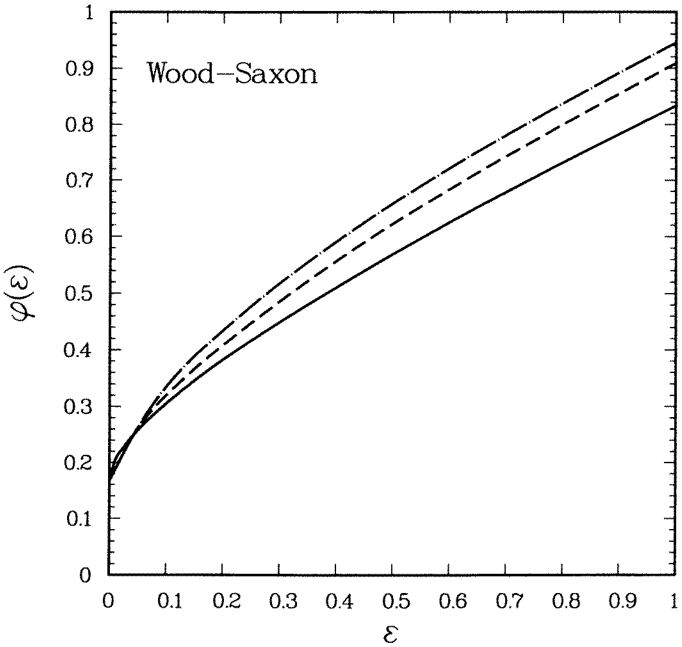

Figure 5. Same as in figure 3 but for the Wood–Saxon potential ($c = 2.5, a = 0.5$): $r_c = 0$ (— · —), $r_c = 1$ (- - - -) and r_c infinite (——).

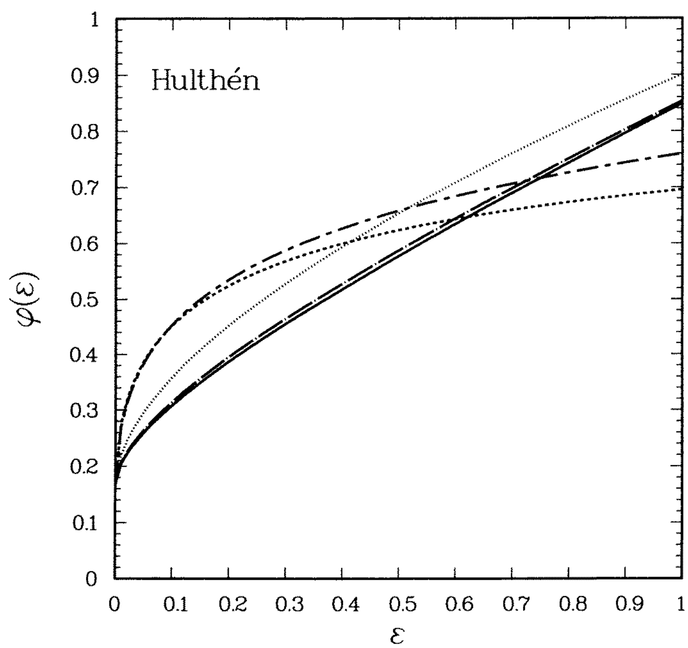

Figure 6. Same as in figure 3 but for the Hulthén potential: $r_c = 0$ (- - - -), $r_c = 0.01$ (— - —), $r_c = 1$ (· · · · · ·), $r_c = 5$ (— · —) and r_c infinite (——).

value of r_c. The case for Hulthén (figure 6) is peculiar in the sense of a non-monotonic behaviour with r_c, and a shape of φ which starts to resemble the other cases as r_c increases.

As expected, the shell-delta results are not so affected by the hard core, unless the energy of the 1p state becomes close to the threshold of the bound state. Even at $\varepsilon = 1$, the spreading is much less than in the case of the square well or the Wood–Saxon potentials. Finally, the striking observation concerns the variation with the hard-core radius. We find that as r_c is increasing, φ reaches rapidly an asymptotic curve independent of the potential. Thus, beyond $r_c = 2, \varphi$ approaches a universal behaviour. In the appendix we show that the limit is given by

$$\varphi \approx \tfrac{1}{6}(1 + 2\sqrt{\varepsilon} + 2\varepsilon). \qquad (24)$$

4. Conclusions

This paper is devoted to the BM inequality in the case of a weakly bound particle moving in a local potential. The inequality relates the rms radius of the ground-state orbital to the lowest dipole energy difference. If the potential admits a single (1s) bound state, we replace the lowest dipole energy difference by the ground-state eigenvalue $-E_0$.

From our investigation, based on few typical potentials in one and three dimensions, we found that the BM inequality is never saturated for a weakly bound particle. In other words it is never close to an equality, in contrast to the case of confining potentials [3, 4]. On the other hand, we have calculated the correction factor φ needed to transform the BM inequality into a dimensional relationship. This correction factor varies with $-E_0$ but it takes a universal value at zero energy. Since this asymptotic value is the lowest one, it is used to establish a lower bound to the rms radius, thus complementary to the BM inequality.

In the one dimension case, φ is found to depend only slightly on the potential. It is not the case in three dimensions, although the correction factors for the square-well and Wood–Saxon potentials are relatively similar. In this respect the Hulthén potential produces a very different shape of φ as function of the ground-state eigenvalue.

However, in the presence of a hard-core component, as the hard-core radius increases, the various φ tend to behave in a uniform way. We showed that indeed as $r_c \to \infty$ the resulting φ is independent of the attractive part of the potential. In practice this behaviour is manifest already at relatively moderate values of r_c.

Appendix

In this appendix, we show the existence of a limiting curve $\varphi(\varepsilon)$ for potentials having a hard-core component when the hard-core radius $r_c \to \infty$. These potentials are defined by

$$\begin{aligned} W(r) &= +\infty \qquad r \leqslant r_c \\ &= V(r - r_c) \qquad r > r_c. \end{aligned} \qquad (25)$$

$V(r)$ are restricted to finite range regular potentials, i.e. such that $\int_b^R |V(r)|\,\mathrm{d}r$, $\int_0^R r|V(r)|\,\mathrm{d}r$ exist for any positive value of b, R denoting the range of the potential.

Since ε, more correctly $E_{0\max}$, is related to the potential strength for which the 1p level is at zero energy, we first discuss the 'critical' strength λ_1 such that the potential $\lambda_1 W$ has a zero energy p-wave bound state. Because of the hard core, it is convenient to translate the radial coordinate by r_c. In this case, the critical λ_1 is found by solving

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}\psi_1(r_c, r) - \left(\frac{2m}{\hbar^2}\lambda_1 V(r) + \frac{2}{(r + r_c)^2}\right)\psi_1(r_c, r) = 0 \qquad (26)$$

imposing the solution to vanish at $r = 0$ and to behave like $(r + r_c)^{-1}$ at infinity.

As r_c becomes increasingly large, the centrifugal contribution vanishes. In this limit, λ_1 tends to λ_0, which corresponds to

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}\psi_0(r) - \frac{2m}{\hbar^2}\lambda_0 V(r)\psi_0(r) = 0 \tag{27}$$

having a zero-energy bound-state solution with the characteristics of an s-wave. The techniques required to establish the critical values λ_1 and λ_0 were reported in [8], and will not be repeated here.

By using translational invariance, $E_{0\max}$, the 1s eigenvalue of the original Schrödinger equation, is obtained from

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}\psi_s(r) - \frac{2m}{\hbar^2}\lambda_1 V(r)\psi_s(r) = -\frac{2m}{\hbar^2}E_{0\max}\psi_s(r) \tag{28}$$

with $\psi_s(0) = 0$ and $\psi_s(\infty) = \text{constant}$.

In [10], we have shown that, as $\lambda_1 \to \lambda_0$, $E_{0\max} \to 0$ according to

$$-E_{0\max} = \beta(\lambda_1 - \lambda_0)^2 \tag{29}$$

where

$$\beta = \frac{2m}{\hbar^2}\left(\frac{\int_0^R \psi_0^2(r)V(r)\,\mathrm{d}r}{\psi_0^2(R)}\right)^2. \tag{30}$$

To evaluate $\lambda_1 - \lambda_0$, we multiply (26) and (27) by ψ_0 and ψ_1, respectively, and take the difference. We get

$$\frac{2m}{\hbar^2}(\lambda_1 - \lambda_0)\int_0^R V(r)\psi_1(r_c, r)\psi_0(r)\,\mathrm{d}r = -2\int_0^\infty \frac{\psi_1(r_c, r)\psi_0(r)}{(r + r_c)^2}\,\mathrm{d}r. \tag{31}$$

The function $\psi_1 \to \psi_0$ uniformly on $[0, R]$ [11], whereas $\psi_0 \simeq \psi_0(R)$ and $\psi_1 \simeq \psi_0(R)(R + r_c)/(r + r_c)$ for $r \geqslant R$. Consequently we are left with

$$\frac{2m}{\hbar^2}(\lambda_1 - \lambda_0)\int_0^R V(r)\psi_0(r)^2\,\mathrm{d}r \simeq -2\int_0^R \frac{\psi_0(r)^2}{(r + r_c)^2}\,\mathrm{d}r + \frac{\psi_0(R)^2}{R + r_c}. \tag{32}$$

Taking into account that ψ_0 is bounded, the integral in the right hand side of equation (32), dominated by a constant times $(1/r_c - 1/(R + r_c))$ behaves like r_c^{-2} and we are left with

$$\frac{2m}{\hbar^2}(\lambda_1 - \lambda_0)\int_0^R V(r)\psi_0(r)^2\,\mathrm{d}r \simeq -\frac{\psi_0(R)^2}{R + r_c}. \tag{33}$$

By combining this result with (29) and (30), we obtain

$$-E_{0\max} \simeq \frac{\hbar^2}{2m}\frac{1}{(R + r_c)^2} \tag{34}$$

together with

$$k_{0\max} \simeq 1/r_c. \tag{35}$$

To calculate the limit of $\varphi(\varepsilon)$ for $\varepsilon = k^2/k_{0\max}^2$, we take $\psi_s(k, r)$ the bound-state wavefunction for the energy $E = -k^2\hbar^2/(2m)$. Since k is lower than $k_{0\max}$, $\psi_s(k, r)$ tends to $\psi_0(r)$ uniformly on $[0, R]$ [11]. For $r > R$, $\psi_s(k, r) = \psi_s(k, R)\exp(k(R - r)) \simeq \psi_0(R)\exp(k(R - r))$. The moments of this wavefunction are given by

$$\int_0^{+\infty} r^n \psi_s(k, r)^2\,\mathrm{d}r \simeq \int_0^R r^n \psi_0(r)^2\,\mathrm{d}r + \psi_0(R)^2\frac{n!}{(2k)^{n+1}}. \tag{36}$$

Therefore the moments are dominated by the contribution of the asymptotic part of the wavefunction. Recalling that

$$\varphi = \frac{1}{3}k^2 \frac{\int_0^{+\infty} \psi_s(k,r)^2 (r+r_c)^2 \, \mathrm{d}r}{\int_0^{+\infty} \psi_s(k,r)^2 \, \mathrm{d}r} \tag{37}$$

we obtain

$$\varphi \simeq \frac{2}{3}k^3(2(2k)^{-3} + 2r_c(2k)^{-2} + r_c^2(2k)^{-1}) = \frac{1}{6}(1 + 2\sqrt{\varepsilon}k_{0\max}r_c + 2\varepsilon k_{0\max}^2 r_c^2) \tag{38}$$

which upon using (35) yields

$$\varphi \simeq \tfrac{1}{6}(1 + 2\sqrt{\varepsilon} + 2\varepsilon). \tag{39}$$

It shows that the function $\varphi(\varepsilon)$ becomes universal as r_c gets large enough. This proof is basically derived for finite-range potentials but it is also valid for the Hulthén potential. For ε close to zero, $\varphi \simeq \frac{1}{6}$ independently of r_c.

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