Chapter 1

Limits on the number of bound states and conditions for their existence

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Abstract

Since the early fifties and the pioneer works of Jost and Pais in 1951 and Bargmann in 1952, the determination of upper and lower limits on the number of bound states of a given potential in the framework of non-relativistic quantum mechanics (Schrödinger equation) and first-quantized mechanics with relativistic kinematics (Klein-Gordon or spinless Salpeter equations), has never ceased to engage the attention of theoretical and mathematical physicists. We propose in this article to review some of the results obtained since these pioneer works and to present some very recent findings as well as some new results. In particular, we will show that very sharp upper and lower limits, where the leading term is the semiclassical estimate of the number of bound states, can be obtained for monotonically increasing central potential with vanishing angular momentum. We will also present some generalizations of these results applicable to non-monotonically increasing potential and non-vanishing angular momentum. These generalizations allow us to obtain upper and lower limits on the total number of bound states of central potentials. These results, initially obtained in three dimensions, are also modified to be applicable in spaces with one and two dimensions. While in one or two dimensions, arbitrary weak potentials always possess at least one bound state, in three dimensions a critical value of the coupling constant, which must be reached

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to allow existence of bound states, exist. Consequently, the potential must be attractive enough to possess bound states. We present necessary and sufficient condition for the existence of bound states for central potentials in three dimensions.

1.1 Introduction and historical survey

The determination in the framework of non-relativistic quantum mechanics of necessary and sufficient conditions for the existence of bound states in a given potential and, more generally, of upper and lower limits on the number of bound states yielded by such a potential, has engaged the attention of theoretical and mathematical physicists since the early fifties, and, notwithstanding the fact that, with modern computers, the numerical evaluation of the number of bound states for a given potential is an easy task, it continues to be actively pursued: see for instance [1-34] as well as the surveys of (some of) these results in [35-37]. In this article, we provide new or recent upper and lower limits on the number of bound states possessed by *central* potentials in one, two and three dimensions and we compare them, for some test potentials, with the exact results and with previously known upper and lower limits. These comparisons indicate that some of these new (or recently found) limits are generally more stringent than hitherto known results and indeed remarkably cogent, especially for potentials possessing many bound states. For discussion about non-central potentials we refer to the excellent review of Blanchard and Stubbe [37]. We also present necessary and sufficient condition for the existence of bound states for central potentials in three dimensions.

Let us now review most of the previous findings, focusing on (what we think to be) the most relevant. Hereafter, except in Sections 1.2.2 and 1.3.2, we use the standard non-relativistic quantum mechanical units such that $\hbar^2/(2m) = 1$, which entails that the potential $V(r)$ has the dimension of an inverse square length. We also assume throughout that the potential $V(r)$ is less singular than the inverse square radius at the origin and that it vanishes asymptotically faster than the inverse square radius, say (for some positive ϵ)

$$\lim_{r\to 0}\left[r^{2-\epsilon}\,V(r)\right] = 0, \tag{1.1a}$$

$$\lim_{r\to \infty}\left[r^{2+\epsilon}\,V(r)\right] = 0. \tag{1.1b}$$

Note that these assumptions entail that the square root of the (modulus of the) potential is integrable both at the origin and at infinity.

We begin this review with results applicable to central potentials in three dimensions (some results are however more general).

Bargmann in 1952 [2] and Schwinger in 1961 [4] have obtained the following upper limit on the number of ℓ-wave bound states possessed by a central potential

in three dimensions:

$$N_\ell < \frac{1}{2\ell+1}\,\mathcal{I}, \tag{1.2a}$$

where $\mathcal{I}$ is defined by

$$\mathcal{I} = \int_0^\infty dr\, r\, V^-(r). \tag{1.2b}$$

The quantity $V^-(r)$ is the absolute value of the negative part of the potential: $V^-(r) = -V(r)\theta[-V(r)]$, where $\theta(x)$ is the usual step function, $\theta(x) = 1$ if $x \geq 0$, $\theta(x) = 0$ if $x < 0$. This result is generally referred to as the Bargmann-Schwinger bound. The upper limit (1.2) was obtained after Jost and Pais in 1951 [1] had shown that the fact that the right-hand side of (1.2) exceed unity is a necessary condition for the existence of bound states (namely, the special case of the Bargmann-Schwinger limit with $N_\ell = 1$). This result (1.2) infer an upper limit on the maximal value, L, of the angular momentum ℓ for which bound states do exist, entailing that for $\ell = L + 1$ the potential does not support any bound states. This upper limit takes the form

$$L \leq L^+_{\rm BS} = \left\{\left\{\frac{1}{2}\,(\mathcal{I}-1)\right\}\right\}, \tag{1.3}$$

where double brace means integer part.

In general, when a bound on N_ℓ like (1.2) is known, it is always possible to infer a limit on L, like (1.3). From these two limits, it is then possible to derive a limit on the total number of bound states. Clearly if N_ℓ^- respectively N_ℓ^+ provide lower, respectively upper, limits on the number N_ℓ of ℓ-wave bound states, and likewise L^-, respectively L^+, provide lower, respectively upper, limits on L, it is plain that the quantities

$$N^\pm = N\left(L^\pm\right), \tag{1.4}$$

where

$$N\,(L) = \sum_{\ell=0}^{L} (2\ell+1)\; N_\ell^\pm, \tag{1.5}$$

provide lower respectively upper limits on the total number N of bound states possessed by the potential $V(r)$. The upper limits (1.2) and (1.3) lead then to the following upper limit on N:

$$N < \frac{1}{2}\,\mathcal{I}\,(\mathcal{I}+1). \tag{1.6}$$

An important property that must ideally satisfy a limit on the number of bound states is the property to be "best possible". This means that it is possible to find a potential that saturate the limit. The Bargmann-Schwinger upper limit is saturate by the potential

$$V(r) = -\sum_{n=1}^{N_\ell} \alpha_n\, \delta(r-\beta_n), \tag{1.7}$$

with an appropriate assignment of the $2N_\ell$ constants α_n and β_n. But while the fact that the formula providing a limit has the property to be best possible entails that there can be no hope to make it more stringent by just modifying some constant appearing in it, it does by no means imply that such a bound provides a stringent limitation for all potentials. Actually, the upper limits (1.2), (1.3) and (1.6) yield poor results for strong potential possessing many bound states. Indeed, an immediate hunch on the accuracy of these limits for strong potentials may be obtained via the introduction of a (dimensionless, positive) "coupling constant" g by setting

$$V(r) = g^2\, v(r), \tag{1.8}$$

where $v(r)$ is assumed to be independent of g, and by recalling that, at large g, N_ℓ grows proportionally to g [35],

$$N_\ell \sim g \quad \text{as} \quad g \to \infty, \tag{1.9}$$

indeed Chadan has shown in 1968 that [14]

$$N_\ell \approx \frac{1}{\pi} \int_0^\infty dr\, \left[V^-(r)\right]^{1/2} \quad \text{as} \quad g \to \infty. \tag{1.10}$$

Here, and always below, we denote with the symbols $\approx$ respectively $\sim$ asymptotic equality respectively proportionality. The analogous asymptotic behaviors of L and of N read

$$L \sim g, \quad \text{as} \quad g \to \infty, \tag{1.11}$$

indeed Simon in 1969 has obtained that [15]

$$L \approx \max_{0 \le r < \infty} \left\{ r \left[V^-(r)\right]^{1/2} \right\} \quad \text{as} \quad g \to \infty, \tag{1.12}$$

and

$$N \sim g^3 \quad \text{as} \quad g \to \infty, \tag{1.13}$$

indeed as shown by Martin in 1972 [17]

$$N \approx \frac{2}{3\pi} \int_0^\infty dr\, r^2\, \left[V^-(r)\right]^{3/2} \quad \text{as} \quad g \to \infty. \tag{1.14}$$

Actually, Martin has derived the exact asymptotic expression (as g diverges) of the total number of bound states in n dimensions

$$N \approx \frac{1}{2^n \pi^{n/2} \Gamma\left(\frac{n}{2}+1\right)} \int d^n x\, \left[V^-(x)\right]^{n/2} \quad \text{as} \quad g \to \infty. \tag{1.15}$$

The asymptotic behavior (1.9) infers that the Bargmann-Schwinger upper bound behaves like g^2 instead of g which entails that the upper limits on L and N have also the incorrect behavior as g goes to infinity.

In 1961, Schwinger has recovered the Bargmann result with the help of a powerful method: the so-called Birman-Schwinger method [4] (see Ref. [3] for the article of Birman). This method is very general and is used in this article to obtain results in non-relativistic as well as in semi-relativistic quantum mechanics. We give the main line of this method in the Appendice 1.3.2. In his article, Schwinger has also obtained with the help of this method an upper limit, different from the limit (1.6), on the total number of bound states of an arbitrary potential:

$$N < \frac{1}{(4\pi)^2} \int d\vec{r}_1 \, d\vec{r}_2 \frac{V^-(\vec{r}_1)\, V^-(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|^2}, \tag{1.16}$$

implying, for central potentials,

$$N < \frac{1}{2} \int_0^\infty dr_1 \, r_1 \, V^-(r_1) \int_0^\infty dr_2 \, r_2 \, V^-(r_2) \, \log \left| \frac{r_1 + r_2}{r_1 - r_2} \right|. \tag{1.17}$$

Here also the upper limit obtained by Schwinger does not possess the correct dependence on the coupling constant g.

The first upper and lower limits featuring the correct behavior as g goes to infinity was obtained by Calogero in 1965 [6]. The upper limit reads

$$N_0 < \frac{2}{\pi} \mathcal{S}, \tag{1.18a}$$

with

$$\mathcal{S} = \int_0^\infty dr \, [V^-(r)]^{1/2}, \tag{1.18b}$$

where N_0 is the number of S-wave ($\ell = 0$) bound states. This result is only valid provided the force associated with the potential $V(r)$ is nowhere repulsive, namely the potential $V(r)$ is a monotonically non-decreasing function of the radius r, $dV(r)/dr > 0$, entailing of course that the potential is everywhere negative. Hence for strongly attractive potentials featuring many bound states the limit (1.18) tends to overestimate N_0 by a factor 2, see (1.10). The main merit of the limits found very recently and reported in the Section 1.2.1 is to remedy this defect (see formulas (1.50) and (1.52) below). The limit (1.18) is nevertheless best possible and saturated by a square-well potential. Some modifications of the inequality (1.18) and of the condition $dV(r)/dr > 0$ on the shape of the potential have been introduced by Chadan *et al.* in 1996 [27]. These modifications lead to less restrictive inequalities but more flexible conditions on the shape of the potential, allowing for some oscillations. The upper limit (1.18) was also uncovered the same year (1965) by Cohn [7]. This upper limit is now called the Calogero-Cohn bound.

The lower limit found by Calogero in 1965 [6] featuring the correct behavior as g diverges, see (1.9), has the following expression

$$N_\ell > \frac{1}{\pi} \max_{0 \le a < \infty} \left\{ \int_0^\infty dr \, \min \left[a^{-1} \left(\frac{r}{a} \right)^{2\ell}, -a \, V(r) \left(\frac{r}{a} \right)^{-2\ell} \right] \right\} - \frac{1}{2}, \tag{1.19}$$

the notation $\min[x, y]$ signifies x if $x \leq y$, y if $y \leq x$. Let us now assume that the equation

$$a^{-1}\left(\frac{r}{a}\right)^{2\ell} = -a\,V(r)\left(\frac{r}{a}\right)^{-2\ell} \tag{1.20}$$

admits one and only one solution, say $r = R(a)$ (as for monotonic potentials), so that the lower limit (1.19) can be rewritten as follows:

$$N_\ell > \frac{1}{\pi}\max_{0\leq a<\infty}\left\{\int_0^{R(a)} dr\, a^{-1}\left(\frac{r}{a}\right)^{2\ell} - \int_{R(a)}^{\infty} dr\, a\,V(r)\left(\frac{r}{a}\right)^{-2\ell}\right\} - \frac{1}{2}, \tag{1.21}$$

where of course $r = R(a)$ is the solution of (1.20). It is then easy, using (1.20), to calculate the maximum in the right-hand side of this inequality and to obtain thereby the following lower limit:

$$N_\ell > \frac{2}{\pi}\frac{\rho\,|V(\rho)|^{1/2}}{2\ell+1} - \frac{1}{2}, \tag{1.22a}$$

with the radius ρ defined to be the solution of the following equation:

$$\rho\,V(\rho) = (2\ell+1)\int_\rho^\infty dr\,\left(\frac{\rho}{r}\right)^{2\ell} V(r). \tag{1.22b}$$

This lower limit presents the correct dependence on g since clearly ρ does not depend on g. It is best possible and the potential that saturates it can be found in the Refs. [6, 35]. Note that this lower limit has been improved in Ref. [31], but we do not report this improvement here.

Calogero also found in 1965 two sufficient conditions for the existence of at least one bound state with angular momentum ℓ (and therefore also at least one bound state for every value of the angular momentum less than ℓ) [8, 9]

$$\int_0^a dr\, r\,|V(r)|\,(r/a)^{2\ell+1} + \int_a^\infty dr\, r\,|V(r)|\,(r/a)^{-(2\ell+1)} > 2\ell+1, \tag{1.23}$$

and

$$a\int_0^\infty dr\,|V(r)|\left[(r/a)^{2\ell} + (r/a)^{-2\ell}\,a^2|V(r)|\right]^{-1} > 1. \tag{1.24}$$

Both these conditions apply provided the potential is nowhere positive; in both of them a is an arbitrary positive constant, and of course the most stringent conditions obtain by minimizing the left-hand sides of (1.23) and (1.24) over all positive values of a. These conditions are also best possible and the potentials that saturates them can be found in the original publications.

It is interesting to note that the result (1.23) is actually a byproduct of a more general sufficient condition for the existence of ℓ-wave bound state also found by Calogero in 1965 [8] and which reads

$$\int_0^\infty dr\,|V(r)|\,r^{-2\ell}\,g_\ell^2(r) > g_\ell(\infty)(2\ell+1), \tag{1.25}$$

with $g_\ell(r)$ restricted by the conditions

$$0 \leq g_\ell(r) \leq r^{2\ell+1}, \tag{1.26a}$$

$$\lim_{r\to 0}\left[r^{2\ell+3+\eta}/g_\ell(r)\right] = 0, \tag{1.26b}$$

$$\frac{dg_\ell(r)}{dr} \geq 0, \tag{1.26c}$$

where η is defined by the behavior of the potential at the origin through

$$V(r) \underset{r\to 0}{\to} \text{const} \times r^\eta, \quad \eta > -2. \tag{1.27}$$

Indeed, the sufficient condition (1.23) is obtained from the general relation (1.25) by choosing

$$\begin{aligned} g_\ell(r) &= r^{2\ell+1} \quad \text{for} \quad r < a \\ &= a^{2\ell+1} \quad \text{for} \quad r \geq a. \end{aligned} \tag{1.28}$$

The next interesting result is due to Glaser *et al.* in 1976 [19] and reads

$$N_\ell < (2\ell+1)^{1-2p} C_p \int_0^\infty \frac{dr}{r} \left[r^2 V^-(r)\right]^p \tag{1.29a}$$

with

$$C_p = \frac{(p-1)^{p-1}\,\Gamma(2p)}{p^p\,\Gamma^2(p)}, \tag{1.29b}$$

and the restriction $p \geq 1$. This upper limit is always characterized by an unsatisfactory dependence on g as g diverges: the right-hand side of (1.29a) is proportional to g^{2p} with $p \geq 1$ rather than to g, hence it always yields a result far from the exact value for strong potentials possessing many bound states. Nevertheless this inequality provides a very accurate necessary condition for the existence of bound by setting $N_\ell = 1$ in (1.29a). Indeed, as we show in the Section 1.3.1, the upper limit (1.29) with $N_\ell = 1$ yields a precise lower bound on the critical value of the coupling constant for which a first bound state appears.

In 1976, Lieb has obtained an upper limit on the total number of bound states applicable to arbitrary potential in three dimensions [18]:

$$N < 0.116 \int d\vec{r}\,[V^-(\vec{r})]^{3/2}, \tag{1.30}$$

(for the origin of the numerical coefficient on the right-hand side of this formula, we refer to the original paper [18]). For central potentials it reads as follows:

$$N < 1.458 \int_0^\infty dr\, r^2\,[V^-(r)]^{3/2}. \tag{1.31}$$

This upper limit on N has the advantage of simplicity but the numerical prefactor is too large (almost 7 times larger than the semi-classical prefactor (1.14)) and better results for central potentials can be obtained with other approaches (see tests in Section 1.2.1). Similar results, but with larger values of the prefactor, has been also obtained by Rozenblum in 1972 [16] and Cwickel in 1977 [21].

In 1977, Martin has found an upper limit on the number of S-wave bound states which features the correct power behavior as g diverges

$$N_0 < \left[\int_0^\infty dr\, r^2\, V^-(r) \int_0^\infty dr\, V^-(r)\right]^{1/4}. \tag{1.32}$$

This limit is applicable to arbitrary potential for which the integrals converge. This limit can thus be viewed as an upper limit on the number of ℓ-wave bound states provided the potential used is the negative part of the effective potential, $V(r) + \ell(\ell+1)/r^2$.

The Calogero-Cohn upper limit (1.18) is obviously also true for $\ell > 0$ but not very stringent. In 1995, Chadan *et al.* has obtained a generalization of this upper limit with an explicit dependence on the angular momentum [25]

$$N_\ell < 1 + \frac{2}{\pi}\mathcal{S} - \left[1 + \frac{4}{\pi^2}\ell(\ell+1)\right]^{1/2}, \tag{1.33}$$

where $\mathcal{S}$ is defined by (1.18b). A less restrictive but neater version of this inequality reads

$$N_\ell < 1 + \frac{2}{\pi}\mathcal{S} - \frac{1}{\pi}(2\ell+1). \tag{1.34}$$

¿From this last relation (1.34) an upper limit on the maximal value, L, of the angular momentum ℓ for which bound states do exist can be obtained

$$L \leq L^+_{\text{CMS}} = \left\{\left\{\mathcal{S} - \frac{1}{2}\right\}\right\}. \tag{1.35}$$

As state above, see (1.5), we can then obtain an upper limit on the total number of bound states with the relations (1.34) and (1.35):

$$N < \frac{2}{3\pi}\left[\mathcal{S}^3 + \frac{3\pi}{2}\mathcal{S}^2 + \left(\frac{3\pi}{2} - \frac{1}{4}\right)\mathcal{S} + \frac{3\pi}{8}\right] < \frac{2}{3\pi}\left(\mathcal{S} + \frac{\pi}{2}\right)^3. \tag{1.36}$$

In 1995, Chadan *et al.*, have (almost) "filled the gap" between the Calogero-Cohn and the Bargmann-Schwinger upper limits with the following upper bound [26]

$$N_\ell < (2\ell+1)^{1-2p}\,\tilde{C}_p \int_0^\infty \frac{dr}{r}|r^2 V(r)|^p, \tag{1.37a}$$

with

$$\tilde{C}_p = p(1-p)^{p-1}, \tag{1.37b}$$

with the restriction $1/2 \leq p < 1$, and it is valid provided the potential is nowhere positive and moreover satisfies for all values of r, $0 \leq r < \infty$, the relation

$$\frac{d}{dr}\left[r^{1-2p}\,|V(r)|^{1-p}\right] \leq 0. \tag{1.38}$$

For $p = 1/2$, the limit (1.37) is equivalent to the Calogero-Cohn upper limit but with a larger prefactor while for $p \uparrow 1$ we recover the Bargmann-Schwinger upper limit.

Contrary to results obtained for spaces with three dimensions and just reviewed above, results in one and two dimensions are scarcer, nevertheless some nice findings exist. One of the first limit of this kind have been obtained by Newton in 1962 [5] (see also Ref. [38]). This is an upper limit applicable to central potentials in two dimensions with $m = 0$ (m is the angular momentum in two dimensions) and reads

$$N_{m=0} < 1 + \frac{1}{\mathcal{I}}\int_0^\infty dr \int_0^r dr'\, rr'\, V^-(r)V^-(r')\,\ln(r/r'), \tag{1.39}$$

where $\mathcal{I}$ is defined by (1.2b). This upper limit does not feature the correct asymptotic behavior as g diverges since it behaves like g^2 instead of g.

In 1977, Klauss [20] and later, in 1983, Newton [24] have found the following upper limit on the number of bound states in one dimension

$$N < 1 + \left[\int_{-\infty}^\infty dx \int_{-\infty}^\infty dy\, xy\, V^-(x)V^-(y)\,|x-y|\right]\left\{\int_{-\infty}^\infty dz\, V^-(z)\right\}^{-1}. \tag{1.40}$$

This upper limit, as the previous one, will not be very stringent for strong potentials due to its bad asymptotic behavior.

In 1978, Glaser *et al.* have obtained a *lower* bound on the total number of bound states applicable to central potential in two dimensions:

$$N > -\frac{1}{4}\int_0^\infty dr\, rV(r). \tag{1.41}$$

Note that this is *not* the negative part of the potential that appears in this inequality but the potential itself.

The problem of finding limits on the number of bound states in space with one and two dimensions has recently be revisited by Chadan *et al.* [29]. The authors have obtained interesting new results. For one spatial dimension the limits read

$$N < 1 + \int_{-\infty}^{+\infty} dx\,|x|\,V^-(x), \tag{1.42}$$

$$N < 1 + \sqrt{2}\left[\int_{-\infty}^{+\infty} dx\, x^2\, V^-(x)\int_{-\infty}^{+\infty} dx\, V^-(x)\right]^{1/4}. \tag{1.43}$$

For two spatial dimensions with central potentials the limits are

$$N_{m=0} < 1 + \int_0^\infty dr\, r\ |\ln(r/R)|\, V^-(r), \tag{1.44}$$

$$N_{m=0} < 1 + \sqrt{2}\left[\int_0^\infty dr\, r\, [\ln(r/R)]^2\ V^-(r) \int_0^\infty dr\, r\, V^-(r)\right]^{1/4}, \tag{1.45}$$

where R is arbitrary and chosen to minimize the result. The limits (1.43) and (1.45) present the correct power behavior as g diverges.

The limits for the one-dimensional case (1.42) and (1.43) are simply obtained from previous limits derived in three dimensions with $\ell = 0$ (see (1.2) and (1.32)). This correspondence is simple to obtain. The one-dimensional zero-energy Schrödinger equation reads

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\psi(x) = 0, \quad x \in (-\infty, \infty), \tag{1.46}$$

with $\psi(-\infty) = 0$. The nodal theorem allows to write that if $V(x)$ has N bound states, then the wave function $\psi(x)$ has N nodes $x_p > -\infty$, $p = 1, \ldots, N$. Let k such that $x_k < 0 < x_{k+1}$. Then the three-dimensional potential, $V_1(r) = V(x)$ with $r = x - x_{k+1}$, has $N - k - 1$ S-wave bound states. Similarly, $V_2(r) = V(x)$ with $r = -(x - x_{k+1})$, has k S-wave bound states. Hence any three-dimensional limit gives a one-dimensional limit. We apply below this method to derived stringent upper and lower limit on the number of bound states in one dimension.

The limits for the two-dimensional case (1.44) and (1.45) are obtained with the help of the following change of variables used in any one-dimensional result:

$$\begin{aligned} x &= \ln(r/R), \quad 0 \le r < \infty \\ V(x) &= r^2\, W(r), \\ \psi(x) &= \phi(r). \end{aligned} \tag{1.47}$$

Indeed, with this change of variable, the one-dimensional zero-energy Schrödinger equation (1.5) becomes

$$\left(-\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + W(r)\right)\phi(r) = 0, \tag{1.48}$$

which is the radial Schrödinger equation in two dimensions with a vanishing angular momentum $m = 0$. The change of variables (1.47) apply to the limits (1.42) and (1.43) leads to the limits (1.44) and (1.45).

Chadan *et al.* also succeed to find an upper limit on the *total* number of bound states applicable to central potential in two dimensions [29]:

$$N < 1 + \int_0^\infty dr\, r\ |\ln(r/R)|\, V^-(r) + \frac{2}{\sqrt{3}}\int_0^\infty dr\, r\, V^-(r). \tag{1.49}$$

1.2 Limits on the number of bound states

In this Section, we give new or recently obtained lower and upper limits on the number of bound states in a central potential. These limits are applicable for one, two and three spatial dimensions. The new limits in one and two dimensions are derived from the results obtained in three dimensions using the method proposed by Chadan *et al.* [29] and explained in Section 1.1. Non-relativistic limits are given in the first part of this Section while limits applicable to semi-relativistic equation (spinless Salpeter and Klein-Gordon equations) are reported in the second part.

1.2.1 Non-relativistic quantum mechanics

Three dimensions

Recently, upper and lower limits on the number of S-wave bound states featuring the correct asymptotic dependence (see (1.10)) were obtained for monotonically increasing potentials [30] ($V^-(r) = -V(r)$). They read

$$N_0 < \frac{\mathcal{S}}{\pi} + \frac{1}{4\pi} \ln\left[\frac{V(p)}{V(q)}\right] + \frac{1}{2}, \tag{1.50a}$$

$$N_0 > \frac{\mathcal{S}}{\pi} - \frac{1}{4\pi} \ln\left[\frac{V(p)}{V(q)}\right] - \frac{3}{2}, \tag{1.50b}$$

where $\mathcal{S}$ is defined by (1.18b) and with the two radii p and q defined as the solutions of the following equations:

$$\int_0^p dr\ [-V(r)]^{1/2} = \frac{\pi}{2} \quad \text{and} \quad \int_q^\infty dr\ [-V(r)]^{1/2} = \frac{\pi}{2}. \tag{1.50c}$$

For regular potentials $p = 0$ can be chosen since $|V(p)| \leq |V(0)|$. In this case, one can show that the constant term in the lower limit (1.50b) can be improved and is equal to -1.

An important difficulty for obtaining analytical formula from (1.50) is the calculation of p and q since primitive of the square root of the potential is needed. A first possibility is simply to use in (1.50c) a potential $\tilde{V}(r)$ such as $|\tilde{V}(r)| \geq |V(r)|$ for all value of r and for which the integrals in (1.50c) have analytical expression. In this way one get $\tilde{p} \leq p$ and $q \leq \tilde{q}$ which can be used in the expression of the limits (1.50a) and (1.50b). This method is illustrated below with the Morse potential (see Section 1.2.1).

Another possibility, useful only for regular potential for which $V(0)$ can be used instead of $V(p)$, is to take advantage of the following lower bound on $|V(q)|$:

$$|V(q)| \geq \left[\frac{\pi}{2W(\alpha)}\right]^{\frac{\alpha}{\alpha-1}}, \tag{1.51a}$$

with

$$W(\alpha) = \left[\int_0^\infty dr \, \frac{|V(r)|^{\alpha/2}}{[V'(r)]^{\alpha-1}} \right]^{\frac{1}{\alpha}}. \tag{1.51b}$$

The interest of the expression (1.51) is that only integration of power of the potential between zero and infinity are involved. The quantity $W(\alpha)$ need of course be finite. If the potential behaves for large r as an exponential, we have the restriction $1 < \alpha < 2$. If the potential behaves for large r as $r^{-\delta}$ ($\delta > 2$), we have the restriction $1 < \alpha < 2\delta/(2+\delta)$. The proof of the lower limit (1.51) is given in Appendice 1.3.2.

The limits (1.50) have been generalized to be applicable to non-monotically increasing potentials [31]. In the original article, they were given for potentials possessing only one minimum (for example, Lennard-Jones or Morse potentials). They read

$$N_0 < \frac{\mathcal{S}}{\pi} + \frac{1}{2\pi} \ln \left[\frac{V^-(r_{\min})}{M} \right] + 1, \tag{1.52a}$$

$$N_0 > \frac{\mathcal{S}}{\pi} - \frac{1}{2\pi} \ln \left[\frac{V^-(r_{\min})}{M} \right] - \frac{3}{2}, \tag{1.52b}$$

where

$$M = \min \left[V^-(p), V^-(q) \right] \tag{1.52c}$$

with the two radii p and q defined as the solutions of the following equations:

$$\int_0^p dr \, \left[V^-(r) \right]^{1/2} = \frac{\pi}{2} \quad \text{and} \quad \int_q^\infty dr \, \left[V^-(r) \right]^{1/2} = \frac{\pi}{2}, \tag{1.52d}$$

and with the additional condition (which might rule out the applicability of these limits to potentials possessing very few bound states, but which is certainly satisfied by potentials that are sufficiently strong to possess several bound states)

$$p \leq r_{\min} \leq q. \tag{1.52e}$$

The radius $r_{\min}$ is the position of the minimal value of the potential. For a regular monotonic potential we have $r_{\min} = 0$, while $r_{\min}$ should be taken to be equal to p for a singular monotonic potential and we recover the limits (1.50) (except for the constant in (1.50a)). For a non-monotonic potential, $r_{\min}$ is, of course, the position where the derivative of potential vanishes.

Let us recall that a simple upper limit L^+ on the largest value L of ℓ for which the potential $V(r)$ possesses bound states (entailing of course that for $\ell > L^+$ the potential $V(r)$ certainly does not possess any ℓ-wave bound state) reads

$$L \leq L^+ = \left\{ \left\{ \sigma - \frac{1}{2} \right\} \right\}, \tag{1.53a}$$

with

$$\sigma = \max[r\sqrt{V^-(r)}], \tag{1.53b}$$

and where the double brace means integer part. [Indeed, it is an immediate consequence – via a standard comparison argument – of the well-known fact that the solution $u(r)$ characterized by the boundary condition $u(0) = 0$ of the ODE $r^2\,u''(r) + c\,u(r) = 0$ features a zero in $0 < r < \infty$ only if the real constant c exceeds $\frac{1}{4}$, $c > \frac{1}{4}$].

It appears that the upper limit L^+ (1.53) is very efficient (see for example tests performed in Ref. [31]). This quantity can thus be used in the formula (1.5) to obtain upper limit an the total number of bound states. In particular we can used L^+ with the upper bound on N_0 (1.52) to obtain:

$$N < \frac{1}{4\pi}(2\sigma+1)^2 \left\{ \mathcal{S} + \frac{1}{2}\log\left[\frac{V^-(r_{\min})}{M}\right] + \pi \right\}, \tag{1.54}$$

with M defined by (1.52c), σ defined by (1.53b), $\mathcal{S}$ defined by (1.18b) and $V^-(r_{\min})$ the minimal value of (the negative part of) the potential. For a monotonic potential this upper limit takes the simpler form

$$N < \frac{1}{4\pi}(2\sigma+1)^2 \left\{ \mathcal{S} + \frac{1}{4}\log\left[\frac{V(p)}{V(q)}\right] + \frac{\pi}{2} \right\}, \tag{1.55}$$

where p and q are defined by (1.50c). It is remarkable that, in spite of the drastic approximation $N_\ell \leq N_0$ used to get these two limits, they turn out, in all the tests performed in Ref. [31] and below, to be more stringent than all previously known results.

The quantity L^+ can also be used with other upper bounds on N_ℓ to improve the upper limit on the total number of bound states. We discuss this possibility below during the tests performed with an exponential potential.

The limits (1.50) and (1.52) are close to semi-classical expressions except for the logarithmic term. Actually, if the potential is everywhere negative and satisfies a given condition, the limits (1.50) and (1.52) can be written under semi-classical expressions. Indeed, let $H(r)$ be defined by the relation

$$H(r) = \frac{5}{4}\left(\frac{V'(r)}{V(r)}\right)^2 - \frac{V''(r)}{V(r)}, \tag{1.56}$$

where appended primes signify of course differentiation with respect to the radius r. The limits (1.50) and (1.52) can then be written in the following form provided $H(r)$ has a given sign:

$$N_0 > \frac{\mathcal{S}}{\pi} - 1 \quad \text{if} \quad H(r) \geq 0 \quad \text{for} \quad 0 \leq r < \infty, \tag{1.57a}$$

$$N_0 < \frac{\mathcal{S}}{\pi} \quad \text{if} \quad H(r) \leq 0 \quad \text{for} \quad 0 \leq r < \infty. \tag{1.57b}$$

This obviously means that, for a given potential, the simplification (1.57) of the limits (1.50) and (1.52) eventually applies either for the lower bound either for the upper bound (but not for both limits).

Several other new limits have been obtained in the Ref. [31], we just report the following lower limit

$$N_\ell > \nu - \frac{\ell}{\pi}\ln\left(\frac{q}{p}\right), \tag{1.58a}$$

where

$$\nu = \mathcal{S} - \frac{1}{4\pi}\ln\left\{\frac{\left[V^-(r_{\min})\right]^2}{V^-(p)V^-(q)}\right\} - \frac{3}{2}. \tag{1.58b}$$

This formula is written for a non-monotonically increasing potential with only one minimum. This lower limit on N_ℓ provides a lower limit, L^-, on L, the maximal value of the angular momentum for which a bound states do exist:

$$L \geq L^- = \left\{\left\{\frac{\nu}{\lambda}\right\}\right\} \tag{1.59a}$$

with

$$\lambda = \frac{1}{\pi}\ln\left(\frac{q}{p}\right) \tag{1.59b}$$

¿From this lower limit on the number of ℓ-wave bound states and the lower limit on L, we can obtain a *lower* limit on the total number of bound states (see (1.5))

$$N > \frac{\nu}{6\lambda^2}(2\nu+\lambda)(\nu+\lambda). \tag{1.60}$$

Up to our knowledge, it was the first time that a lower limit on the total number of bound state in three dimensions was obtained.

To prove the accuracy of the limits reported in this Section, we test them with two typical potentials: the exponential potential (hereafter referred to as E)

$$V(r) = -g^2\,R^{-2}\,\exp\left(-\frac{r}{R}\right), \tag{1.61}$$

and the Morse potential [39] (hereafter referred to as M)

$$V(r) = -g^2\,R^{-2}\,\left\{2\exp\left[-\left(\frac{r}{R}-\alpha\right)\right] - \exp\left[-2\left(\frac{r}{R}-\alpha\right)\right]\right\}. \tag{1.62}$$

The first test is performed with the E potential (1.61). In this case the exact number of bound states for $\ell = 0$ coincides with the number of zeros of the zeroth-order Bessel function $J_0(x)$ in the interval $0 < x \leq 2g$ (see, for example, Ref. [40], p. 196). The exact number $N_{\ell>0}$ of bound states for this potential is computed numerically.

For $\ell = 0$, the upper limit (1.50a) reads

$$N_0 < \frac{2}{\pi}g + \frac{1}{2\pi}\ln\left(\frac{4}{\pi}g\right) + \frac{1}{2}. \tag{1.63}$$

For this potential, the lower limit (1.50b) can be improved since the function $H(r)$ defined by (1.56) is always positive. Thus we have

$$N_0 > \frac{2}{\pi} g - 1. \tag{1.64}$$

To obtain information for $\ell > 0$ we consider the limits (1.52) with the effective potential $V_{\ell,\mathrm{eff}} = V(r) + \ell(\ell+1)/r^2$, they read:

$$N_\ell < \frac{1}{\pi} F(g,\ell;x_-,x_+) + \frac{1}{2\pi} \log \left| \frac{V_{\ell,\mathrm{eff}}^{\min}}{M} \right| + 1, \tag{1.65a}$$

$$N_\ell > \frac{1}{\pi} F(g,\ell;x_-,x_+) - \frac{1}{2\pi} \log \left| \frac{V_{\ell,\mathrm{eff}}^{\min}}{M} \right| - \frac{3}{2}, \tag{1.65b}$$

where

$$F(g,\ell;a,b) = \int_a^b \frac{dx}{x} \sqrt{g^2 x^2 \exp(-x) - \ell(\ell+1)}, \tag{1.65c}$$

and

$$M = \min\left[|V_{\ell,\mathrm{eff}}(p)|, |V_{\ell,\mathrm{eff}}(q)| \right] \tag{1.65d}$$

where p and q are solutions of

$$F(g,\ell;x_-,p/R) = \frac{\pi}{2}, \quad F(g,\ell;q/R,x_+) = \frac{\pi}{2}, \tag{1.65e}$$

where $x_\pm$ are the two solutions of

$$\ell(\ell+1) = g^2\, x_\pm^2\, \exp(-x_\pm), \tag{1.65f}$$

and where $V_{\ell,\mathrm{eff}}^{\min}$ is the minimal value of the effective potential.

The lower limit (1.58) has a much simpler expression:

$$N_\ell > \frac{2}{\pi} g - \frac{1}{2\pi} \ln\left(\frac{4}{\pi} g\right) - \frac{3}{2} - \frac{\ell}{\pi} \ln\left[\frac{\ln x}{\ln(1-x)}\right], \tag{1.66}$$

with $x = \pi/(4g)$.

Results for previously known limits are listed below. The Bargmann-Schwinger upper limit (1.2) takes the simple form

$$N_\ell < \frac{g^2}{2\ell+1}. \tag{1.67}$$

The Calogero-Cohn upper limit (1.18) is given by

$$N_0 < \frac{4}{\pi} g. \tag{1.68}$$

The upper limit (1.33) found by Chadan *et al.* read

$$N_\ell < \frac{4g}{\pi} + 1 - \sqrt{1 + \frac{4\,\ell\,(\ell+1)}{\pi^2}}. \tag{1.69}$$

The upper limit (1.32) found by Martin read for $\ell = 0$

$$N_0 < 2^{1/4}\, g. \tag{1.70}$$

But this limit take a more complicated form for $\ell > 0$:

$$N_\ell < (AB)^{1/4} \tag{1.71a}$$

where A and B are given by

$$\begin{aligned} A &= g^2 \left[\exp(-x_-)(x_-^2 + 2x_- + 2) - \exp(-x_+)(x_+^2 + 2x_+ + 2)\right] \\ &- \ell(\ell+1)(x_+ - x_-), \end{aligned} \tag{1.71b}$$

$$B = g^2 \left[\exp(-x_-) - \exp(-x_+)\right] - \ell(\ell+1)\left(\frac{1}{x_-} - \frac{1}{x_+}\right), \tag{1.71c}$$

with x_- and x_+ given by (1.65f). The upper limit (1.29) obtained by Glaser *et al.* takes the form

$$N_\ell \leq g^{2p}(2\ell+1)^{(1-2p)}\,\frac{C_p \Gamma(2p)}{p^{2p}}, \tag{1.72}$$

with C_p defined by (1.29b). The Calogero lower bound (1.22) is only cogent for $\ell = 0$ (see below) and reads

$$N_0 > \frac{2g}{\pi\sqrt{e}} - \frac{1}{2}, \tag{1.73}$$

A comparison between exact results for the S-wave ($\ell = 0$) case, recent limits and previously known results is reported in the Fig 1.1. This shows clearly that the limits (1.63) and (1.64) are very stringent and seem difficult to improve significantly.

Comparisons between various limits on $N_{\ell>0}$ and exact results are presented in Table 1.1. We refer to the name of the limits given in this Table for the discussion. The BS limit gives poor results when g becomes large but becomes slightly better as ℓ grows. The CMS gives better restrictions when ℓ is small but behaves like the BS limit when ℓ grows. The M limit overestimates the number of bound states by a factor 2 when ℓ is small; it is no better for larger ℓ, yet better than the BS and CMS limits. The GGMT limit (with, in each case, the optimized value of the parameter p, see (1.29)) gives similar results to those yielded by the BS limit when ℓ is small and becomes better and equivalent to the M limit for larger values of ℓ. The results obtained with the Chadan *et al.* (1.37) limit are uninteresting hence not reported: indeed, the values of p which minimize the value of the limit are either $p = 1/2$ for small values of ℓ (in which case this limit is analogous but less stringent than the Calogero-Cohn limit, see (1.18)), or $p = 1$ for larger values of ℓ (and this yields the

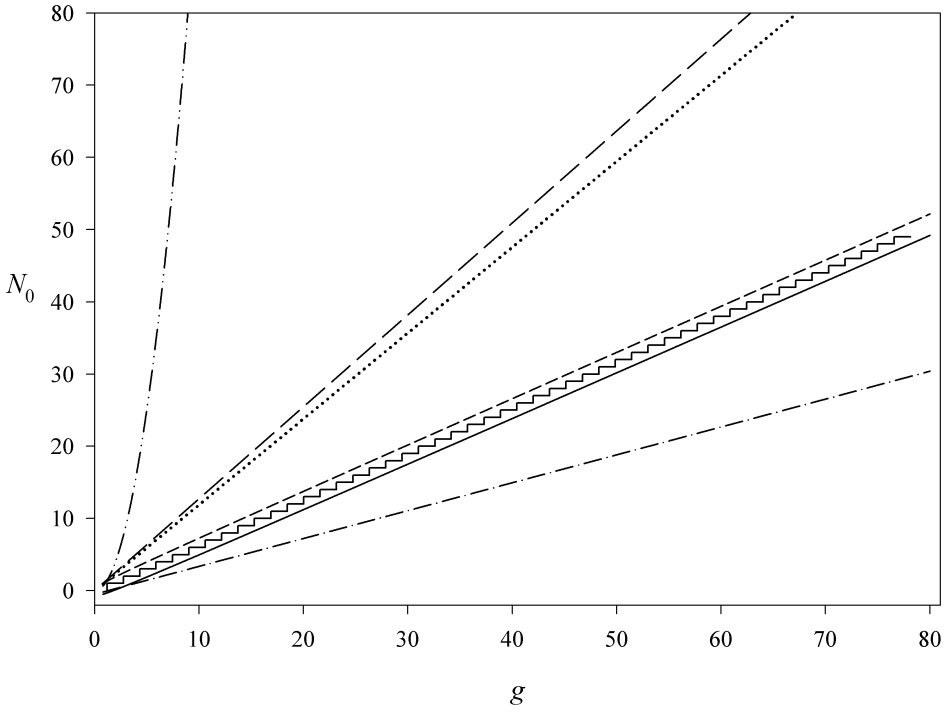

Figure 1.1: Comparison between the exact number of S-wave ($\ell = 0$) bound states for the E potential (1.61) (ladder curve), the limits (1.63) (short dash) and (1.64) (solid), the Calogero (1.73) (dash dot) lower limits, the Bargmann-Schwinger (1.67) (dash dot dot), the Calogero-Cohn (1.68) (dash) and Martin (1.70) (dot) upper limits.

Table 1.1: Comparison for the E potential (1.61) between the exact number $N_{\ell>0}$ of bound states (column Ex), various upper and lower limits on N_ℓ previously known (Bargmann-Schwinger (1.67): BS; Chadan *et al.* (1.69): CMS; Martin (1.71): M; Glaser *et al.* (1.72): GGMT) and new upper and lower limits on N_ℓ (upper limit (1.65a): $N_{\rm up}$; lower limit (1.65b): $N_{\rm lo}^{(1)}$; lower limit (1.66): $N_{\rm lo}^{(2)}$), for several values of g and ℓ.

g	ℓ	$N_{\rm lo}^{(2)}$	$N_{\rm lo}^{(1)}$	Ex	$N_{\rm up}$	BS	CMS	M	GGMT
8	1	3	3	4	5	21	9	8	21
	3	1	1	2	3	9	8	5	6
13	2	4	5	7	8	33	15	13	31
	6	0	2	3	4	13	13	7	7
18	3	6	7	9	10	46	21	18	43
	9	0	2	4	4	17	17	9	8
24	4	8	10	12	13	64	28	24	60
	12	0	4	5	6	23	23	13	11
29	5	9	13	15	16	76	34	29	71
	15	0	4	6	7	27	28	15	13
35	6	11	16	18	19	94	41	35	88
	18	0	6	7	8	33	33	18	16
40	7	12	18	20	21	106	47	40	100
	21	0	6	8	9	37	38	20	18

BS limit). The new limits $N_{\rm up}$ and $N_{\rm lo}^{(1)}$ clearly yield the most stringent results. The $N_{\rm lo}^{(2)}$ lower limit works reasonably well for small values of ℓ but becomes poor for higher values of the angular momentum. Finally, we note that the results obtained with the Calogero lower limit (1.22) for $\ell > 0$ are not reported because they are very poor. This limit gives $N_\ell \geq 1$ for small value of ℓ and $N_\ell \geq 0$ for large value of ℓ. This defect comes from the presence of the factor $1/(2\ell+1)$ which for instance implies that this lower bound becomes three times smaller when ℓ goes from 0 to 1 while the actual number of bound states N_ℓ decreases generally only by one or two units.

We now test the limits on the total number of bound states N with the E potential. We will not test the Schwinger limit (1.16) due to its bad behavior at large g. We do however test the Bargmann-Schwinger limit (1.6) which yields the same incorrect behavior but is simpler to compute.

The upper limit (1.55) takes the simple form

$$N < \frac{1}{8}\left(\frac{4g}{e}+1\right)^2\left(\frac{4g}{\pi}+\frac{1}{\pi}\log\frac{4g}{\pi}+1\right). \tag{1.74}$$

The lower limit (1.60) reads

$$N > \frac{\nu}{6}\left(2\left(L^-\right)^2+7L^-+6\right), \tag{1.75a}$$

with L^- and ν given by

$$L^- = \left\{\left\{\frac{\nu}{\lambda}\right\}\right\}, \tag{1.75b}$$

with

$$\nu = \frac{2g}{\pi}-\frac{1}{2\pi}\log\left[\frac{1-x}{x}\right]-\frac{3}{2}, \tag{1.75c}$$

$$\lambda = \frac{1}{\pi}\log\left[\frac{\log x}{\log(1-x)}\right], \tag{1.75d}$$

and $x = \pi/(4g)$.

Results for previously known limits are listed below. The Bargmann-Schwinger upper limit (1.6) takes the simple form

$$N < \frac{1}{2}g^2(g^2+1). \tag{1.76}$$

The simple upper limit (1.31) obtained by Lieb reads

$$N < 0.864\, g^3. \tag{1.77}$$

The upper limit (1.36) obtained by Chadan *et al.* thanks to an extension of the Calogero-Cohn upper limit to $\ell > 0$ takes the form

$$N < 1.698\,(g^3+2.356\,g^2+1.116\,g+0.1473). \tag{1.78}$$

The Bargmann-Schwinger (1.76) and the Chadan *et al.* (1.78) upper limits can be improved: instead of using the limit on L provided by these limits (L^+_{BS} (1.3) and L^+_{CMS} (1.35)), we can use the nice upper limit L^+ (1.53); the *improved* limits obtained in this manner are:

$$N < \frac{1}{2} g^2 \left(\frac{4g}{e} + 1 \right), \tag{1.79}$$

$$N < 0.5202 \, (g^3 + 2.179 \, g^2 + 1.726 \, g + 0.4806). \tag{1.80}$$

Fig. 1.2 presents a comparison between the various limits and the exact result. It shows that the limits on the *total* number of bound states which can be expressed in a neat form are not very stringent. [Indeed, the best results are yielded by the upper limit (1.74) which is obtained using only a limit on the number of S-wave bound states, N_0, and the simple limit L^+ on the maximal value L of ℓ for which bound states do exist]. There are at least three reasons for this. First, most of the limits do not contain the appropriate functional of the potential (as identified by the asymptotic behavior at large g of N, see (1.14)): only the Lieb limit, see (1.31), features the correct form, but the numerical factor is not optimal indeed too large (by approximately a factor 7). The second reason is that for every value of ℓ, there is a round-off error introduced by the limit; to obtain the limit on the total number of bound states we sum all these errors. The third reason is that to be able to make the summation over the values of ℓ we must have an explicit dependence of the limits on ℓ, and this entails that we cannot use some of the limits we found; in particular we cannot use the upper and lower limits (1.52a) and (1.52b) (with $V(r)$ replaced by the effective potential), which are quite stringent, to obtain a neat formula.

The second potential we use to test the new limits is the M potential (1.62). This is a non-monotonic potential for which the number N_0 of S-wave ($\ell = 0$) bound states is known; we indeed consider for this potential only the $\ell = 0$ case. The exact formula for the number of S-wave bound states for the M potential is

$$N_0 = \left\{ \left\{ g + \frac{1}{2} \right\} \right\}, \tag{1.81}$$

where $\{\{x\}\}$ means integer part of x. Note that the exact relation (1.81) is independent of the value of the constant α which appears in the potential (see (1.62)).

For this potential, the limits (1.52) can be computed (almost completely) analytically:

$$N_0 \;<\; g - \frac{1}{2\pi} \log s + 1, \tag{1.82}$$

$$N_0 \;>\; g + \frac{1}{2\pi} \log s - \frac{3}{2}, \tag{1.83}$$

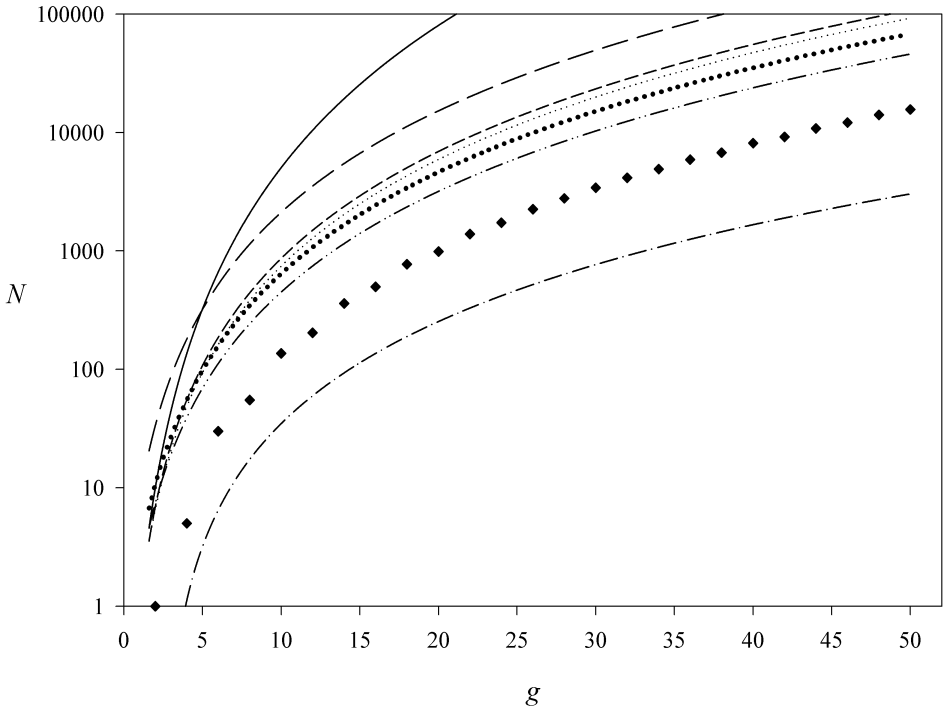

Figure 1.2: Comparison for the E potential (1.61) between the exact value of the total number of bound states N (diamond), the upper limits obtained by Bargmann-Schwinger (1.76) (solid), Lieb (1.77) (short dash), Chadan *et al.* (1.78) (long dash), the *improved* Bargmann-Schwinger (1.79) (dot), *improved* Chadan *et al.* (1.80) upper limits (sparse dot), the limits (1.74) (dash dot dot) and the lower limits (1.75) (dash dot).

with $s = \min(2y - y^2, 2x - x^2)$ and x, y solutions of

$$\pi - \sqrt{2y - y^2} - 2\arcsin\left(\frac{y}{2}\right) = \frac{\pi}{2g}, \tag{1.84}$$

$$\sqrt{2x - x^2} + 2\arcsin\left(\frac{x}{2}\right) = \frac{\pi}{2g} \tag{1.85}$$

The calculation of the cutoff radii p and q, see (1.52d), cannot be evaluated analytically. But one can compute upper and lower limits, $\tilde{p} < p$ and $\tilde{q} > q$, on these radii by using only the attractive part of the potential in the definition (1.52d) of p and q. When $\tilde{p}$ and $\tilde{q}$ are used in place of p and q we obtain the (marginally less stringent) limits

$$N_0 < g + \frac{1}{2\pi}\log\left[\frac{z^4}{4(z^2-1)}\right] + 1, \tag{1.86}$$

$$N_0 > g - \frac{1}{2\pi}\log\left[\frac{z^4}{4(z^2-1)}\right] - \frac{3}{2}, \tag{1.87}$$

with $z = 8g/\pi$. As mentioned in above, validity of the inequalities $\tilde{p} \leq r_{\min} \leq \tilde{q}$ is required in order to use the limits (1.86) and (1.87); this leads to the restriction $g \geq \pi\sqrt{2}/(8(\sqrt{2}-1)) \cong 1.34$.

The previously known limits applicable to this potential are listed below. The Bargmann-Schwinger upper limit (1.2) takes the form:

$$N_0 \leq 2g^2\left(\alpha + \log 2 + \frac{3}{2}\right). \tag{1.88}$$

The upper limit (1.32) found by Martin reads

$$N_0 \leq \sqrt{2}g(\alpha^2 + (3 - 2\log 2)\alpha + 1.901)^{1/4}; \tag{1.89}$$

The Calogero lower bound (1.19) reads

$$N_0 > -\frac{1}{2} + \frac{2}{\pi}g\,T(\alpha), \tag{1.90a}$$

$$T(\alpha) = \max_{0\leq\gamma\leq 1}\left\{\frac{1}{\gamma}\left[e^{\alpha} - \frac{e^{2\alpha}}{4} - \sqrt{1-\gamma^2} + \frac{\gamma^2}{2}\log\left(\frac{1+\sqrt{1-\gamma^2}}{1-\sqrt{1-\gamma^2}}\right)\right]\right\}. \tag{1.90b}$$

Note that for $\alpha > \alpha_0 \cong 1.386$, with $4\exp(\alpha_0) = \exp(2\alpha_0)$, this lower limit (1.90) is trivial because $T(\alpha)$ is then negative.

Fig. 1.3 displays these limits as a function of g. Note that some limits depend on α while the exact result does not. We tested the results for the $\alpha = 1$ case (not $\alpha = 0$, in order to have a non-monotonic potential). It is clear from this figure that the limits (1.86) and (1.87) are quite cogent. This remains true even for large values of g: for instance, when the exact number N_0 of bound states is 5000, these upper and lower limits restrict its value to the rather small interval $[4996, 5003]$. In this case the Bargmann-Schwinger upper limit exceeds $1.5\ 10^8$, the Martin upper limit only informs us that $N < 10307$, the Calogero lower limit that $N > 2879$.

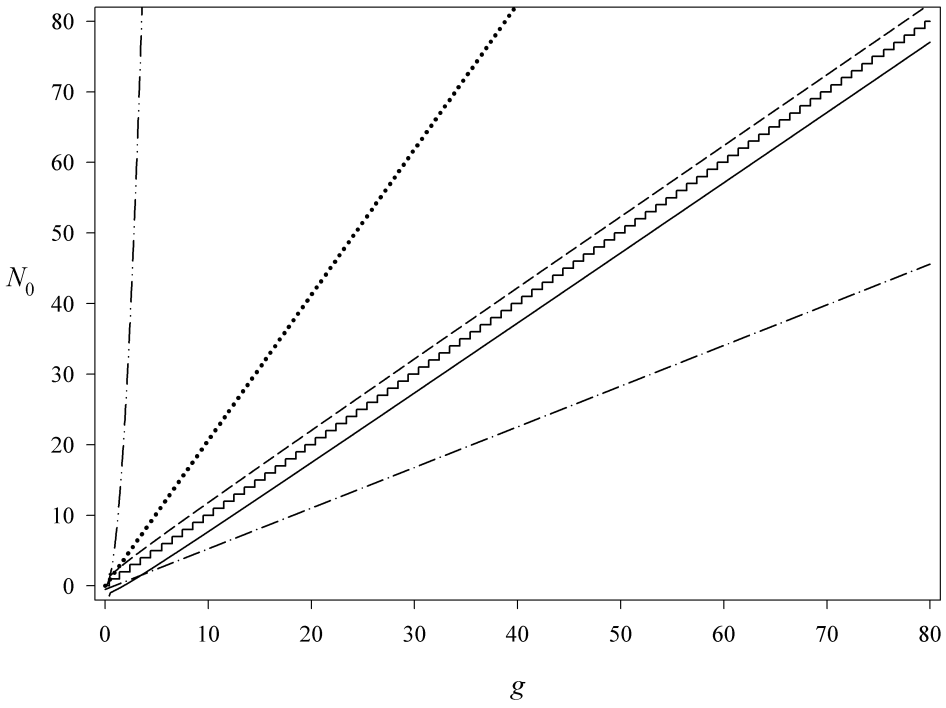

Figure 1.3: Comparison for the M potential (1.62) between the exact value (1.81) of the number of S-wave bound states N_0 (ladder), the Bargmann-Schwinger (1.88) (dash dot dot), Martin (1.89) (dot) upper limits, the upper limit (1.86) (short dash) and the Calogero lower limits (1.90) (dash dot) and the lower limit (1.87) (solid) (all with $\ell = 0$ and $\alpha = 1$).

Ideas of the proofs

We propose to give in this Section, the main line of the proof of the upper and lower limits (1.50). We refer to the original article [30, 31] for more details and proofs of other limits.

Let $u(r)$ be the zero-energy S-wave Schrödinger wave function, characterized by the second order ordinary differential equation

$$u''(r) - V(r)u(r) = 0, \tag{1.91}$$

with boundary condition

$$u(0) = 0. \tag{1.92}$$

It is well known (see, for instance, Ref. [35]) that the number of zeros of the solution of (1.91) with (1.92) in the interval $0 \leq r < \infty$ coincides with the number N_0 of S-wave bound states supported by the potential $V(r)$ (we always exclude, for simplicity, the marginal case of a potential that features a "zero-energy bound state or resonance"). Let us indicate with z_n the successive zeros of $u(r)$, and with b_n the successive zeros of $u'(r)$ (namely, the locations of the successive extrema of the wave function $u(r)$),

$$u(z_n) = 0, \quad u'(b_n) = 0. \tag{1.93}$$

It is then clear that, since we suppose the potential $V(r)$ to be nowhere positive,

$$V(r) = -|V(r)|, \tag{1.94}$$

the zero-energy wave function $u(r)$ is an everywhere convex function of r, entailing the "interlacing" relations

$$0 = z_0 < b_1 < z_1 < b_2 < \cdots < z_{N_0-1} < b_{N_0} < z_{N_0} < \infty. \tag{1.95}$$

Note that these formulas imply that $u'(r)$ does not vanish in the interval $z_{N_0} \leq r < \infty$, namely $b_{N_0+1} < \infty$ does not exist (otherwise it would be inevitably followed by $z_{N_0+1} < \infty$ and this is excluded since N_0 is the number of zeros of $u(r)$).

Following Refs. [6, 30, 31, 35] we now introduce a function $\eta(r)$ defined via the relation

$$\tan[\eta(r)] = |V(r)|^{1/2} \frac{u(r)}{u'(r)}. \tag{1.96a}$$

with

$$\eta(0) = 0, \tag{1.96b}$$

and the requirement that $\eta(r)$ be a continuous function of r (to lift the $\mathrm{mod}(\pi)$ ambiguity entailed by the definition (1.96)). It is then clear that the properties (1.95) together with the definition (1.96) imply the relations

$$\eta(z_n) = n\pi, \quad \eta(b_{n+1}) = (2n+1)\pi/2, \quad n = 0, 1, \ldots, N_0 - 1, \tag{1.97a}$$

$$\eta(z_{N_0}) = \eta(\infty) = N_0\pi, \tag{1.97b}$$

and that the value of $\eta(r)$ inside the intervals (1.95) lies between the values taken at the extremal points of these intervals, namely, for $z_n \leq r \leq b_{n+1}$ with $n = 0, \ldots, N_0 - 1$, $n\pi \leq \eta(r) \leq (2n+1)\pi/2$, and for $b_n \leq r \leq z_n$ with $n = 1, \ldots, N_0$, $(2n-1)\pi/2 \leq \eta(r) \leq n\pi$, except of course for the last interval, $z_{N_0} \leq r < \infty$, where $N_0\pi \leq \eta(r) < (2N_0+1)\pi/2$. Note that these results also imply that, for all values of r,

$$0 \leq \eta(r) < \left(N_0 + \frac{1}{2}\right)\pi, \tag{1.97c}$$

(indeed the value at which the second inequality was violated would qualify as b_{N_0+1} , which, as already noted, would then inevitably be followed by z_{N_0+1} , violating the hypothesis that the number of zeros be N_0).

Moreover, from (1.91) we obtain via (1.96a) and (1.94) the nonlinear first-order differential equation

$$\eta'(r) = |V(r)|^{1/2} - \frac{V'(r)}{4|V(r)|}\sin[2\eta(r)], \tag{1.98}$$

which, together with the "initial condition" (1.96b), determines the function $\eta(r)$ and, therefore, via (1.97b), the number N_0 of S-wave bound states. This equation will be our main tool to derive (upper and lower) limits on N_0. It is indeed clear from (1.98) that

$$\eta'(r) \leq |V(r)|^{1/2} + \frac{V'(r)}{4|V(r)|}, \tag{1.99a}$$

$$\eta'(r) \geq |V(r)|^{1/2} - \frac{V'(r)}{4|V(r)|}. \tag{1.99b}$$

Let us now focus first on the derivation of the upper limit (1.50a). To this end we integrate (1.99a) from b_1 to z_{N_0+1}, and via (1.97a) we get

$$\left(N_0 - \frac{3}{2}\right)\pi \leq \int_{b_1}^{z_{N_0-1}} dr\,|V(r)|^{1/2} + \frac{1}{4}\ln\left|\frac{V(b_1)}{V(z_{N_0-1})}\right|. \tag{1.100}$$

On the other hand in the intervals $0 \leq r \leq b_1$ and $z_{N_0-1} \leq r \leq b_{N_0}$ (where $\sin[2\eta(r)]$ is non-negative, see (1.97a)] (1.99a) can be replaced by the more stringent inequality

$$\eta'(r) \leq |V(r)|^{1/2}, \tag{1.101}$$

and the integration of this inequality over these intervals yields

$$\frac{\pi}{2} \leq \int_0^{b_1} dr\,|V(r)|^{1/2}, \tag{1.102a}$$

$$\frac{\pi}{2} \leq \int_{z_{N_0-1}}^{b_{N_0}} dr\,|V(r)|^{1/2}. \tag{1.102b}$$

Hence by summing (1.100), (1.102a) and (1.102b) (and dividing by π) we get

$$N_0 - \frac{1}{2} \leq \frac{1}{\pi}\int_0^{b_{N_0}} dr\,|V(r)|^{1/2} + \frac{1}{4\pi}\ln\left|\frac{V(b_1)}{V(z_{N_0-1})}\right|, \tag{1.103}$$

and therefore a fortiori (thanks to the monotonicity of $V(r)$)

$$N_0 < \frac{1}{\pi}\int_0^{\infty} dr\,|V(r)|^{1/2} + \frac{1}{4\pi}\ln\left|\frac{V(p)}{V(q)}\right| + \frac{1}{2}, \tag{1.104}$$

provided

$$p \leq b_1, \tag{1.105a}$$

$$q \geq z_{N_0-1}. \tag{1.105b}$$

With the definitions (1.50c) of p and q, it is clear that the relations (1.105) are satisfied which complete the proof for the upper bound (1.50a).

The proof for the lower limit (1.50b) is similar. For a regular potential, we integrate the inequality (1.99b) from 0 to q and we use the relation (1.97c). For a singular potential, we integrate the inequality (1.99b) from p to q and we use also the relation (1.97c).

One and two dimensions

The upper and lower limits (1.52) presented in the previous Section 1.2.1 can be generalized to be applicable to potentials possessing more than one minimum. With an inspection of the proof given in the original article [31], it is easy to see that a possible generalization (not the most stringent but perhaps the neater version) takes the form

$$N_0 < \frac{\mathcal{S}}{\pi} + \frac{\nu}{2\pi}\,\ln\left[\frac{V^-(R_{\min})}{M}\right] + 1, \tag{1.106a}$$

$$N_0 > \frac{\mathcal{S}}{\pi} - \frac{\nu}{2\pi}\,\ln\left[\frac{V^-(R_{\min})}{M}\right] - \frac{3}{2}, \tag{1.106b}$$

where

$$M = \min\left[V^-(p), V^-(q), V^-(r^1_{\max}), \ldots, V^-(r^{\nu-1}_{\max})\right], \tag{1.106c}$$

where $R_{\min}$ is the position of the absolute minima of the potential, $r^i_{\max}$ is the position of the ith maxima of the potential ($0 < r^1_{\max} < \ldots < r^{\nu-1}_{\max} < \infty$) and ν is the number of minima of the potential. The additional necessary condition for the applicability of these limits reads now

$$p \leq r^1_{\min} \quad \text{and} \quad r^{\nu}_{\min} \leq q, \tag{1.106d}$$

where $r^i_{\min}$ is the position of the ith minima ($0 \leq r^1_{\min} < \ldots < r^{\nu}_{\min} < \infty$) and p and q are still given by (1.52d). Different versions of the limits (1.106) are possible, but the difference is only located in the logarithmic term and thus plays a minor role.

¿From the limits (1.106) we could obtain limits on the number of bound states in one dimension using the method proposed by Chadan *et al.* and explained in the Section 1.1. But in doing so we would obtain only an upper bound with moreover a large constant term. We prefer to derive explicitely upper and lower limits in one dimensions from the corresponding Schrödinger equation without any reference to limits applicable in three dimensions.

Let $u(x)$ be the zero-energy Schrödinger wave function in one dimension, characterized by the second order ordinary differential equation

$$u''(x) - V(x)u(x) = 0, \tag{1.107}$$

with boundary condition

$$u(-\infty) = 0. \tag{1.108}$$

It is well known that the number of zeros of the solution of (1.107) with (1.108) in the interval $-\infty < x < \infty$ coincides with the number N of bound states supported by the potential $V(x)$. We will use the same notation than whose used in Section 1.2.1. Let us indicate with z_n the successive zeros of $u(x)$, and with b_n the successive zeros of $u'(x)$ (namely, the locations of the successive extrema of the wave function $u(x)$),

$$u(z_n) = 0, \quad u'(b_n) = 0. \tag{1.109}$$

We introduce a function $\eta(x)$ defined via the relation

$$\tan[\eta(x)] = |V(x)|^{1/2} \frac{u(x)}{u'(x)}. \tag{1.110}$$

The function $\eta(x)$ satisfies the equation

$$\eta'(x) = |V(x)|^{1/2} - \frac{V'(x)}{4|V(x)|} \sin[2\eta(x)]. \tag{1.111}$$

We will now consider potentials that satisfies the condition

$$V(x) > 0 \quad \text{for} \quad x < x_-, \tag{1.112a}$$

$$V(x) < 0 \quad \text{for} \quad x_- < x < x_+, \tag{1.112b}$$

$$V(x) > 0 \quad \text{for} \quad x_+ < x. \tag{1.112c}$$

This condition entails that

$$\eta(x_-) = 0, \tag{1.113}$$

as well as the fact that $u(x)$ is concave in the interval $-\infty < x < x_-$, hence it has no zero in that interval, hence

$$x_- < b_1 < z_1. \tag{1.114}$$

Likewise the fact that $u(x)$ is also concave in the interval $x_+ < x < \infty$, hence it has no extremum in that interval, entails

$$z_{N-1} < b_N < x_+. \tag{1.115}$$

Now we integrate (1.111) from z_1 to z_{N-1} to get

$$\eta(z_{N-1}) - \eta(z_1) = (N-2)\pi =$$
$$= \int_{z_1}^{z_{N-1}} dx\ \left[V^-(x)\right]^{1/2} - \frac{1}{4}\sum_{i=0}^{2\nu-1}\int_{x_{k_i}}^{x_{k_{i+1}}} dx\,\frac{V'(x)}{4|V(x)|}\sin[2\eta(x)], \tag{1.116}$$

where $x_{k_0} = z_1$, $x_{k_{2\nu}} = z_{N-1}$ and x_{k_i} is the position of the extrema of the potential between x_- and x_+. Thus, in the sum of the relation (1.116) we have 2ν integrals and for each integral, $V'(x)$ has a given sign. This allows an easy majorization or minorization of the right-hand side of (1.116). For a majorization, we replace $\sin[2\eta(x)]$ by 1 whenever $V'(x)$ is negative and by -1 when $V'(x)$ is positive. The contrary applies for a minorization. We then simply obtain

$$(N-2)\pi < \int_{z_1}^{z_{N-1}} dx\ \left[V^-(x)\right]^{1/2} + \frac{1}{2}\ln\left[\frac{\mathcal{A}}{\mathcal{B}}\right], \tag{1.117a}$$

with

$$\mathcal{A} = \prod_{i=1}^{\nu} V^-(x^i_{\min}) \quad \text{and} \quad \mathcal{B} = (V^-(z_1)V^-(z_{N-1}))^{1/2}\prod_{i=1}^{\nu-1} V^-(x^i_{\max}) \tag{1.117b}$$

and where $x^i_{\max}$ is the position of the ith maxima of the potential ($x_+ < x^1_{\max} < \ldots < x^{\nu-1}_{\max} < x_+$) and $x^i_{\min}$ is the position of the ith minima of the potential ($x_+ < x^1_{\min} < \ldots < x^{\nu}_{\min} < x_+$).

We now need to find quantities p and q, defined only in terms of the potential, such that $p \leq z_1$ and $q \geq z_{N-1}$ (to majorize the integral appearing in (1.117a)) and also such that $|V^-(p)| \leq |V^-(z_1)|$ and $|V^-(q)| \leq |V^-(z_{N-1})|$ (to majorize the logarithmic term of the inequality (1.117a)). Let us first consider the "favorable" case (which obtains for a sufficiently attractive potential): $z_1 \leq x^1_{\min}$ and $z_{N-1} \geq x^{\nu}_{\min}$. In this case, we integrate (1.111) from b_1 to z_1 and since in this interval both $V'(x)/|V(x)|$ and $\sin[2\eta(x)]$ are *negative*, we infer

$$\eta(z_1) - \eta(b_1) = \frac{\pi}{2} \leq \int_{b_1}^{z_1} dx\ \left[V^-(x)\right]^{1/2}, \tag{1.118}$$

hence *a fortiori* (see (1.114))

$$\int_{-\infty}^{z_1} dx\ \left[V^-(x)\right]^{1/2} > \frac{\pi}{2}. \tag{1.119}$$

If we define p via the formula

$$\int_{-\infty}^{p} dx \, \left[V^-(x)\right]^{1/2} = \frac{\pi}{2}, \tag{1.120}$$

then we conclude (by comparing (1.119) with (1.120)) that $p < z_1$. Moreover, since we have supposed $z_1 \leq x^1_{\min}$, we have also $|V(p)| < |V(z_1)|$. We then integrate (1.111) from z_{N-1} to b_N, and taking advantage of the fact that in this interval both $V'(x)/|V(x)|$ and $\sin[2\eta(x)]$ are *positive*, we infer

$$\eta(b_N) - \eta(z_{N-1}) = \frac{\pi}{2} \leq \int_{z_{N-1}}^{b_N} dx \, \left[V^-(x)\right]^{1/2}, \tag{1.121}$$

hence *a fortiori* (see (1.115))

$$\frac{\pi}{2} < \int_{z_{N-1}}^{\infty} dx \, \left[V^-(x)\right]^{1/2}. \tag{1.122}$$

Analogously, if we define q via the formula

$$\int_{q}^{\infty} dx \, \left[V^-(x)\right]^{1/2} = \frac{\pi}{2}, \tag{1.123}$$

we conclude that $q > z_{N-1}$. Moreover, since we have supposed $z_{N-1} \geq x^\nu_{\min}$, we have also $|V(q)| < |V(z_{N-1})|$. Thus if these two relations, $z_1 \leq x^1_{\min}$ and $z_{N-1} \geq x^\nu_{\min}$, hold, we obtain

$$N < \frac{1}{\pi} \int_{-\infty}^{\infty} dx \, \left[V^-(x)\right]^{1/2} + \frac{1}{2} \ln \left[\frac{\mathcal{A}}{\mathcal{B}}\right] + 1, \tag{1.124a}$$

where $\mathcal{A}$ is still defined by (1.117b) and where

$$\mathcal{B} = (V^-(p)V^-(q))^{1/2} \prod_{i=1}^{\nu-1} V^-(x^i_{\max}), \tag{1.124b}$$

where we have used the equations (1.120) and (1.123).

We need now to consider the cases where $z_1 > x^1_{\min}$ and/or $z_{N-1} < x^\nu_{\min}$ and to prove that it is still possible to define quantities p and q such as $p < z_1$ and $q > z_{N-1}$ and such as a majorization of $\mathcal{B}$ is possible. This difficulty is easily in two step solved. Firstly, We simply impose the additional requirement on p and q:

$$p \leq x^1_{\min} \quad \text{and} \quad x^\nu_{\min} \leq q. \tag{1.125}$$

This indeed ensure that $p < z_1$ and $q > z_{N-1}$. Indeed, we have just proved above that it was the case provided that $z_1 \leq x^1_{\min}$ and $z_{N-1} \geq x^\nu_{\min}$. Now if one (or both) of these last conditions is not satisfy (which could be the case for weak potentials),

the conditions $p < z_1$ and $q > z_{N-1}$ are still satisfy thanks to the relations (1.125), this ensure the majorization of the integral of (1.117a). Secondly, we must now majorize $\mathcal{B}$. We have shown above that the relations $z_1 \leq x^1_{\min}$ and $z_{N-1} \geq x^\nu_{\min}$ entails that $|V^-(p)| \leq |V^-(z_1)|$ and $|V^-(q)| \leq |V^-(z_{N-1})|$. It is obvious that, if $z_1 > x^1_{\min}$, then

$$|V^-(z_1)| \geq M, \tag{1.126}$$

where

$$M = \min\left[V^-(p), V^-(q), V^-(x^1_{\max}), \ldots, V^-(x^{\nu-1}_{\max})\right]. \tag{1.127}$$

Similarly, if $z_{N-1} < x^\nu_{\min}$, then $|V^-(z_{N-1})| \geq M$.

We choose now to write the neater upper limit by replacing all factors in the expression of $\mathcal{B}$ by M and to replace all factors in the expression of $\mathcal{A}$ by $V^-(X_{\min})$, where $X_{\min}$ is the position of the absolute minima of the potential. The upper limit on the number of bound states in spaces with one dimensions reads

$$N < \frac{1}{\pi}\int_{-\infty}^{\infty} dx\ \left[V^-(x)\right]^{1/2} + \frac{\nu}{2\pi}\ln\left[\frac{V^-(X_{\min})}{M}\right] + 1, \tag{1.128}$$

with M defined by (1.127) and provided the potential satisfies (1.112) (note also that ν, the number of minima of the potential between x_- and x_+ must be finite).

The lower limit is obtained in the same way except that we integrate (1.111) between p and q defined by (1.120) and (1.123). We have

$$\eta(q) - \eta(p) \geq \int_p^q dx\ \left[V^-(x)\right]^{1/2} - \frac{1}{2}\ln\left[\frac{\mathcal{A}}{\mathcal{B}}\right]. \tag{1.129}$$

Now since $\eta(p) \geq 0$ and $\eta(q) < (N + 1/2)\pi$ (otherwise, if the last inequality was violated, this would ensure the existence of b_{N+1} and then of z_{N+1}, which is not possible since we have supposed that the potential possess only N bound states), we obtain

$$N > \frac{1}{\pi}\int_{-\infty}^{\infty} dx\ \left[V^-(x)\right]^{1/2} - \frac{\nu}{2\pi}\ln\left[\frac{V^-(X_{\min})}{M}\right] - \frac{3}{2}, \tag{1.130}$$

where we have used the definitions of p and q.

We are now in position to derive limits for spaces with two dimensions. The change of variable (1.47) applied to the limits (1.128) and (1.130) leads to the following limits applicable to spaces with two dimensions provided the potential is central and that the angular momentum, m is equal to zero:

$$N_{m=0} < \frac{1}{\pi}\int_0^{\infty} dr\,[V^-(r)]^{1/2} + \frac{\nu}{2\pi}\ln\left[\frac{V^-(R_{\min})}{M}\right] + \frac{\nu}{\pi}\ln\left[\frac{R_{\min}}{\bar{R}_{\min}}\right] + 1, \tag{1.131a}$$

$$N_{m=0} > \frac{1}{\pi}\int_0^{\infty} dr\,[V^-(r)]^{1/2} - \frac{\nu}{2\pi}\ln\left[\frac{V^-(R_{\min})}{M}\right] - \frac{\nu}{\pi}\ln\left[\frac{R_{\min}}{\bar{R}_{\min}}\right] - \frac{3}{2}, \tag{1.131b}$$

where M, $R_{\min}$, p and q are defined as for the formulas (1.106), and where $\bar{R}_{\min}$ is the radius among p, q, $r^1_{\max}$, ..., $r^{\nu-1}_{\max}$, for which $V^-(\bar{R}_{\min})$ take the minimal value. Note that the last logarithmic term in (1.131) could be negative. Note also that when $R_{\min}$ is vanishing, it should be replaced by p.

It is well known that a correspondence exists between spaces with two and three dimensions when the potential is central (this is easily seen from the Schrödinger equation). The formal change of angular momentum, $m = \ell + 1/2$, applied to results applicable in three dimensions yields formulas for two dimensions. In particular, the relation (1.53) (see also (1.164) below) becomes

$$m \leq m^+ = \{\{\sigma\}\}\,, \tag{1.132}$$

with σ defined by (1.53b). We are now in position to obtain a limit on the total number of bound states for a central potential in two dimensions (remember that for $m = 0$ the multiplicity equals 1 while for $m > 0$ the multiplicity equals 2). Trivially, we have

$$N \leq N_{m=0} + 2\sum_{m=1}^{m^+} N_{m=0} < (1 + 2\sigma)N_{m=0}. \tag{1.133}$$

Thus any upper limit on $N_{m=0}$, for example (1.131a), provides an upper limit on N.

We see that the formulas (1.128) and (1.130) for one spatial dimensions and the formulas (1.131) for two spatial dimensions (with $m = 0$) have the correct asymptotic expression (see (1.15) with $n = 1$). Thus, for potentials strong enough to bind several bound states, the new limits will be better than those presented in Section 1.1. Consequently, we do not present any test since the situation is comparable to what we have presented in Section 1.2.1.

The situation is different for the upper limit on the total number of bound states in two dimensions. We then compare, as a test, the leading term of our upper limit on N (1.133) with (1.131a), with the upper limit of Chadan *et al.* (1.49) and with the exact asymptotic expression of N (see (1.15) with $n = 2$)

$$N \approx \frac{1}{2}\int_0^\infty dr\, r\, V^-(r). \tag{1.134}$$

For a square-well potential, $V(r) = -g^2 R^{-2}\,\theta(R - r)$, we found that our limit gives

$$N \approx 0.318\, g^2. \tag{1.135}$$

The limit (1.49) of Chadan *et al.* takes the asymptotic form

$$N \approx 0.751\, g^2. \tag{1.136}$$

The exact asymptotic expression is

$$N \approx \frac{1}{4}\, g^2. \tag{1.137}$$

Clearly for g large enough our limit will be better. The same calculation can be performed for an exponential potential, $V(r) = -g^2 R^{-2} \exp(-r/R)$, and we found for our bound that

$$N \approx 0.937\, g^2. \tag{1.138}$$

The limit of Chadan *et al.* (1.49) yields

$$N \approx 1.78\, g^2, \tag{1.139}$$

while the exact asymptotic expression is

$$N \approx \frac{1}{2}\, g^2. \tag{1.140}$$

Again, as for the square-well potential, our limit will be more stringent for g large enough.

1.2.2 Semi-relativistic quantum mechanics

Klein-Gordon equation

In the context of first-quantized mechanics with relativistic kinematics, a zero-spin particle of (positive) mass m moving in an external potential $W(\vec{r})$, which is the fourth-component of a relativistic 4-vector, can be described (in self-evident notation, and with the choice of units $\hbar = c = 1$ throughout this Section 1.2.2!) by the following Klein-Gordon equation:

$$\left(\vec{p}^{\,2} + m^2\right) \Psi(\vec{r}) = \left[E - W(\vec{r})\right]^2 \Psi(\vec{r}) \tag{1.141}$$

In the spherically-symmetrical case, $W(\vec{r}) = W(r)$, the zero-kinetic-energy (namely, $E = m$) S-wave radial equation coincides with the corresponding equation for the Schrödinger case, (1.91), with the following definition of $V(r)$ in terms of $W(r)$:

$$V(r) = 2mW(r) - W^2(r). \tag{1.142}$$

Note that, if the potential $W(r)$ is monotonically non-decreasing and vanishes at infinity (and is therefore non-positive, $W(r) = -|W(r)|$), the same property holds as well for the potential $V(r)$. And the following conditions on the behavior of at the origin and at infinity are clearly sufficient to guarantee the validity of (1.1):

$$\lim_{r\to 0} \left[r^{1-\epsilon}\, W(r)\right] = 0, \tag{1.143a}$$

$$\lim_{r\to \infty} \left[r^{1+\epsilon}\, W(r)\right] = 0. \tag{1.143b}$$

All the results reported above in the Schrödinger context can therefore be immediately taken over to the Klein-Gordon case. Note however that, as a consequence of the relation (1.142), if one introduces a coupling constant g as a measure of the strength of the potential by setting $W(r) = g^2 w(r)$, then one sees that in the Klein-Gordon case as g diverges the number of S-wave bound states grows proportionally to g^2 (rather than proportionally to g as is the case in the Schrödinger context).

Spinless Salpeter equation

We present in this Section results about the spinless Salpeter equation characterized by a pseudo-differential operator. The spinless Salpeter equation is a simple relativistic version of the Schrödinger equation which can be obtained, with some approximations, from the covariant Bethe-Salpeter equation [41, 42] and takes the form

$$\left[\sqrt{\vec{p}^{\,2}+m^2}+V(\vec{r})\right]\,\Psi(\vec{r})=M\,\Psi(\vec{r}), \tag{1.144}$$

where m is the mass of the particle and M is the mass of the eigenstate ($M=m+E$, E is the binding energy). We restrict our attention to time component vector potentials. This equation is generally used when kinetic relativistic effects cannot be neglected and when the particles under consideration are bosons or when the spin of the particles is neglected or is only taken into account via spin-dependent interactions. Despite its apparent complexity, this equation is often preferred to the Klein-Gordon equation. The equation (1.144) appears, for example, in mesons and baryons spectroscopy in the context of potential models (see for example [43, 44, 45, 46, 47, 48, 49, 50]).

Due to the pseudo-differential nature of the kinetic energy operator, few exact results are known about this equation. Most of these results have been obtained for a Coulomb potential (for example, upper and lower bounds on energy levels) [51, 52, 53, 54, 55]. Recently, upper and lower limits on energy levels have been obtained for some other particular interactions [56].

Conversely to the Schrödinger equation, for which a fairly large number of results giving both upper and lower limits on the number of bound states can be found in the literature (see Section 1.1), only one (very nice) result, concerning the total number of bound states, is known for the spinless Salpeter equation [57]

$$N<K\int d\vec{r}\,\left[V^-(\vec{r})(V^-(\vec{r})+2m)\right]^{3/2}, \tag{1.145}$$

with $K=0.239$ for arbitrary values of m and $K=0.103$ for $m=0$. This inequality shows that N grows with strength of the potential, g ($V(\vec{r})=g^2v(\vec{r})$), at most as g^6.

In contrast with previous Sections, we also present here results applicable to non-central potential. To obtain an upper limit on the total number of bound states of the spinless Salpeter equation we use the Birman-Schwinger method (see Appendice 1.3.2). We then need to calculate the Green function of the kinetic energy operator. Similar calculations have already been performed previously [58, 59]. In contrast to calculations found in [59], we need here to calculate the Green function of the following operator

$$T\left(\vec{p}^{\,2}\right)=\sqrt{\vec{p}^{\,2}+m^2}-m. \tag{1.146}$$

This is done by performing the integral

$$G(m,\Delta) = \frac{1}{(2\pi)^3}\int d\vec{p}\,\frac{\exp(-i\,\vec{p}\cdot\vec{\Delta})}{\sqrt{p^2+m^2}-m}, \tag{1.147}$$

where $\vec{\Delta} = \vec{r} - \vec{r}\,'$. We find that

$$G(m,\Delta) = \frac{m}{4\pi\Delta}\left[1+\frac{2}{\pi}F(m\Delta)\right] \equiv \frac{m}{4\pi\Delta}\,H(m\Delta), \tag{1.148a}$$

with

$$F(y) = \int_y^\infty \frac{dz}{z}\,K_1(z) + \frac{\pi}{2}, \tag{1.148b}$$

where $K_\nu(y)$ is a modified Bessel function (see for example [60, p. 374]). The symmetrical kernel, see (1.201), is then given by

$$K(m,\vec{r},\vec{r}\,') = [V^-(\vec{r})]^{1/2} G(m,\Delta)[V^-(\vec{r}\,')]^{1/2}. \tag{1.149}$$

The Birman-Schwinger method yields the following upper limit on the total number of bound states of the spinless Salpeter equation

$$N < \frac{1}{\alpha^n}\int d\vec{r}_1\ldots d\vec{r}_n\,V^-(\vec{r}_1)\ldots V^-(\vec{r}_n)\,G(m,\Delta_{12})\ldots G(m,\Delta_{n1}), \tag{1.150}$$

where $\Delta_{ij} = |\vec{r}_i - \vec{r}_j|$ and $n \geq 4$ (the integral diverges for smaller values of n). We have introduced in (1.150) the parameter α which takes the value 1 respectively 2 for one respectively two (identical) particle problems.

Now, we need to calculate the Green function (1.148) in a closed form, that is to say, to compute $F(y)$, see (1.148b). An integration by part leads to

$$F(y) = K_1(y) + \frac{\pi}{2} - \int_y^\infty dz\,K_0(z). \tag{1.151}$$

To obtain an upper limit for the number of bound states, a majorization of the kernel (1.149) is enough. Since the Bessel function $K_0(z)$ is positive for $0 \leq z < \infty$, and that its integration between 0 and ∞ is equal to $\pi/2$ (see [60, p. 486]), the integral in (1.151) is not only positive but also small compared to the other terms of this equation. Indeed, in the region ($y \approx 0$) where this integral takes its maximal value ($\pi/2$), this quantity is still small compared to the value taken by the *singular* Bessel function $K_1(y)$. Thus the majorization obtained by replacing the integral in (1.151) by 0, namely

$$F(y) \leq K_1(y) + \frac{\pi}{2}, \tag{1.152}$$

should not spoil too much the upper limit. Another majorization, which leads to a simpler kernel, is obtained by replacing the Bessel function $K_1(y)$ by $1/y$. This

additional approximation is however exact in the case of a vanishing mass ($m = 0$) since $mK_1(my) = 1/y$ in this limit. The kernel is then given by

$$\begin{aligned} G(m, \Delta_{ij}) &\leq \frac{m}{2\pi\Delta_{ij}} + \frac{mK_1(m\Delta_{ij})}{2\pi^2\Delta_{ij}} = G^{(1)}(m, \Delta_{ij}) && \text{(1.153a)} \\ &\leq \frac{m}{2\pi\Delta_{ij}} + \frac{1}{2\pi^2\Delta_{ij}^2} = G^{(2)}(m, \Delta_{ij}). && \text{(1.153b)} \end{aligned}$$

The upper limit (1.150) can then be used with either $G^{(1)}(m, \Delta_{ij})$ or $G^{(2)}(m, \Delta_{ij})$. Of course, using the function $G^{(1)}(x, y)$ yields more stringent results than those obtained by using the function $G^{(2)}(x, y)$.

We will discuss more specifically the case of a central potential below but we already write here the upper limit (1.150), using the kernel $G^{(2)}(x, y)$, for this class of potentials. In this way, we introduce some quantities which will be useful later. Integrating over angular variables, the limit (1.150) reads

$$N < \sum_{\nu=0}^{\infty}(2\nu + 1) \int_0^{\infty} dr_1 \dots dr_n \, V^-(r_1) \dots V^-(r_n) \, A_\nu(m, r_1, r_2) \dots A_\nu(m, r_n, r_1), \tag{1.154a}$$

with

$$A_\nu(m, x, y) = \frac{1}{\alpha} \frac{4\pi}{2\nu + 1} \, xy \, a_\nu(m, x, y), \tag{1.154b}$$

and

$$\begin{aligned} a_\nu(m, x, y) &= \frac{m}{2\pi} \, r_<^\nu \, r_>^{-(\nu+1)} + \frac{1}{2\pi^{3/2}} \frac{\Gamma(\nu + 1)}{\Gamma(\nu + 1/2)} \frac{(xy)^\nu}{(x + y)^{2(\nu+1)}} \times \\ &\times \; F\left(\nu + 1, \nu + 1, 2(\nu + 1), \frac{4xy}{(x + y)^2}\right), && \text{(1.154c)} \end{aligned}$$

where $r_< = \min[x, y], r_> = \max[x, y]$ and $F(a, b, c, z)$ is the hypergeometric function.

A simpler upper limit can be obtained with additional approximations in the ultra-relativistic case ($m = 0$). Using n times ($n \geq 4$) the Hölder inequality we obtain

$$\begin{aligned} N &< B(n, p, p') \left[\int_0^{\infty} dr \, r^{2(p-1)/p} \, V^-(r)\right] \left[\int_0^{\infty} dr \, [V^-(r)]^{pp'}\right]^{1/(pp')} \times \\ &\times \left[\int_0^{\infty} dr \, r^{(p'-1)/p'} \, [V^-(r)]^p\right]^{1/p} \left[\int_0^{\infty} dr \, r^{p-1} \, [V^-(r)]^p\right]^{(n-3)/p}, && \text{(1.155a)} \end{aligned}$$

with the constant $B(n, p, p')$ given by

$$B(n, p, p') = \sum_{\nu=0}^{\infty}(2\nu + 1) \, [C(\nu, p/(p - 1))]^{n-1} \, C(\nu, pp'/(p' - 1)), \tag{1.155b}$$

and

$$C(\nu,q) = \frac{1}{\alpha\sqrt{\pi}}\frac{\Gamma(\nu+1)}{2^{2\nu+2}\Gamma(\nu+3/2)}\cdot$$

$$\cdot\left[\int_0^1 dx\,(1+x^{-2})\left(z^{\nu+1}F(\nu+1,\nu+1,2(\nu+1),z)\right)^q\right]^{1/q}, \tag{1.155c}$$

with $z = 4x/(1+x)^2$, $p > 1$ and $p' > 1$. All the complexity of the problem is now located in the calculation of the constant $B(n,p,p')$. Analytical calculations for small values of ν and numerical investigations up to $\nu = 100$ seems to prove that for all values of ν we have

$$C(\nu,2) = 1/(\alpha\sqrt{2\nu+1}), \tag{1.156a}$$

$$C(\nu,3) \leq 1/[\alpha(2\nu+1)^{1/3}]. \tag{1.156b}$$

In this case, we find that $B(n,2,3) \leq (1-2^{-w})\zeta(w)$, with $w = (3n-7)/6$ and $\zeta(x)$ is the Riemann Zeta function. This implies $n \geq 5$ to obtain non-trivial results and in particular $B(5,2,3) \leq 2.172$.

We are now focusing on central potentials. To obtain an upper limit on the number of ℓ-wave bound states of the spinless Salpeter equation, we need to derive the radial expression of the symmetrical kernel (1.149). This can be achieved by performing similar calculations than those done in Ref. [59, p. 2255-2257]. We have (see the original article for more details [34])

$$G_\ell(m,r,r') = \frac{mrr'}{2}\int_0^\pi d\theta'\,\sin\theta'\,\frac{H(m\Delta)}{\Delta}\,P_\ell(\cos\theta'), \tag{1.157}$$

where $H(x)$ is defined by (1.148a) and $P_\ell(\cos\theta)$ are Legendre polynomials. The symmetrical kernel is then given by

$$K_\ell(m,r,r') = [V^-(r)]^{1/2}\,G_\ell(m,r,r')\,[V^-(r')]^{1/2}. \tag{1.158}$$

We can now again use the Birman-Schwinger method, see Appendice 1.3.2, to obtain an upper limit on the number of ℓ-wave bound states. With the help of the majorization (1.152) we have

$$N_\ell < \int_0^\infty dr_1\ldots dr_n\,V^-(r_1)\ldots V^-(r_n)\,T_\ell(m,r_1,r_2)\ldots T_\ell(m,r_n,r_1), \tag{1.159a}$$

with

$$\alpha\,T_\ell(m,r,r') = \frac{1}{\pi}\mathcal{G}_\ell(m,r,r') + \mathcal{S}_\ell(m,r,r'), \tag{1.159b}$$

and

$$\mathcal{G}_\ell(m,r,r') = m\int_{|r-r'|}^{r+r'} dy\,K_1(my)\,P_\ell\left(\frac{r^2+r'^2-y^2}{2rr'}\right), \tag{1.159c}$$

$$\mathcal{S}_\ell(m,r,r') = m\int_{|r-r'|}^{r+r'} dy\, P_\ell\left(\frac{r^2+r'^2-y^2}{2rr'}\right) = \frac{2m}{2\ell+1}\, r_<^{\ell+1}\, r_>^{-\ell}, \tag{1.159d}$$

where $r_< = \min[r,r']$ and $r_> = \max[r,r']$. The kernel $\mathcal{S}_\ell(m,r,r')$ is actually the Green function of the non-relativistic kinetic energy operator and takes a simple form while the kernel $\mathcal{G}_\ell(m,r,r')$ can be calculated analytically for each value of ℓ [58, 59]. We have, here also, introduced in (1.159b) the parameter α which takes the value 1 respectively 2 for one respectively two (identical) particle problems. We can use an additional approximation and majorize $K_1(y)$ by $1/y$. In this case, $T_\ell(m,r,r')$ is replaced by $A_\ell(m,r,r')$, see (1.154b). Note that $T_\ell(0,r,r') = A_\ell(0,r,r')$ since in this limit ($m \to 0$) $mK_1(my) = 1/y$.

Obviously simplifications occur in the ultra-relativistic case ($m = 0$). With the help of the Hölder inequality we obtain

$$\begin{aligned} N_\ell \;&<\; \tilde{B}(n,\ell,p,p')\left[\int_0^\infty dr\, r^{2(p-1)/p}\, V^-(r)\right]\left[\int_0^\infty dr\, [V^-(r)]^{pp'}\right]^{1/(pp')} \times \\ &\times \left[\int_0^\infty dr\, r^{(p'-1)/p'}\, [V^-(r)]^p\right]^{1/p}\left[\int_0^\infty dr\, r^{p-1}\, [V^-(r)]^p\right]^{(n-3)/p}, \end{aligned} \tag{1.160a}$$

with

$$\tilde{B}(n,\ell,p,p') = [C(\ell,p/(p-1))]^{n-1}\, C(\ell,pp'/(p'-1)), \tag{1.160b}$$

and where $n \geq 2$, $p > 1$, $p' > 1$ and $C(\ell,q)$ defined by (1.155c). The upper limit on the total number of bound states that can be obtained from the upper limit on the number of ℓ-wave bound states (1.160) is very similar to the upper limit (1.155) except that the sum would stop at $\ell = L$ (the largest value of the angular momentum ℓ for which bound states do exist) and that n is only restricted to be greater than two!

For some clarity reasons we also gives here a necessary condition for the existence of bound states obtained from (1.160) which allows us to derive an interesting upper limit on the total number of bound states of the spinless Salpeter equation for central potentials.

Taking the limit $n \to \infty$ in the relation (1.160), we obtain the following necessary condition for the existence of at least one ℓ-wave bound state:

$$\int_0^\infty \frac{dr}{r}\, \left[C(\ell,p/(p-1))\, r\, V^-(r)\right]^p \geq 1. \tag{1.161}$$

This simple relation yields a lower limit, $g_{\rm c}^{\rm lo}$, on the (numerically) exact critical value of g, $g_{\rm c}$, for which a first bound state appears, $g_{\rm c} \geq g_{\rm c}^{\rm lo}$ *and* yields an upper limit L^+ on L. We can obtain a simpler expression by considering now the limit $p \to \infty$. We find that a necessary condition for the existence of at least one ℓ-wave bound state is also given by

$$C(\ell,1)\, \mathcal{M} \geq 1, \tag{1.162a}$$

Table 1.2: Values of the function $c(\ell)$, see (1.163), for several values of ℓ. Note that $c(0) = \infty$ and $c(\infty) = \sqrt{2\pi}$.

ℓ	$c(\ell)$	ℓ	$c(\ell)$	ℓ	$c(\ell)$	ℓ	$c(\ell)$
1	3.205	8	2.557	15	2.531	40	2.515
2	2.795	9	2.550	16	2.529	50	2.513
3	2.678	10	2.545	17	2.528	60	2.512
4	2.625	11	2.541	18	2.526	70	2.511
5	2.596	12	2.538	19	2.525	80	2.511
6	2.578	13	2.535	20	2.524	90	2.510
7	2.566	14	2.533	30	2.518	100	2.510

where

$$\mathcal{M} = \max[r\, V^-(r)]. \tag{1.162b}$$

This last necessary condition have only a sense for $\ell > 0$ because $C(0,1)$ diverges. Of course, this does not mean that there always exist bound states for $\ell = 0$. For this value of the angular momentum, one needs to use the relation (1.161) to draw conclusions about existence of bound states. The constant $C(\ell, 1)$ (see (1.155c)) can be rewritten as

$$C(\ell,1) = \frac{1}{\alpha\sqrt{\pi}} \frac{\Gamma(\ell+1)}{\Gamma(\ell+3/2)} \frac{c(\ell)}{\sqrt{2\ell+1}}. \tag{1.163}$$

The interest of this rewritten is that the function $c(\ell)$ varies very slowly with ℓ and can then be easily and usefully tabulated, see Table 1.2. A possible simple majorization of $c(\ell)$ is $c(\ell) < \sqrt{2\pi} + a\ell^b$ with $a = 0.7$ and $b = -1.18$ (valid at least for $1 \leq \ell \leq 100$). Note also that the necessary condition (1.162) is the ultra-relativistic counterpart of the well known non-relativistic necessary condition (see for example [61])

$$(\ell + 1/2)^{-2} \max[r^2\, 2mV^-(r)] \geq 1, \tag{1.164}$$

which yields the non-relativistic upper limit (1.53) on L.

We are now able to obtain an upper limit on the total number of bound states, applicable only to central potentials in the ultra-relativistic regime, which possess the correct g^6 asymptotic behavior. We choose in (1.160) $n = 2$, $p = 2$ and $p' \to \infty$ and with the help of (1.156a) (which is certainly correct up to $\ell = 100$) we obtain

$$N_\ell < \frac{1}{\alpha^2(2\ell+1)}\, \tilde{\mathcal{M}}\, \mathcal{I}, \tag{1.165a}$$

with

$$\tilde{\mathcal{M}} = \max[V^-(r)], \tag{1.165b}$$

$$\mathcal{I} = \int_0^\infty dr\, r\, V^-(r). \tag{1.165c}$$

To some extend, the limit (1.165) is the ultra-relativistic counterpart of the non-relativistic Bargmann-Schwinger upper bound (1.2). The upper limit on N is obtained with a summation over the right-hand side of (1.165a) from $\ell = 0$ to $\ell = L$ taking into account the multiplicity of each ℓ-wave bound states. To this end, an upper limit on L is needed. The best limit, which behaves linearly with the strength of potential, is obtained, not from (1.165a), but instead from the simple relation (1.162). We have

$$N < \frac{1}{\alpha^2}(L^+ + 1)\,\tilde{\mathcal{M}}\,\mathcal{I}. \tag{1.166}$$

The optimal value for L^+ is obtained by solving (1.162) but a neater, if generally less stringent, upper limit L^{++} ($L^+ \leq L^{++}$) is given by

$$L^{++} = \frac{1}{4}\left(\sqrt{1+8s^2} - 1\right) \leq \frac{s}{\sqrt{2}}, \tag{1.167a}$$

with

$$s = \frac{c(1)}{\alpha\sqrt{\pi}}\,\mathcal{M}. \tag{1.167b}$$

The expression (1.167) for the upper limit on L is obtained using (1.162), (1.163) and the second part of the inequalities $\sqrt{x+1} \geq \Gamma[x+3/2]/\Gamma[x+1] \geq \sqrt{x}$ for $x \geq 0$. $c(1)$ could even be replaced by $c(L^{++})$ in (1.167b). The transcendental equation obtained would then be solved very quickly after few iterations thanks to the slow variation of $c(\ell)$ as a function of ℓ. If we believe that the relation (1.156a) is always true for all values of the angular momentum, we can write the asymptotic expression of the upper limit (1.166) when the strength of the potential, g, goes to infinity:

$$N(g \to \infty) < \frac{1}{\alpha^3}\mathcal{M}\,\tilde{\mathcal{M}}\,\mathcal{I}, \tag{1.168}$$

where $c(\infty)$ were used to obtain the asymptotic expression of L^+, $L^+ \approx \mathcal{M}/\alpha$, where the symbol $\approx$ means asymptotic equality. This last expression is useful to compare the upper limit (1.166) with the Daubechies upper limit (1.145) since we clearly have

$$\int_0^\infty dr\, r^2\,[V^-(r)]^3 \leq \mathcal{M}\,\tilde{\mathcal{M}}\,\mathcal{I}. \tag{1.169}$$

This last inequality means that the upper limit (1.145) would always be better than the limit (1.166) if its coefficient was equal to 1. Since the coefficient is greater than unity, $4\pi K = 1.294 > 1$, there is some room for the limit (1.166) to be more stringent. A square-well potential is an example:

$$V(r) = -V_0\,\theta[(R_1 - r)(r - R_2)], \tag{1.170}$$

where $R_2 \geq R_1$ are two arbitrary positive radius and $\theta(x)$ is the step function. When the ratio of the radius, R_1/R_2, is in the interval $[0.4859, 1)$, the upper limit (1.166) is better than the Daubechies upper limit.

Actually, with the upper limit (1.160) on N_ℓ (with $n = 2$) and the upper limit, L^+, on L obtained with (1.162) (or with L^{++}), we have a family of upper limit depending on two parameters p and p' which, being less neat than the limit (1.166), could prove to be more stringent.

1.3 Conditions for the existence of bound states

In Section 1.1, we have reviewed the most relevant results concerning the limits on the number of bound states supported by a central potential $V(r)$. It is well known that, in three dimensions, a critical value, g_c, for strength g of the potential should be reached to obtain a first bound states $g \geq g_c$. Necessary conditions for the existence of at least one bound state are obtained from upper limits on N_0 or N (N is the total number bound states) by setting $N_0 = 1$ or $N = 1$ which yields lower limits on the critical value of g. Similarly, sufficient conditions for the existence of at least one bound state are obtained from lower limits on N_0 or N by setting $N_0 = 1$ or $N = 1$ which yield upper limits on g_c.

As indicated in Section 1.1, an important theorem for classifying the numerous limits on the number of bound states was found by Chadan [14], and generalized by Martin [17], and gives the asymptotic behavior of the number of bound states as the strength, g, of the central potential goes to infinity:

$$N \approx \frac{g^{1/2}}{\pi} \int_0^\infty dr\, v(r)^{1/2} \quad \text{as} \quad g \to \infty, \tag{1.171}$$

where the symbol $\approx$ means asymptotic equality and $V^-(r) = -g\, v(r)$ (note that we use here g as coupling constant instead of g^2 in previous Sections!). This result implies that any upper and lower limit which could yield cogent results should behave asymptotically as $g^{1/2}$. More importantly, the relation (1.171) gives the functional of the potential, that is to say the coefficient in front of $g^{1/2}$, that appears in the asymptotic behavior. Upper and lower limits featuring the correct $g^{1/2}$ dependency was first obtained in the Ref. [6] (see (1.18) and (1.19)). Upper and lower limits featuring the correct asymptotic behavior (1.171) was first derived in Refs. [30, 31] (see (1.50) and (1.52)). In practice, the asymptotic regime is reached very quickly when the strength of the potential is large enough to bind two or three bound states.

The situation is completely different when one consider the transition between 0 and 1 bound state and in particular upper and lower limit on the critical value of the strength of the potential, g_c, for which a first bound state appears. In this case, there is no theorem to know in advance which limit yield the most stringent restriction on g_c. It is then of interest to obtain various limits, since the limit yielding the most stringent restriction change from one potential to another.

In the next Section 1.3.1, we present very recent necessary and sufficient conditions for existence of bound states. In all tests we performed, it appears that, among previously known results, the most stringent necessary conditions for the existence

of bound states is given by the Glaser *et al.* relation (1.29). We will thus only refer to this result to test our new results. The situation is less clear for sufficient conditions but as we will see, we do not need precise comparison in this case. In Section 1.3.2, we present a necessary conditions for existence of bound states applicable to the spinless Salpeter equation for which few results are known.

1.3.1 Non-relativistic quantum mechanics

The necessary conditions for the existence of bound states derived in this section is obtained with the help of a simple extension of the Birman-Schwinger method (see Appendice 1.3.2). The Schrödinger equation for a central potential $V(r)$ reads

$$\left(-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}\right)u_\ell(r)=(E-V(r))\,u_\ell(r). \tag{1.172}$$

The Green function, $G(\Delta)\equiv g_\ell(r,r')$, of the kinetic energy operator (see (1.197)) takes the explicit form

$$g_\ell(r,r')=\frac{1}{2\ell+1}r_<^{\ell+1}\,r_>^{-\ell}, \tag{1.173}$$

where $r_<=\min[r,r']$ and $r_>=\max[r,r']$. The symmetrical kernel $K(\mathbf{r},\mathbf{r}')\equiv K_\ell(r,r')$ (see (1.201)) reads

$$K_\ell(r,r')=[V^-(r)]^{1/2}\,g_\ell(r,r')\,[V^-(r')]^{1/2}. \tag{1.174}$$

The expression of the iterated kernels is given by (see (1.203))

$$K_\ell^{(n)}(s,t)=\int_0^\infty du\;K_\ell(s,u)\,K_\ell^{(n-1)}(u,t), \tag{1.175a}$$

with

$$K_\ell^{(1)}(s,t)\equiv K_\ell(s,t), \tag{1.175b}$$

and $n=1,2,\ldots$. Finally, the upper limits on the number of ℓ-wave bound states reads

$$N_\ell<\int_0^\infty dr\,K_\ell^{(n)}(r,r), \tag{1.176}$$

with $n=1,2,\ldots$.

In his article, Schwinger consider only the case $n=1$ for the equation (1.176) which yields the Bargmann-Schwinger upper limit (1.2). Indeed, greater values of n would yield upper limits which possess a worse dependency on the strength of the potential g than the upper limit (1.2) and which would be very poor for strong potentials. But it appears that, as illustrated below, the larger the value n the better the lower limit on the critical value of strength of the potential.

The necessary conditions for the existence of ℓ-wave bound states obtained from (1.176) read respectively for $n = 1, 2, 3$:

$$\frac{1}{2\ell+1}\int_0^\infty dr\, r\, V^-(r) \geq 1, \tag{1.177}$$

$$\frac{2}{(2\ell+1)^2}\int_0^\infty dr_1\, r_1^{-2\ell}\, V^-(r_1)\int_0^{r_1} dr_2\, r_2^{2\ell+2}\, V^-(r_2) \geq 1, \tag{1.178}$$

$$\frac{6}{(2\ell+1)^3}\int_0^\infty dr_1\, r_1^{-2\ell}\, V^-(r_1)\int_0^{r_1} dr_2\, r_2\, V^-(r_2)\int_0^{r_2} dr_3\, r_3^{2\ell+2}\, V^-(r_3) \geq 1, \tag{1.179}$$

The improvements of the lower limits on g_c implied by the relations (1.178) and (1.179) over the lower limit inferred by the well known relation (1.177) are illustrated below for a square-well potential and an exponential potential.

The sufficient condition is obtained with the help of a generalization of the comparison theorem proved recently and where the comparison potentials intersect (Theorem 7 of Ref. [62]). The new theorem reads

Theorem. *If two monotonic potentials $V_1(r)$ and $V_2(r)$ cross twice for $r > 0$ at $r = r_1, r_2$ $(r_1 < r_2)$ with*

$$(i)\quad V_1(r) < V_2(r) \quad for \quad 0 < r < r_1 \quad and$$
$$(ii)\quad \int_0^{r_2} dy\,[V_1(y) - V_2(y)]\, y^2 \leq 0,$$

then $E_1 < E_2$, where $E_{1,2}$ are the ground states of the potentials $V_{1,2}(r)$.

As comparison potential $V_2(r)$, we choose a simple square-well

$$V_2(r) = -V_0\,\theta(R - r), \tag{1.180}$$

where $\theta(x)$ is the step function. Moreover, we choose this potential such as a zero-energy bound state exists: $V_0R^2 = \pi^2/4$. This implies that the potential $V_1(r)$ possesses at least one bound state. For this particular choice of $V_2(r)$ we have $r_2 = R$. We write the potential $V_1(r)$ under the form

$$V_1(r) = -gs^{-2}\, v(r/s, k), \tag{1.181}$$

where k are the other parameters of the potential. The hypothesis (ii) above yields the following upper bound g_c^up on the critical coupling constant g_c

$$g_\mathrm{c}^\mathrm{up} = \frac{\pi^2}{12}\,\frac{\alpha}{\int_0^\alpha dy\, y^2\, v(y,k)}, \tag{1.182}$$

where $\alpha = R/s$. The best restriction is obviously obtained with the value of α minimizing the right-hand side of (1.182). The upper limit can thus be written as

$$g_\mathrm{c}^\mathrm{up} = \frac{\pi^2}{12}\,\frac{1}{\alpha^2\, v(\alpha,k)}, \tag{1.183a}$$

where α is the unique solution of

$$\int_0^\alpha dy\, y^2\, v(y,k) = \alpha^3 v(\alpha,k). \tag{1.183b}$$

The definition (1.183b) of α has a simple geometric significance which implies that $\alpha > \max[y^2 v(y,k)]$.

Obviously, we have used a very particular comparison potential $V_2(r)$ to write a neat formula for the upper limit on the critical coupling constant g_c. In practice, a better upper limit could be obtained by the use of a more appropriate comparison potential for which the exact value of the critical coupling constant is known (and for which the conditions (i) and (ii) apply!).

We propose now to test these necessary and sufficient conditions for existence of bound states. The first potential we consider to test the limits is a square-well potential that we write in the convenient form

$$V(r) = -gR^{-2}\,\theta(1 - r/R). \tag{1.184}$$

The sufficient condition (1.183), applicable only for $\ell = 0$, is saturated for this potential (with $\alpha = 1$) and thus leads to the exact result. The necessary conditions (1.177)-(1.179) give the following lower limits

$$g_c^{\rm lo} = 2(2\ell+1), \tag{1.185}$$
$$g_c^{\rm lo} = (2\ell+1)[2(2\ell+3)]^{1/2}, \tag{1.186}$$
$$g_c^{\rm lo} = (2\ell+1)[(2\ell+3)(2\ell+5)]^{1/3}. \tag{1.187}$$

The comparison between the new lower limits on g_c, the limit (1.29) and the exact results is reported in Table 1.3 and shows that the new limits are quite cogent and converge quickly to the exact result especially for small value of ℓ.

The last test is performed with an exponential potential written as

$$V(r) = -gR^{-2}\,\exp(-r/R). \tag{1.188}$$

For $\ell = 0$, the sufficient condition (1.183) leads to $g_c^{\rm up} = 2.118$ while the exact result is given by $g_c = z_0^2/4 \cong 1.4458$ ($z_0 = 2.4048$ is the first zero of the Bessel function $J_0(x)$). The upper limit is not very stringent for this potential because the comparison potential that we choose (a square-well) is very different from an exponential potential. The upper limit yields more cogent result, for example, for a Wood-Saxon potential. For an exponential potential a better upper limit can be obtained with the Calogero lower bound (1.22): $g_c^{\rm up} = 1.677$.

The comparison between the news lower limits on g_c, the limit (1.29) and the exact result is reported in the Table 1.4. The new lower limits on g_c are quite cogent and converge quickly to the exact results especially for small value of ℓ, but this convergence is slower than in the case of a square-well potential.

Table 1.3: Comparison between the exact values of the critical coupling constant g_c of a square-well potential for various values of ℓ and the lower limits, $g_c^{lo} \leq g_c$, obtained with the relations (1.185)-(1.187), the lower limit obtained with the relation (1.176) with $n = 4$ and $N_\ell = 1$ (calculated numerically) and the lower limit obtained with the formula (1.29) (with the optimal value of p).

ℓ	$n = 1$	$n = 2$	$n = 3$	$n = 4$	Eq. (1.29)	Exact
0	2	2.4495	2.4662	2.4672	2.3593	2.4674
1	6	9.4868	9.8132	9.8592	9.1220	9.8696
2	10	18.708	19.895	20.120	18.454	20.191
3	14	29.699	32.383	32.981	30.245	33.217
4	18	42.214	47.064	48.272	44.425	48.831
5	22	56.089	63.788	65.868	60.947	66.954

Table 1.4: Comparison between the exact values of the critical coupling constant g_c of an exponential potential for various values of ℓ and the lower limits, $g_c^{lo} \leq g_c$, obtained with the relations (1.185)-(1.187), the lower limit obtained with the relation (1.176) with $n = 4$ and $N_\ell = 1$ (calculated numerically) and the lower limit obtained with the formula (1.29) (with the optimal value of p).

ℓ	$n = 1$	$n = 2$	$n = 3$	$n = 4$	Eq. (1.29)	Exact
0	1	1.4142	1.4422	1.4453	1.4383	1.4458
1	3	6.2700	6.8546	6.9913	7.0232	7.0491
2	5	13.145	15.257	15.804	16.277	16.313
3	7	21.593	26.265	27.364	29.218	29.259
4	9	31.363	39.616	41.296	45.849	45.893
5	11	42.297	55.120	57.480	66.173	66.219

1.3.2 Semi-relativistic quantum mechanics

As explained in Section 1.2.2, results for the Klein-Gordon equation can be obtained from results applicable to Schrödinger with the help of a simple correspondence, see (1.142). We will then discuss here results concerning the spinless Salpeter equation. Actually the relevant necessary conditions have essentially been given in Section 1.2.2 but we recall them explicitely here for completeness and for a potential written as $V(r) = -gR^{-1}v(r/R)$. We also perform some tests of these formulas.

The first necessary condition is obtained from the Daubechies upper limit and reads

$$4\pi K g^3 \int_0^\infty dx\, x^2 \left[v(x)(v(x) + 2\beta/g)\right]^{3/2} > 1, \tag{1.189}$$

with $K = 0.239$ for arbitrary values of m, $K = 0.103$ for $m = 0$ and where $\beta = mR$.

The second necessary condition is derived from the upper limit (1.159) with $\ell = 0$

$$\frac{g^2}{(\pi\alpha)^2} \int_0^\infty dx\, v(x) \int_0^\infty dy\, v(y) \times$$
$$\times \left[(K_0(\beta|x-y|) - K_0(\beta(x+y))) + \pi\beta(x+y-|x-y|)\right]^2 > 1. \tag{1.190}$$

Simplifications obviously occur in the case of a vanishing mass and the limit reads

$$\frac{g^2}{(\pi\alpha)^2} \int_0^\infty dx\, v(x) \int_0^\infty dy\, v(y)\, \ln^2 \left|\frac{x+y}{x-y}\right| > 1. \tag{1.191}$$

The third necessary condition is only applicable in the ultra-relativistic regime ($m = 0$) is (see (1.161))

$$\int_0^\infty \frac{dr}{r}\, \left[C(\ell, p/(p-1))\, r\, V^-(r)\right]^p \geq 1. \tag{1.192}$$

The last necessary condition is also only applicable in the ultra-relativistic regime ($m = 0$) and for $\ell > 0$ reads (see (1.162))

$$C(\ell, 1)\, \mathcal{M} \geq 1, \tag{1.193a}$$

where

$$\mathcal{M} = \max[r\, V^-(r)]. \tag{1.193b}$$

We test these limits with two simple central potentials. This first one is an exponential potential

$$v(x) = \exp(-x). \tag{1.194}$$

The second one is a Pöschl-Teller potential

$$v(x) = \frac{1}{\cosh^2 x}. \tag{1.195}$$

Table 1.5: Comparison, for the exponential and the Pöschl-Teller potentials, between the lower limit g_c^{lo} on the critical values g_c yielded by the limits (1.190) and (1.191), the lower limit $g_{c,D}^{lo}$, of g yielded by the Daubechies upper limit (1.189) and the exact critical value g_c, obtained by solving numerically the spinless Salpeter equation.

	Exponential			Pöschl-Teller		
β	g_c^{lo}	$g_{c,D}^{lo}$	g_c	g_c^{lo}	$g_{c,D}^{lo}$	g_c
0	4.443	4.370	5.574	4.126	3.886	5.008
1	1.223	0.6574	1.361	1.512	0.8631	1.742
2	0.6739	0.3374	0.7133	0.8912	0.4582	0.9598
3	0.4604	0.2261	0.4804	0.6233	0.3092	0.6549
4	0.3487	0.1698	0.3616	0.4769	0.2329	0.4956
5	0.2803	0.1360	0.2898	0.3854	0.1867	0.3981

The comparison between the (numerically) exact results, g_c, and the lower limits on g_c, obtained from (1.189), (1.190) and (1.191) is displayed in Table 1.5 for a two-particles problem ($\alpha = 2$). The results obtained with the upper limits (1.190) and (1.191) are rather satisfactory especially when β is large and are always better than the results obtained with the Daubechies upper limit (1.189).

We can also test the necessary condition (1.192) (valid only when $m = 0$) for $\ell = 0$ by the computation of g_c^{lo}. we obtain $g_c^{lo} = 4$ for the exponential potential and $g_c^{lo} = 3.685$ for the Pöschl-Teller potential.

We also test the relations (1.192) and (1.193) by computing the lower limit g_c for $\ell > 0$ with the potentials (1.194) and (1.195). The comparison of these lower limits with the (numerically) exact critical coupling constant is given in the Table 1.6. The lower limits yielded by the relation (1.192) are always better than those obtained with the relation (1.193) but the differences become smaller as ℓ grows. These lower limits are quite satisfactory compared to the exact results and the relative differences between these quantities decrease from 22% to 10% for ℓ increasing from 1 to 5 for both potentials.

To conclude, we compare the upper limit, L^+, obtained with (1.193), with the exact largest value, L, of the angular momentum for which bound states do exist. The results obtained for an exponential and the Pöschl-Teller potential are reported in the Table 1.7. The bounds on L obtained with (1.193) are very stringent for both potentials. These excellent results are not so surprising since the same strong limitations on L are obtained with the non-relativistic counterpart of (1.193) (see (1.53)).

Table 1.6: Comparison, for the exponential and the Pöschl-Teller potentials, between the lower limit on the critical values g_c yielded by the limits (1.192) ($g_{c,I}^{lo}$) and (1.193) ($g_{c,II}^{lo}$) and the exact critical value g_c, obtained by solving numerically the spinless Salpeter equation.

	Exponential			Pöschl-Teller		
ℓ	$g_{c,I}^{lo}$	$g_{c,II}^{lo}$	g_c	$g_{c,I}^{lo}$	$g_{c,II}^{lo}$	g_c
1	8.524	6.922	10.98	7.437	5.687	9.545
2	13.67	12.81	16.39	11.59	10.53	14.04
3	19.03	18.46	21.81	15.91	15.17	18.52
4	24.44	24.02	27.24	20.30	19.73	22.99
5	29.88	29.53	32.67	24.73	24.27	27.46

Table 1.7: Comparison, for the exponential and the Pöschl-Teller potentials, between the upper limit, L^+, obtained with (1.193), with the exact largest value, L, (obtained by solving numerically the spinless Salpeter equation) of the angular momentum for which bound states do exist.

	Exponential		Pöschl-Teller	
g	L^+	L	L^+	L
10	1	0	1	1
20	3	2	4	3
30	5	4	6	5
40	6	6	8	7
50	8	8	10	10
100	17	17	21	21
150	27	26	33	32
200	36	35	44	43

Appendix A: Birman-Schwinger method

Birman [3] and Schwinger [4] have shown how to obtain an upper limit on the number of bound states once the Green function of the kinetic energy operator of a wave equation is known. In this section, we recall briefly the main line of the method; for more details see the original articles [3, 4].

Let $T\left(\vec{p}^{\,2}\right)$ be a general kinetic energy operator and let

$$\left[T\left(\vec{p}^{\,2}\right) + V(\vec{r})\right]\Psi(\vec{r}) = E\,\Psi(\vec{r}) \tag{1.196}$$

be the wave equation, in three dimensions, that satisfy the wave function $\Psi(\vec{r})$ (eigenstates) and where E is the energy (eigenvalues). Let $G(\Delta)$ be the Green function of $T\left(\vec{p}^{\,2}\right)$:

$$T\left(\vec{p}^{\,2}\right)G(\Delta) = \delta^3(\vec{\Delta}\,), \tag{1.197}$$

where $\vec{\Delta} = \vec{r} - \vec{r}\,'$, $\Delta = |\vec{\Delta}|$ and $\delta^3(\vec{x}\,)$ is the Dirac function. We can write (1.196), with $E = 0$, using this Green function as

$$\Psi(\vec{r}) = -\int d\vec{r}\,'\,G(\Delta)\,V(\vec{r}\,')\,\Psi(\vec{r}\,'). \tag{1.198}$$

Since the purpose of the method is to obtain an upper limit on the number of bound states, we can replace $V(\vec{r})$ by $-V^-(\vec{r})$ where $V^-(\vec{r})$ is the negative part of the potential obtained by setting the positive part of the potential equal to zero. Indeed, a decrease of the potential in some region must lower the energies of the bound states and therefore cannot lessen their number. Moreover, we introduce the parameter $0 < \lambda \leq 1$ by the substitution $V^-(\vec{r}) \to \lambda V^-(\vec{r})$. As λ increases from 0, we reach a critical value, λ_1, at which a bound state first appears with a vanishing binding energy, $E = 0$. With further growth of λ, the energy of this state decreases until we reach a second critical value, λ_2, at which a second bound state appears and so on. When λ has attained the value unity and, $\lambda_N \leq 1 < \lambda_{N+1}$, there are N bound states.

We now introduce, to obtain a symmetrical kernel, a new wave function as

$$\Phi(\vec{r}) = [V^-(\vec{r})]^{1/2}\,\Psi(\vec{r}). \tag{1.199}$$

The equation (1.198) becomes

$$\Phi(\vec{r}) = \lambda\int d\vec{r}\,'\,K(\vec{r},\vec{r}\,')\,\Phi(\vec{r}\,'), \tag{1.200}$$

where $K(\vec{r},\vec{r}\,')$ is given by

$$K(\vec{r},\vec{r}\,') = [V^-(\vec{r})]^{1/2}\,G(\Delta)\,[V^-(\vec{r}\,')]^{1/2}. \tag{1.201}$$

If the kernel is positive, we have $0 < \lambda_1 < \lambda_2 < \cdots < \lambda_N \leq 1$ and $0 < \lambda_k < \infty$ (λ_k denotes each eigenvalue of (1.200)). It is well known that the trace of the iterated kernels equals the sum of the eigenvalues of the integral equation (1.200) as follow

$$\sum_{k=1}^{\infty} \frac{1}{(\lambda_k)^n} = \int d\vec{r}\, K^{(n)}(\vec{r}, \vec{r}), \tag{1.202}$$

where the iterated kernel $K^{(n)}(\vec{s}, \vec{t})$ is given by

$$K^{(n)}(\vec{s}, \vec{t}) = \int d\vec{u}\, K(\vec{s}, \vec{u}\,)\, K^{(n-1)}(\vec{u}, \vec{t}), \tag{1.203a}$$

with

$$K^{(1)}(\vec{s}, \vec{t}) \equiv K(\vec{s}, \vec{t}), \tag{1.203b}$$

and $n = 1, 2, \ldots$. Now it is plain that the following inequalities hold

$$\sum_{k=1}^{\infty} \frac{1}{(\lambda_k)^n} \geq \sum_{k=1}^{N} \frac{1}{(\lambda_k)^n} > N, \tag{1.204}$$

where N is the number of bound states. From (1.202), (1.203) and (1.204) we find that an upper limit on the total number of bound states of the wave equation (1.196) is given by

$$N < \int d\vec{r}\, K^{(n)}(\vec{r}, \vec{r}). \tag{1.205}$$

Appendix B: Proof of the lower bound on $|V(q)|$

¿From the definition (1.50c) of q we have

$$\frac{\pi}{2} = \int_q^{\infty} dr\, |V(r)|^{1/2} \equiv \int_q^{\infty} dr\, \frac{|V(q)|^{1/2}}{[V'(r)]^{1/\beta}}\, [V'(r)]^{1/\beta}. \tag{1.206}$$

Now we use the Hölder inequality with $1/\alpha + 1/\beta = 1$, $\alpha > 1$. We obtain

$$\frac{\pi}{2} \leq \left[\int_q^{\infty} dr\, \frac{|V(q)|^{1/2}}{[V'(r)]^{1/\beta}} \right]^{\frac{1}{\alpha}} \left[\int_q^{\infty} dr\, V'(r) \right]^{\frac{1}{\beta}}. \tag{1.207}$$

The last integral is equal to $|V(q)|$ and knowing that $\beta = \alpha/(\alpha - 1)$, we obtain the lower bound (1.51).

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