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Critical strength of attractive central potentials

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Abstract

We obtain several sequences of necessary and sufficient conditions for the existence of bound states applicable to attractive (purely negative) central potentials. These conditions yield several sequences of upper and lower limits on the critical value, $g_c^{(\ell)}$, of the coupling constant (strength), g , of the potential, $V(r) = -gv(r)$, for which a first ℓ -wave bound state appears, which converges to the exact critical value.

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1. Introduction

Since the pioneering works of Jost and Pais in 1951 [1] and Bargmann in 1952 [2], the determination of upper and lower limits on the number of bound states of a given potential, having spherical symmetry $V(r)$, in the framework of non-relativistic quantum mechanics is still of interest. A fairly large number of results of this kind can be found in the literature for the Schrödinger equation (see, for example, [3–18]) and for results applicable to one and two dimension spaces (see, for example, [19–23]).

An important theorem for classifying these results was found by Chadan [8] and gives the asymptotic behaviour of the number of ℓ -wave bound states as the strength, g , of the central potential $V(r) = gv(r)$ goes to infinity:

$$N_\ell \approx \frac{g^{1/2}}{\pi} \int_0^\infty dr v^-(r)^{1/2} \quad \text{as } g \rightarrow \infty, \quad (1)$$

where the symbol \approx means asymptotic equality, $V^-(r) = gv^-(r)$ and $v^-(r) = \max(0, -v(r))$ (see also [24] for a generalization of relation (1)). This result implies that any upper and lower limit on N_ℓ which could yield cogent results should behave asymptotically as $g^{1/2}$. More importantly, relation (1) gives the functional of the potential, that is to say, the coefficient in front of $g^{1/2}$ that appears in the asymptotic behaviour. Upper and lower limits on the number

of ℓ -wave bound states featuring the correct $g^{1/2}$ dependency was first obtained in [6]. Upper and lower limits on N_ℓ featuring the correct asymptotic behaviour (1) was first derived in [17, 18]. 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 considers the transition between zero and one bound state. In contrast to one and two dimension cases where any attractive potential, satisfying adequate integrability conditions, has at least one bound state, in the three-dimensional case, the potential acquires a bound state only if it is attractive (negative) enough. Thus, for central potential, for example, there exists a ‘critical’ value, $g_c^{(\ell)}$, of the coupling constant (strength), g , of the potential, $V(r) = gv(r)$, for which a first ℓ -wave bound state appears. The determination of this critical value requires to solve the zero energy Schrödinger equation [3, 25, 26]. To circumvent the exact calculation of the Jost function at zero energy, upper and lower bounds are very helpful. From now on, use will be made of the standard quantum-mechanical units $\hbar = 2\mu = 1$ where μ is the reduced mass of the particles.

In 1976, Glaser *et al* obtained a strong necessary condition for the existence of a ℓ -wave bound state in an arbitrary central potential in three dimensions [9]:

$$(\forall p \geq 1) \quad \frac{(p-1)^{p-1} \Gamma(2p)}{(2\ell+1)^{2p-1} p^p \Gamma^2(p)} \int_0^\infty \frac{dr}{r} [r^2 V^-(r)]^p \geq 1. \quad (2)$$

This relation yields a lower limit on the critical value $g_c^{(\ell)}$, by making a minimization over $p \geq 1$, which was shown to be very accurate (see, for example, [9, 16, 28]).

Other necessary conditions for the existence of bound states can be found in the literature (see, for example, [7, 11, 28] and for reviews see [10, 17, 18]), but in general, the relation (2) yields the strongest restriction on $g_c^{(\ell)}$ (in some cases, the relations obtained in [28] can, however, be better).

Sufficient conditions for the existence of bound states, yielding upper limits on the critical value of the strength of the potential, are scarcer. Two sufficient conditions for the existence of at least one bound state with angular momentum ℓ have been found by Calogero in 1965 [5, 6]

$$(\forall R > 0) \quad \int_0^R dr r |V(r)| (r/R)^{2\ell+1} + \int_R^\infty dr r |V(r)| (r/R)^{-(2\ell+1)} > 2\ell + 1, \quad (3)$$

and

$$(\forall R > 0) \quad R \int_0^\infty dr |V(r)| [(r/R)^{2\ell} + (r/R)^{-2\ell} R^2 |V(r)|]^{-1} > 1. \quad (4)$$

These two conditions apply provided the potential is nowhere positive, $V(r) = -|V(r)|$. The most stringent conditions are obtained by minimizing the left-hand sides of (3) and (4) over all positive values of R . Some other sufficient conditions for the existence of bound states can be found in the literature (see, for example, [16, 28] and for reviews see [10, 17, 18]). A sufficient condition which does not require the spherical symmetry for the potential V was proposed in 1980 by Chadan [29] (see also [30]). When the potential is central and purely attractive, the inequality

$$\text{Tr } K^{(2)} \geq \text{Tr } K^{(1)}, \quad (5)$$

where

$$\begin{aligned} K^{(1)}(r, r') &= \inf(r, r')^{\ell+1} \sup(r, r')^{-\ell} V(r') \\ K^{(n)}(r, r') &= \int_0^\infty ds K^{(1)}(r, s) K^{(n-1)}(s, r'), \end{aligned} \quad (6)$$

implies the existence of at least a bound state for the potential $V(r)$. In the case where $V(r)$ has some changes of sign, condition (5), is replaced by

$$\text{Tr } K^{(4)} \geq \text{Tr } K^{(2)}, \quad (7)$$

which implies that one of the potentials $\pm V(r)$ has at least one bound state.

Recently, an upper limit on the critical strength has been found, originating from a variational technique [31]:

$$g_c^{(\ell)} \leq \lambda \int_0^\infty dx F(2p-1; x) \left[\int_0^\infty dy F(p; y) y^{-\lambda} \int_0^y dz F(p; z) z^\lambda \right]^{-1}, \quad (8)$$

with $F(q; x) = x^q v(x)^{(q+1)/2}$, $v(x) \geq 0$, $\lambda = \ell + 1/2$ and $q > 0$ which was found to be very accurate. Clearly more accurate upper limits could be obtained but depending strongly on the choice of the trial wavefunction.

This paper follows a different scheme. To circumvent the difficulty to guess a trial (strongly potential dependent) wavefunction for variational methods we propose upper and lower limits originating from iterative procedures, all designed to converge towards the exact result. The methods proposed by Chadan enter this category of iterative convergent procedures. Also, Lassaut and Lombard [16] worked in this sense some years ago, but the procedure was constrained by the condition $g_c^{(\ell)} \int_0^\infty dr r |V(r)| < 2(2\ell + 1)$, which is not verified when the convexity of the potential is too high or when the angular momentum ℓ increases. We thus propose in this paper sequences of upper and lower limits of the critical value, $g_c^{(\ell)}$, which converge towards the critical coupling constant without any restriction on the possible values of $g_c^{(\ell)}$. The advantage of our procedure, based upon the Riesz theorem [32, 33] in what concerns the upper limits, is that there is no need to start from a conveniently chosen wavefunction. Indeed, the improvements are simple for these sequences: one just needs to calculate the next order. Note that the basic idea of sequences of lower limits for $g_c^{(\ell)}$ have already been explored in [28].

The paper is organized as follows. In section 2 we derive the upper limits on the critical value $g_c^{(\ell)}$. In section 3 the algorithm for generating both lower and upper limits is discussed. In section 4 our proposal of upper and lower bounds are tested against the exact values for common potentials. Our conclusions are presented in section 5.

2. Upper limits on the critical strength

From now on, we assume that $V(r)$ is locally integrable and such that

$$\int_0^\infty dr r |V(r)| < \infty, \quad (9)$$

remembering that we consider purely attractive potentials namely satisfying $V(r) \leq 0$. Following Birman and Schwinger [3, 25, 26] the critical values of the strength of the potential correspond to the occurrence of an eigenstate with a vanishing energy. In this paper we consider the zero energy Schrödinger equation that we write into the form of an integral equation incorporating the boundary conditions

$$u_\ell(r) = - \int_0^\infty dr' g_\ell(r, r') V(r') u_\ell(r'), \quad (10)$$

where $g_\ell(r, r')$ is the Green function of the kinetic energy operator and is explicitly given by

$$g_\ell(r, r') = \frac{1}{2\ell + 1} r_{<}^{\ell+1} r_{>}^{-\ell}, \quad (11)$$

where $r_< = \inf(r, r')$ and $r_> = \sup(r, r')$. An important technical difficulty appears if the potential possesses some changes of sign (see relation (12) below). This is overcome for the derivation of necessary conditions, or of upper bounds on the number of bound states, by replacing the potential by its negative part $V(r) \rightarrow V^-(r) = \max(0, -V(r))$. Indeed, the potential $V^-(r)$ is more attractive than $V(r)$ and thus a necessary condition for the existence of bound states in $V^-(r)$ is certainly a valid necessary condition for $V(r)$. This procedure can no longer be used to obtain sufficient conditions. For this reason we consider potentials that are nowhere positive, $V(r) = -gv(r)$, with $v(r) \geq 0$.

To obtain a symmetrical kernel we now introduce the function $\psi_\ell(r)$ as follows

$$\psi_\ell(r) = \sqrt{v(r)}u_\ell(r). \quad (12)$$

Equation (10) becomes

$$\psi_\ell(r) = g \int_0^\infty dr' K_\ell(r, r')\psi_\ell(r'), \quad (13)$$

where the symmetric kernel $K_\ell(r, r')$ is given by

$$K_\ell(r, r') = \sqrt{v(r)}g_\ell(r, r')\sqrt{v(r')}. \quad (14)$$

Relation (13) is thus an eigenvalue problem with a symmetric kernel and, for each value of ℓ , the smallest characteristic numbers are just the critical values $g_c^{(\ell)}$. The higher characteristic numbers correspond to the critical values of the strength for which a second, a third, \dots , ℓ -wave bound state appears. The kernel (14) acting on the Hilbert space $L^2(\mathbb{R})$ is a Hilbert–Schmidt kernel [34] for the class of potentials defined by (9), i.e. satisfies the inequality

$$\int_0^\infty \int_0^\infty dx dy K_\ell(x, y)K_\ell(x, y) < \infty. \quad (15)$$

Consequently the eigenvalue problem (13) always possesses at least one characteristic number [35] (in general, this problem has an infinity of characteristic numbers).

We propose now to solve the eigenvalue problem (13) using iterative methods.

2.1. Iterative power method

Let us write, for simplicity, relation (13) under the form

$$\psi_\ell = g\mathcal{K}_\ell\psi_\ell, \quad (16)$$

where \mathcal{K}_ℓ denotes the symmetric linear operator, operating on the Hilbert space $L^2(\mathbb{R})$, which is in this paper the integral operator generated by the so-called Birman–Schwinger [3, 25] kernel K_ℓ , equation (14).

Since the kernel $K_\ell(r, r')$ is Hilbert–Schmidt, \mathcal{K}_ℓ is a compact operator [27]. As \mathcal{K}_ℓ is symmetric the Riesz theorem applies [32, 33]. For *each* value of the angular momentum ℓ , the set of eigenvalues $1/g_p$, $1 \leq p$, (which in the present case are all positive) can be ordered according to a sequence tending to zero, $1/g_1 \geq 1/g_2 \geq \dots \geq 1/g_p \geq \dots \geq 0$. There exists an orthonormal basis in $L^2(\mathbb{R})$, labelled by $\varphi_p(r)$, $p \geq 1$, each $\varphi_p(r)$ being associated with $1/g_p$, and for each function $\phi_\ell(r) \in L^2(\mathbb{R})$

$$\mathcal{K}_\ell\phi_\ell = \sum_{p=1}^{\infty} \langle \mathcal{K}_\ell\phi_\ell | \varphi_p \rangle \varphi_p = \sum_{p=1}^{\infty} \langle \phi_\ell | \mathcal{K}_\ell \varphi_p \rangle \varphi_p = \sum_{p=1}^{\infty} \frac{1}{g_p} \langle \phi_\ell | \varphi_p \rangle \varphi_p, \quad (17)$$

where the symbol $\langle f | g \rangle$ denotes the scalar product $\int_0^\infty dr f(r)g(r)$. For the sake of simplicity we have dropped the indices (ℓ) which should appear on g_p and on $\varphi_p(r)$.

The positivity of the eigenvalues originates [33] from the fact that \mathcal{K}_ℓ is positive i.e.

$$(\forall \phi_\ell \in L^2(\mathbb{R})) \quad \langle \phi_\ell | \mathcal{K}_\ell \phi_\ell \rangle \geq 0. \tag{18}$$

In the present case, where the potential has the spherical symmetry, there is no degeneracy and we have strict inequalities for the eigenvalues

$$\frac{1}{g_1} > \frac{1}{g_2} > \dots > \frac{1}{g_p} > \dots > 0. \tag{19}$$

This is due to the fact that the eigenstates are solutions of a linear second order equation with constraints at the origin and infinity.

Now, we introduce the iterated kernel $K_\ell^{(n)}(s, t)$ of $K_\ell(s, t)$

$$K_\ell^{(n)}(s, t) = \int_0^\infty du K_\ell(s, u) K_\ell^{(n-1)}(u, t) \quad n \geq 2, \tag{20}$$

with

$$K_\ell^{(1)}(s, t) = K_\ell(s, t). \tag{21}$$

We can then compute the scalar product between ϕ_ℓ and $\mathcal{K}_\ell^{(n)}\phi_\ell$, and find

$$\langle \phi_\ell | \mathcal{K}_\ell^{(n)} \phi_\ell \rangle = \langle \mathcal{K}_\ell^{(n)} \phi_\ell | \phi_\ell \rangle = \sum_{p=1}^\infty \frac{1}{g_p^n} \langle \phi_\ell | \varphi_p \rangle^2. \tag{22}$$

Therefore, we obtain the following convexity-type relation:

$$\begin{aligned} \langle \phi_\ell | \mathcal{K}_\ell^{(n+1)} \phi_\ell \rangle \langle \phi_\ell | \mathcal{K}_\ell^{(n-1)} \phi_\ell \rangle - \langle \phi_\ell | \mathcal{K}_\ell^{(n)} \phi_\ell \rangle^2 &= \sum_{p < q=1}^\infty \frac{1}{(g_p g_q)^{n-1}} \left(\frac{1}{g_p} - \frac{1}{g_q} \right)^2 \langle \phi_\ell | \varphi_p \rangle^2 \langle \phi_\ell | \varphi_q \rangle^2, \\ &\geq 0. \end{aligned} \tag{23}$$

Since the left-hand side of this latter equality is positive we conclude that the sequence

$$n \mapsto \delta_n = \frac{\langle \phi_\ell | \mathcal{K}_\ell^{(n+1)} \phi_\ell \rangle}{\langle \phi_\ell | \mathcal{K}_\ell^{(n)} \phi_\ell \rangle} \quad n \geq 1, \tag{24}$$

with

$$\delta_0 = \frac{\langle \phi_\ell | \mathcal{K}_\ell \phi_\ell \rangle}{\langle \phi_\ell | \phi_\ell \rangle}, \tag{25}$$

is always *increasing*.

On the other hand, taking into account (22) and (24) we have

$$\delta_n = \frac{1}{g_1} \frac{\sum_{p=1}^\infty \left(\frac{g_1}{g_p}\right)^{n+1} \langle \phi_\ell | \varphi_p \rangle^2}{\sum_{p=1}^\infty \left(\frac{g_1}{g_p}\right)^n \langle \phi_\ell | \varphi_p \rangle^2}. \tag{26}$$

Due to the strict inequalities (19) and the Parseval formula

$$\|\phi_\ell\|_2^2 = \sum_{p=1}^\infty \langle \phi_\ell | \varphi_p \rangle^2, \tag{27}$$

the sequence δ_n converges to $1/g_1$, where $g_1 = g_c^{(\ell)}$ is the lowest critical value of the coupling constant of the potential, except when $\langle \phi_\ell | \varphi_1 \rangle$ is zero. This procedure, known in the literature as the iterated power method, yields the maximal eigenvalue of the problem considered, i.e. in the present case to the lowest critical value $g_c^{(\ell)} = g_1$. Any starting positive (non-zero) squared integrable function $\phi_\ell(r)$ is appropriated. Indeed the function $\varphi_1(r)$ has no node which ensures that the scalar product $\langle \phi_\ell | \varphi_1 \rangle$ is not zero. (In our numerical studies, presented in section 4 use is made of the choice $\phi_\ell(r) = r^{\ell+1} \sqrt{v(r)}$). Moreover since $n \mapsto \delta_n$ is increasing we get upper bounds for $g_c^{(\ell)}$ namely $g_c^{(\ell)} < \dots < 1/\delta_p < \dots < 1/\delta_2 < 1/\delta_1$.

There exist other iterative methods in the literature and we discuss briefly two variants of them in the following two sections.

2.2. Kellogg's method

In this section, we consider the method proposed by Kellogg for the compact operator \mathcal{K}_ℓ [36, 33]. We construct the following sequence of functions:

$$\phi_\ell^{(n+1)}(r) = \int_0^\infty dr' K_\ell(r, r') \phi_\ell^{(n)}(r'), \tag{28}$$

where $K_\ell(r, r')$ is given by (14). This latter relation is schematically written as

$$\phi_\ell^{(n+1)} = \mathcal{K}_\ell \phi_\ell^{(n)}. \tag{29a}$$

For non-zero $\phi_\ell^{(0)}(r)$, Kellogg considers the following sequence of numbers:

$$\gamma_{n+1} = \frac{\|\phi_\ell^{(n)}\|_2}{\|\phi_\ell^{(n+1)}\|_2} \quad n \geq 1, \tag{29b}$$

where $\|\phi_\ell^{(n)}\|_2$ is the L^2 norm of the function $\phi_\ell^{(n)}(r)$.

We keep our conventions namely $\varphi_1(r), \varphi_2(r), \dots$, still denote the eigenfunctions of problem (16) and $g_1 < g_2 < \dots$ are the corresponding characteristic numbers.

Suppose that $\phi_\ell^{(0)}(r)$ is orthogonal to the functions $\varphi_1(r), \varphi_2(r), \dots, \varphi_{k-1}(r)$ but not orthogonal to the function $\varphi_k(r)$. Then the sequence γ_n converges towards g_k with the property that $g_k \leq \gamma_n$. Moreover the sequence of functions $\phi_\ell^{(n)}(r)/\|\phi_\ell^{(n)}\|_2$ converges to $\varphi_k(r)$ in $L^2(\mathbb{R})$ [33]. Consequently there exists a subsequence of $n \mapsto \phi_\ell^{(n)}(r)/\|\phi_\ell^{(n)}\|_2$ which converges almost everywhere to $\varphi_k(r)$.

The convergence of γ_n is illustrated simply here, where we are interested in the smallest characteristic number $g_c^{(\ell)}$. Still we choose a positive (non-zero) squared integrable function $\phi_\ell^{(0)}(r)$, which, according to our previous discussion, is not orthogonal to $\varphi_1(r)$. The sequence of numbers γ_n provides us upper bounds for $g_c^{(\ell)}$ because this sequence is *decreasing* and converges to $g_c^{(\ell)}$. The monotony of the sequence $n \mapsto \gamma_n$ is related to the following equation, derived from (22):

$$\|\phi_\ell^{(n)}\|_2^2 = \langle \mathcal{K}_\ell^{(n)} \phi_\ell^{(0)} | \mathcal{K}_\ell^{(n)} \phi_\ell^{(0)} \rangle = \sum_{p=1}^\infty \frac{1}{g_p^{2n}} \langle \phi_\ell^{(0)} | \varphi_p \rangle^2, \tag{30}$$

which leads to the inequality

$$(\gamma_{n+2}^2 - \gamma_{n+1}^2) \|\phi_\ell^{(n+2)}\|_2^2 \|\phi_\ell^{(n+1)}\|_2^2 = - \sum_{p < q=1}^\infty \frac{1}{(g_p g_q)^{2n}} \left(\frac{1}{g_p^2} - \frac{1}{g_q^2} \right)^2 \langle \phi_\ell^{(0)} | \varphi_p \rangle^2 \langle \phi_\ell^{(0)} | \varphi_q \rangle^2, \tag{31}$$

$$\leq 0.$$

The positivity of γ_n asserts $\gamma_{n+2} \leq \gamma_{n+1}$.

On the other hand we can check easily that γ_n converges to $g_c^{(\ell)}$ for n going to infinity. Indeed, taking into account definitions (29b) and (30) we have

$$\gamma_n^2 = g_1^2 \frac{\sum_{p=1}^\infty \left(\frac{g_1}{g_p}\right)^{2n} \langle \phi_\ell^{(0)} | \varphi_p \rangle^2}{\sum_{p=1}^\infty \left(\frac{g_1}{g_p}\right)^{2n+2} \langle \phi_\ell^{(0)} | \varphi_p \rangle^2}, \tag{32}$$

which, using (19) and (27), shows clearly the convergence.

In section 4, use will be made of the iterative procedure (28) but for the functions $u_\ell^{(n)}(r)$, defined by $u_\ell^{(n)}(r) = \phi_\ell^{(n)}(r)/\sqrt{v(r)}$, namely

$$u_\ell^{(n+1)}(r) = \int_0^\infty dr' v(r') g_\ell(r, r') u_\ell^{(n)}(r'),$$

$$= \frac{r^{-\ell}}{2\ell + 1} \int_0^r dr' r'^{\ell+1} v(r') u_\ell^{(n)}(r') + \frac{r^{\ell+1}}{2\ell + 1} \int_r^\infty dr' r'^{-\ell} v(r') u_\ell^{(n)}(r'), \tag{33}$$

with $u_\ell^{(0)}(r) = r^{\ell+1}$. The sequence γ_n is given by

$$\gamma_{n+1} = \sqrt{\frac{\int_0^\infty dr v(r) [u_\ell^{(n)}(r)]^2}{\int_0^\infty dr v(r) [u_\ell^{(n+1)}(r)]^2}}. \tag{34}$$

2.3. Kolomý's method

The second variant of iterative methods was proposed by Kolomý [37] who constructed the sequence of functions

$$\phi_\ell^{(n+1)} = \frac{\langle \mathcal{K}_\ell \phi_\ell^{(n)} | \phi_\ell^{(n)} \rangle}{\| \mathcal{K}_\ell \phi_\ell^{(n)} \|_2^2} \mathcal{K}_\ell \phi_\ell^{(n)}, \tag{35a}$$

and consider the sequence of numbers

$$\beta_{n+1} = \frac{\langle \mathcal{K}_\ell \phi_\ell^{(n)} | \phi_\ell^{(n)} \rangle}{\| \mathcal{K}_\ell \phi_\ell^{(n)} \|_2^2}. \tag{35b}$$

The factor $(\langle \mathcal{K}_\ell \phi_\ell^{(n)} | \phi_\ell^{(n)} \rangle) / (\| \mathcal{K}_\ell \phi_\ell^{(n)} \|_2^2)$ in (35a) is useless as far as the series of number (35b) is concerned. In this paper, where our interest is focused on the lowest eigenvalue of the problem, we simply drop the normalization factor in (35a), namely we consider

$$\phi_\ell^{(n+1)} = \mathcal{K}_\ell \phi_\ell^{(n)}, \tag{36}$$

coupled with (35b).

When the starting trial function $\phi_\ell^{(0)}(r)$ is a positive (non-zero) squared integrable function, it is not orthogonal to $\varphi_1(r)$. Then the sequence β_n converges to g_1 with $g_1 \leq \beta_n$. We still obtain a sequence of upper bounds for $g_c^{(\ell)}$. Indeed the sequence $n \mapsto \beta_n$ is decreasing since

$$\begin{aligned} (\beta_{n+2} - \beta_{n+1}) \| \mathcal{K}_\ell \phi_\ell^{(n+1)} \|_2^2 \| \mathcal{K}_\ell \phi_\ell^{(n)} \|_2^2 &= - \sum_{p < q=1}^\infty \frac{1}{(g_p g_q)^{2n-1}} \left(\frac{1}{g_p} - \frac{1}{g_q} \right)^2 \left(\frac{1}{g_p} + \frac{1}{g_q} \right) \\ &\quad \times \langle \phi_\ell^{(0)} | \varphi_p \rangle^2 \langle \phi_\ell^{(0)} | \varphi_q \rangle^2 \\ &\leq 0. \end{aligned} \tag{37}$$

On the other hand we can check easily that β_n converges to $g_1 = g_c^{(\ell)}$ for n going to infinity. Indeed, taking into account definitions (35b) and (17), we have

$$\beta_{n+1} = g_1 \frac{\sum_{p=1}^\infty \left(\frac{g_1}{g_p} \right)^{2n+1} \langle \phi_\ell^{(0)} | \varphi_p \rangle^2}{\sum_{p=1}^\infty \left(\frac{g_1}{g_p} \right)^{2n+2} \langle \phi_\ell^{(0)} | \varphi_p \rangle^2}, \tag{38}$$

which, using (19) and (27), shows clearly the convergence.

For the sake of convenience, we rewrite the iterative procedure (36) in terms of the function $u_\ell^{(n)}(r)$, defined by $u_\ell^{(n)}(r) = \phi_\ell^{(n)}(r) / \sqrt{v(r)}$. Using (35b), the sequence β_n reads

$$\beta_{n+1} = \frac{\int_0^\infty dr v(r) u_\ell^{(n)}(r) u_\ell^{(n+1)}(r)}{\int_0^\infty dr v(r) [u_\ell^{(n+1)}(r)]^2}. \tag{39}$$

As we show in section 4, both iterative procedures depicted in 2.2 and 2.3 converge very rapidly, when use is made of the initial function $\phi_\ell^{(0)}(r) = r^{\ell+1} \sqrt{v(r)}$. However, to decrease the number of iterations, more flexible function $\phi_\ell^{(0)}(r)$, obeying to the desired conditions, positivity and squared integrability, could be very helpful. This is explored in the following section.

2.4. Combination of iterative and variational methods

The variational method we propose is based upon the theorem [38, 39] which states that for a symmetric compact operator,

$$\sup_{\psi} [\langle \mathcal{K}_{\ell} \psi | \psi \rangle] = \frac{1}{|g_1|}, \quad (40)$$

under the constraint that ψ is squared integrable and normalized to unity ($\|\psi\|_2 = 1$). Since in this paper the kernel we consider is positive we have $|g_1| = g_1$. The maximal value of (40) is reached for $\psi(r) = \varphi_1(r)$, the eigenfunction associated with the smallest eigenvalue $g_1 = g_c^{(\ell)}$. Consequently, for any function $\psi(r)$, normalized to unity, we obtain the following upper limit:

$$g_c^{(\ell)} \leq \langle \mathcal{K}_{\ell} \psi | \psi \rangle^{-1}. \quad (41)$$

This method was used in [31] to obtain the upper limit (8) using the trial function

$$\psi(r) = A[r^{2p-1}v(r)^p]^{1/2}, \quad p > 0. \quad (42)$$

The degree of flexibility increases with

$$\psi(r) = A[r^p v(r)^q]^{1/2}, \quad (43)$$

where still (p, q) are varied in the domain ensuring that $\psi(r) \in L^2(\mathbb{R})$ and A is a normalization factor designed to have $\|\psi\|_2 = 1$. When we combine the iterative methods together with the variational one, we construct a sequence of functions which automatically converges in $L^2(\mathbb{R})$ to the exact zero energy wavefunction. This means that the variational method (40) can be used with all iterated $\psi^{(i)} = \mathcal{K}_{\ell}^{(i)} \psi$, $i = 1, 2, \dots$, of $\psi(r)$, equation (43).

These possibilities are tested in section 4 and shown to greatly improve the convergence towards the exact result.

3. Upper and lower limits on the critical strength

Now, let us introduce another method which provides both lower and upper limits of the critical value required. Note that this method has some link with the iterative power method discussed above.

In this section we restrict to the S-wave case since the determination of the critical value for the potential $V(r)$ in the ℓ -wave is equivalent to the determination of the critical value for the potential

$$W_{\ell}(r) = \frac{1}{(2\ell + 1)^2} \frac{V(r^{1/(2\ell+1)})}{r^{4\ell/(2\ell+1)}} \quad (44)$$

in the S-wave [16].

Theorem. Let $V(r)$ be a central potential with $V(r) = -gv(r)$, $v(r) \geq 0$. Let the functions $\psi_n(r)$ defined by the following recurrence relation:

$$\psi_n(r) = \int_0^{\infty} dr' g(r, r') v(r') \psi_{n-1}(r') \quad n \geq 1 \quad (45)$$

with $\psi_0(r) = r$ and $g(r, r') = \inf(r, r')$. Let α_n and ω_n be two sequences defined as follows:

$$\alpha_n = \lim_{r \rightarrow 0} \frac{\psi_{n+1}(r)}{\psi_n(r)} = \frac{\psi'_{n+1}(0)}{\psi'_n(0)} = \frac{\int_0^{\infty} dr v(r) \psi_n(r)}{\int_0^{\infty} dr v(r) \psi_{n-1}(r)} \quad n \geq 1, \quad (46)$$

where the prime denotes the derivative with respect to r and

$$\omega_n = \lim_{r \rightarrow \infty} \frac{\psi_{n+1}(r)}{\psi_n(r)} = \frac{\int_0^\infty dr r v(r) \psi_n(r)}{\int_0^\infty dr r v(r) \psi_{n-1}(r)} \quad n \geq 1. \tag{47}$$

Then, the two sequences α_n and ω_n converge to $1/g_c^{(0)}$, $g_c^{(0)}$ being the critical value of the strength of the potential $V(r)$ for which a first S-wave bound state appears. The α_n sequence is decreasing while the ω_n sequence is increasing.

The proof that ω_n is increasing and converges towards the desired value is rather simple. The change of function $\phi_0^{(n)}(r) = \sqrt{v(r)}\psi_n(r)$ in the iterative process (45) leads to

$$\phi_0^{(n+1)}(r) = \int_0^\infty dr' K_0(r, r') \phi_0^{(n)}(r') \quad n \geq 1, \tag{48}$$

with $\phi_0^{(0)}(r) = r\sqrt{v(r)}$ and $K_0(r, r') = \sqrt{v(r)} \inf(r, r') \sqrt{v(r')}$. Clearly we recover

$$\phi_0^{(n+1)} = \mathcal{K}_0 \phi_0^{(n)} = \mathcal{K}_0^{(n+1)} \phi_0^{(0)} \quad n \geq 0, \tag{49}$$

in terms of the iterated kernel $\mathcal{K}_0^{(n)}$ (see section 2.1). As

$$\lim_{r \rightarrow \infty} \psi_n(r) = \int_0^\infty dr r v(r) \psi_{n-1}(r) \quad n \geq 1, \tag{50}$$

is in fact the scalar product

$$\lim_{r \rightarrow \infty} \psi_n(r) = \langle \phi_0^{(0)} | \phi_0^{(n-1)} \rangle, \tag{51}$$

we deduce that $\omega_n = \delta_{n-1}$ when the starting function in (24) is $\phi_0(r) = r\sqrt{v(r)}$. This shows that ω_n is an increasing sequence converging to $1/g_c^{(0)}$.

Now, let us consider the sequence α_n . We show in the appendix that $n \mapsto \alpha_n$ is a decreasing sequence which converges to $1/g_c^{(0)}$. In the appendix we relate all the $\psi'_n(0)$ entering the definition of α_n to the Jost function for $V(r)$ at zero energy. This is of some interest in the measure where we obtain lower limits for $g_c^{(0)}$ circumventing the constraint $g_c^{(0)} \int_0^\infty dr r |v(r)| < 2$ of [16].

The sequences α_n and ω_n are simple enough to write the first members explicitly. First of all we remark that

$$\alpha_0 = \int_0^\infty dx x v(x), \tag{52}$$

which is just the Bargmann–Schwinger necessary condition for the existence of bound states. We also have $\omega_0 = 0$. The next order yields the following relation:

$$\begin{aligned} \frac{\int_0^\infty dx x v(x)}{\int_0^\infty dx v(x) \int_0^\infty dy \inf(x, y) y v(y)} &= \frac{1}{\alpha_1} \leq g_c^{(0)} \leq \frac{1}{\omega_1} \\ &= \frac{\int_0^\infty dx x^2 v(x)}{2 \int_0^\infty dx x v(x) \int_0^x dy y^2 v(y)}. \end{aligned} \tag{53}$$

4. Tests of the bounds on some common potentials

In this section, we propose to test the accuracy of the various upper and lower limits obtained in sections 2 and 3 with three potentials: a square well (SW) potential,

$$V(r) = -gR^{-2}\theta(1 - r/R); \tag{54}$$

Table 1. Comparison between the coefficient γ_n obtained by the Kellogg method, with $\phi_0^{(0)} = r\sqrt{v(r)}$, and the exact results for the potentials (54)–(56).

Potential	γ_1	γ_2	γ_3	γ_4	Exact
E ($\ell = 0$)	1.532 3	1.448 0	1.445 9	1.445 8	1.445 8
PE ($\ell = 0$)	0.704 63	0.677 18	0.676 69	0.676 68	0.676 68
SW ($\ell = 0$)	2.485 3	2.467 6	2.467 4	2.467 4	2.467 4
SW ($\ell = 1$)	10.247	9.888 5	9.870 7	9.869 7	9.869 6
SW ($\ell = 2$)	21.635	20.317	20.202	20.192	20.191
SW ($\ell = 3$)	36.630	33.620	33.278	33.227	33.217
SW ($\ell = 4$)	55.210	49.745	49.000	48.864	48.831
SW ($\ell = 5$)	77.374	68.669	67.322	67.039	66.954

Table 2. Comparison between the coefficient β_n obtained by the Kolomý method, with $\phi_0^{(0)} = r\sqrt{v(r)}$, and the exact results for the potentials (54)–(56).

Potential	β_1	β_2	β_3	β_4	Exact
E ($\ell = 0$)	1.467 4	1.446 5	1.445 82	1.445 80	1.445 8
PE ($\ell = 0$)	0.682 70	0.676 82	0.676 69	0.676 68	0.676 68
SW ($\ell = 0$)	2.470 6	2.467 44	2.467 4	2.467 4	2.467 4
SW ($\ell = 1$)	10.000	9.877 0	9.870 1	9.869 6	9.869 6
SW ($\ell = 2$)	20.811	20.253	20.198	20.192	20.191
SW ($\ell = 3$)	34.851	33.439	33.252	33.223	33.217
SW ($\ell = 4$)	52.105 3	49.372	48.935	48.852	48.831
SW ($\ell = 5$)	72.567 2	68.022	67.192	67.039	66.954

an exponential (E) potential

$$V(r) = -gR^{-2} \exp(-r/R); \quad (55)$$

a non-monotonic potential (PE potential)

$$V(r) = -gR^{-3}r \exp(-r/R). \quad (56)$$

In these potentials, the radius R is arbitrary (but positive). Due to the scaling property, which does not affect the critical value $g_c^{(\ell)}$, the radius R appearing in the potential can be set to unity.

In order to test the reliability of the different methods when the convexity of the potential increases, we perform simple analytical calculations (that we do not report here) involving the SW potential (54), when the angular momentum ℓ increases. We also study the E and the PE potentials only for the S-wave.

In order to examine to what extent our recursive procedure leads rapidly to the exact result, the exact value of the critical coupling constants of the potentials, $g_c^{(\ell)}$, and its approximated upper and lower limits investigated in sections 2 and 3 are depicted in tables 1 to 4. More precisely, the Kellogg coefficients γ_n are shown in table 1, the Kolomý coefficient are reported in table 2. The results obtained by the variational method and its iterated are given in table 3. In table 4, we report the results obtained by lower and upper limits discussed in section 3. As a further information, we give in table 5 the results for α_4 and ω_4 which are compared to those obtained by formulae (2)–(4) and (8) for the three potentials (54)–(56).

In all cases, a few iterations are enough to obtain strong restrictions on the possible values of $g_c^{(\ell)}$, especially for low value of the angular momentum.

Table 3. Comparison between the upper limit on $g_c^{(\ell)}$ obtained by the variational method, the combination of the variational, and the Kellogg method and the exact value of $g_c^{(\ell)}$. The variational wavefunctions $\phi_\ell(r)$ are $r \exp(-qr)$ for the E and the PE potentials and r^p for the SW potential.

Potential	ϕ_ℓ	$\mathcal{K}_\ell \phi_\ell$	Exact
E ($\ell = 0$)	1.446 76	1.445 82	1.445 80
PE ($\ell = 0$)	0.685 43	0.676 72	0.676 68
SW ($\ell = 0$)	2.474 7	2.467 4	2.467 4
SW ($\ell = 1$)	9.993 4	9.871 0	9.869 6
SW ($\ell = 2$)	20.604	20.201	20.191
SW ($\ell = 3$)	34.099	33.253	33.217
SW ($\ell = 4$)	50.357	48.915	48.831
SW ($\ell = 5$)	69.295	67.117	66.954

Table 4. Comparison between the coefficient α_n and ω_n obtained by the new iterative method and the exact results for the potentials (54)–(56).

Potential	α_1^{-1}	α_2^{-1}	α_3^{-1}	α_4^{-1}	Exact	ω_4^{-1}	ω_3^{-1}	ω_2^{-1}	ω_1^{-1}
E ($\ell = 0$)	1.333 3	1.421 1	1.440 8	1.444 8	1.445 8	1.446 5	1.449 5	1.467 4	1.600 0
PE ($\ell = 0$)	0.64000	0.670 09	0.675 58	0.676 50	0.676 68	0.676 82	0.677 55	0.682 70	0.727 27
SW ($\ell = 0$)	2.400 0	2.459 0	2.466 4	2.467 3	2.467 4	2.467 4	2.467 7	2.470 6	2.500 0
SW ($\ell = 1$)	8.571 4	9.483 9	9.763 8	9.841 9	9.869 6	9.877 0	9.900 0	10.000	10.500
SW ($\ell = 2$)	15.556	18.271	19.452	19.921	20.191	20.252	20.381	20.811	22.500
SW ($\ell = 3$)	22.909	28.077	30.813	32.149	33.217	33.439	33.801	34.851	38.500
SW ($\ell = 4$)	30.462	38.506	43.336	46.041	48.831	49.372	50.121	52.105	58.500
SW ($\ell = 5$)	38.133	49.336	56.671	61.201	66.954	68.022	69.322	72.567	82.500

Table 5. Comparison between previously known upper and lower limits (2)–(4) and (8) on $g_c^{(\ell)}$ and the exact results for the potentials (54)–(56).

Potential	Equation (2)	Equation (3)	Equation (4)	Equation (8)	Exact	α_4^{-1}	ω_4^{-1}
E ($\ell = 0$)	1.438 3	1.675 5	1.544 2	1.446 7	1.445 8	1.444 8	1.446 5
PE ($\ell = 0$)	0.674 21	0.764 98	0.865 47	0.676 91	0.676 68	0.676 50	0.676 82
SW ($\ell = 0$)	2.359 3	2.666 7	4.000 0	2.474 7	2.467 4	2.467 3	2.467 4
SW ($\ell = 1$)	9.122 0	11.719	10.068	9.993 4	9.869 6	9.841 9	9.877 0
SW ($\ell = 2$)	18.454	25.413	20.895	20.604	20.191	19.921	20.252
SW ($\ell = 3$)	30.245	43.570	35.424	34.099	33.217	32.149	33.439
SW ($\ell = 4$)	44.425	66.089	53.519	50.357	48.831	46.041	49.372
SW ($\ell = 5$)	60.947	92.909	75.114	69.295	66.954	61.201	68.022

5. Conclusions

In this paper we have presented in section 2 several iterative procedures yielding sequences of upper limits on the critical value, $g_c^{(\ell)}$, of the coupling constant (strength), g , of the potential, $V(r) = -gv(r)$, for which a first ℓ -wave bound state appears. In section 3 we have obtained a method yielding both upper and lower limits on $g_c^{(\ell)}$. All these sequences converge rather rapidly to the exact critical value as shown by the tests presented in section 4. Due to the construction of the sequences, for example $\beta_n = 1/\omega_{2n}$, the convergence of the sequences obtained in section 2 is faster than those of section 3. However, results which are closest to the exact values are obtained, with minimal numerical efforts, from the combination of variational and iterative methods.

Note that the results presented in this paper, of similar accuracy than the results given by other methods, can always be improved when use is made of a supplementary iteration. The accuracy of the results that we obtain can be measured by the difference $1/\omega_n - 1/\alpha_n$.

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Appendix. Monotony of the sequence α_n

In this appendix we study the sequence α_n defined by (46). As made for ω_n , we express α_n in terms of a scalar product. We know that $\psi_{n+1}(r) \simeq r \int_0^\infty dr v(r) \psi_n(r)$, $n \geq 1$ at the vicinity of $r = 0$, so that its first derivative is the scalar product

$$\psi'_{n+1}(0) = \langle q_0 | \phi_0^{(n)} \rangle \quad (\text{A.1})$$

with $q_0(r) = \sqrt{v(r)}$ and $\phi_0^{(n)}(r) = \sqrt{v(r)} \psi_n(r)$.

The proof of the monotony is made in two steps. First we show that the inverse of the Jost function at zero energy, given, for example, in equations (13) and (14) of [16], in terms of the coupling constant g is simply the series

$$\frac{1}{f_0(g, 0)} = \sum_{n=0}^{\infty} \psi'_n(0) g^n \quad (\text{A.2})$$

which converges for $g < g_c^{(0)}$. It can be easily verified by considering $\tilde{\psi}_n(r)$, defined by the recurrence relation (45) but where the first term $\tilde{\psi}_0(r)$ is equal to unity. Equation (45) becomes

$$\begin{aligned} \tilde{\psi}_n(r) &= M_n - \int_r^\infty dr' (r' - r) v(r) \tilde{\psi}_{n-1}(r') \quad n \geq 1 \\ M_n &= \int_0^\infty dr r v(r) \tilde{\psi}_{n-1}(r) \quad n \geq 1. \end{aligned} \quad (\text{A.3})$$

Introducing $\tilde{\phi}_0^{(n)}(r) = \tilde{\psi}_n(r) \sqrt{v(r)}$, $\phi_0^{(n)}(r) = \psi_n(r) \sqrt{v(r)}$ and $q_0(r) = \sqrt{v(r)}$ we have, due to the symmetry of the scalar product,

$$\begin{aligned} M_n &= \langle \psi_0^{(0)} | \tilde{\phi}_0^{(n-1)} \rangle = \langle \psi_0^{(0)} | \mathcal{K}_0^{(n-1)} \tilde{\phi}_0^{(0)} \rangle = \langle \psi_0^{(0)} | \mathcal{K}_0^{(n-1)} q_0 \rangle = \langle q_0 | \mathcal{K}_0^{(n-1)} \psi_0^{(0)} \rangle \\ &= \langle q_0 | \psi_0^{(n-1)} \rangle = \int_0^\infty dr v(r) \psi_{n-1}(r) = \psi'_n(0). \end{aligned} \quad (\text{A.4})$$

This allows us to define M_n for $n = 0$ and we have $M_0 = 1$.

On the other hand, it has been shown that the zero energy Jost function could be written as [16]

$$f_0(g, 0) = \sum_{n=0}^{\infty} (-)^n a_n g^n, \quad (\text{A.5})$$

with

$$a_n = \int_0^\infty dr_1 r_1 v(r_1) \int_{r_1}^\infty dr_2 (r_2 - r_1) v(r_2) \cdots \int_{r_{n-1}}^\infty dr_n (r_n - r_{n-1}) v(r_n) \quad n \geq 2 \quad (\text{A.6})$$

and $a_0 = 1, a_1 = \int_0^\infty dr r v(r)$. We have the following relation between M_n and a_n :

$$\sum_{p=0}^n M_{n-p} a_p (-)^p = 0 \quad n \geq 1, \tag{A.7}$$

whereas for $n = 0, a_0 M_0 = 1$. This shows that the series $\sum_{n=0}^\infty M_n g^n$ is equal to $1/f(0, g)$ for $g < g_c^{(0)}$. Indeed, relation (A.7) is just the relation that exists between Taylor's coefficients of the functions $f(x)$ and $1/f(x)$.

Secondly we prove the following lemma:

Lemma. *Let the series*

$$F(g) = \sum_{n=0}^\infty \beta_n g^n \tag{A.8}$$

be convergent for $g < R, (R > 0)$, such that $\beta_0 = 1$ and

$$\begin{aligned} (\forall n \geq 0) \quad \beta_n > 0 \\ (\forall n \geq 0) \quad \beta_{n+2} \beta_n \leq \beta_{n+1}^2. \end{aligned} \tag{A.9}$$

Then, for every $\lambda > 0$, the series

$$G(g) = \sum_{p=0}^\infty \beta_p g^p \times \sum_{q=0}^\infty \lambda^q g^q = \sum_{n=0}^\infty \gamma_n g^n \tag{A.10}$$

convergent for $g < \tilde{R} = \inf(R, 1/\lambda)$ is such that $\gamma_0 = 1$ and has the property

$$\begin{aligned} (\forall n \geq 0) \quad \gamma_n > 0 \\ (\forall n \geq 0) \quad \gamma_{n+2} \gamma_n \leq \gamma_{n+1}^2. \end{aligned} \tag{A.11}$$

The proof of the lemma originates from the definition of γ_n

$$\gamma_n = \sum_{p=0}^n \beta_p \lambda^{n-p} \tag{A.12}$$

which asserts that $\gamma_0 = 1$ and $\gamma_n > 0$ since λ and β_n are positive (see (A.9)). The second property in (A.11) is satisfied if and only if the following relation is satisfied for $n \geq 0$:

$$\sum_{p=0}^{n+2} \beta_p \lambda^{n+2-p} \sum_{q=0}^n \beta_q \lambda^{n-q} - \left(\sum_{p=0}^{n+1} \beta_p \lambda^{n+1-p} \right)^2 \leq 0. \tag{A.13}$$

Inequality (A.13) is equivalent to the requirement that

$$(\beta_{n+2} - \beta_{n+1} \lambda) \sum_{p=0}^n \beta_p \lambda^{n-p} - \beta_{n+1}^2 \leq 0, \tag{A.14}$$

which is manifestly satisfied when

$$(\forall n, 1 \leq p \leq n) \quad \beta_{n+2} \beta_p - \beta_{n+1} \beta_{p+1} \leq 0. \tag{A.15}$$

Relation (A.9) and the positivity of β_n imply that this latter inequality, which originates from the iteration of (A.9) when n is lowered up to p , is verified.

Now we use the fact that, for any $g < g_1 = g_c^{(0)}$ the Jost function can be written as [27]

$$f_0(g, 0) = \prod_{n=1}^\infty \left(1 - \frac{g}{g_n} \right) \tag{A.16}$$

where the g_n still denote the characteristic numbers of the eigenvalue problem considered. Product (A.16) exists for $g < g_1$ when each series $\sum_{n=0}^{\infty} g_n^{-p}$ converges for every integer $p \geq 1$, which is true when the (positive) trace of the iterated kernel $K_0^{(n)}(r, r')$ is finite. Equation (A.16) implies that for any $g < g_1$ we have

$$\frac{1}{f_0(g, 0)} = \prod_{n=1}^{\infty} \sum_{p=0}^{\infty} \left(\frac{g}{g_n}\right)^p = \lim_{N \rightarrow \infty} S_N \quad S_N = \prod_{n=1}^N \sum_{p=0}^{\infty} \left(\frac{g}{g_n}\right)^p. \quad (\text{A.17})$$

Since all the quantities in (A.17) are positive we can write, for $g < g_1$

$$S_N = \sum_{p=0}^{\infty} s_p^{(N)} g^p \quad (\text{A.18})$$

where $s_0^{(N)} \equiv 1$. Now assuming that for some N , the following property holds:

$$(\forall p \geq 0) \quad s_{p+2}^{(N)} s_p^{(N)} - (s_{p+1}^{(N)})^2 \leq 0 \quad (\text{A.19})$$

according to the lemma, the property still holds for $N + 1$ as well. Note that the radius of convergence \tilde{R} of the lemma is always minorated by $g_1 > 0$. For $N = 1$, $s_p^{(1)}$ is simply $1/g_1^p$ and property (A.19) is valid. For $N = 2$, $s_p^{(2)} = \sum_{k=0}^p g_1^{-k} g_2^{k-p}$ and it can be verified that property (A.19) is again valid. Therefore, for every $N \geq 2$ property (A.19) is also valid and in particular for N going to infinity. The comparison between (A.2) and (A.17) shows that $\psi'_n(0) = s_n^{(\infty)}$. From relation (A.19) we obtain

$$(\forall n \geq 0) \quad \frac{\psi'_{n+2}(0)}{\psi'_{n+1}(0)} \leq \frac{\psi'_{n+1}(0)}{\psi'_n(0)}, \quad (\text{A.20})$$

which, with definition (46) of α_n , proves that the sequence α_n is decreasing.

Since α_n is decreasing and positive it converges towards some $\alpha \geq 0$. On the other hand we know that the radius of convergence of the series $1/f(g, 0)$ is g_1 . Using the d'Alembert rule for the series of positive numbers $(\psi'_n(0))_{n \geq 0}$ we have $1/g_1 = \lim_{n \rightarrow \infty} \psi'_{n+1}(0)/\psi'_n(0) = \alpha$ so that α_n converges towards $1/g_1 = 1/g_c^{(0)}$.

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