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A sufficient condition for the existence of bound states for scalar spherically symmetric potentials

M Lassaut and R J Lombard

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

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Abstract. We consider the class of three-dimensional attractive finite range or similar potentials $\lambda W(r)$, depending on a strength constant λ. Beyond a 'critical' value, λ_c, the potential $\lambda W(r)$ has at least one bound state. For the s-wave, we propose simple bounds for λ_c obtained by formally solving the Schrödinger equation for the zero energy bound state. The various bounds are compared with the exact value λ_c for a set of usual potentials. They are also compared with bounds derived in earlier works by Glaser *et al* and by Calogero. We show that the $\ell \neq 0$ case is solved by equations very similar to $\ell = 0$ ones.

1. Introduction

The number of bound states produced by a given potential is a standard question of quantum mechanics, which is discussed in many textbooks (see, for instance [1, 2]). Perhaps the most familiar relationship is the Bargmann inequality,

$$n_\ell \leqslant \frac{1}{2\ell+1}\int_0^{+\infty} r|V(r)|\,\mathrm{d}r \tag{1}$$

it proves very useful when deciding whether the spectrum of $V(r)$ is finite. However, because it is an inequality, and moreover an upper bound on the number of bound states, it cannot ensure the occurrence of at least one bound state. Sufficient conditions exist, which answer this question [1]. One of them was proposed years ago by Calogero [3]. On the other hand, optimal conditions have been obtained by Glaser *et al* [4] for the absence of bound states by using variational techniques, which reads

$$\frac{(p-1)^{p-1}\Gamma(2p)}{p^p\Gamma^2(p)(2\ell+1)^{2p-1}}\int_0^{+\infty}|r^2V(r)|^p\frac{\mathrm{d}r}{r} < 1 \qquad 1 \leqslant p \leqslant \tfrac{3}{2}. \tag{2}$$

The purpose of the present work is to provide a simple and efficient criterion for the existence of a single bound state. It is derived for spherically symmetric potentials $\lambda W(r)$ depending on a strength constant λ. The method is based on results reported in a previous work [5], devoted to the behaviour of the eigenvalue at the transition between zero and one bound state. This transition occurs at a 'critical' value of the strength constant λ_c, corresponding to a bound state at zero energy. We show that an estimate can provide an upper bound of λ_c for a large class of potentials.

Let us mention a recent paper by Chadan *et al* [6] that deals with a generalization of the Calogero–Cohn bound. Their method is quite different from ours and provides

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

an upper bound to the number of bound states. The efficiency of the bound, provided by equation (2), as well as Calogero's sufficiency condition, will be compared with the criterion we are advocating in the present work.

The paper is organized as follows. In section 2 an upper bound for λ_c is proposed for the s-wave and extended to higher waves. In section 3 our proposal of an upper bound for λ_c is tested against the exact value for some potentials. Conclusions are presented in section 4.

2. Existence of an upper bound on λ_c

We consider spherically symmetric scalar potentials, $\lambda W(r)$, having at most a finite number of bound states for a finite value of the strength constant λ. This class comprises potentials not too singular at the origin and decreasing fast enough at infinity, i.e. such that $\int_0^{+\infty} r|W(r)|\,\mathrm{d}r$ and $\int_b^{+\infty} |W(r)|\,\mathrm{d}r$, $b > 0$ are finite.

The Schrödinger equation reads :

$$\left(-\frac{\hbar^2}{2m}\triangle + \lambda W(r)\right)\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}). \tag{3}$$

Here, m is the mass of the single particle experiencing the potential $W(r)$, and $\psi(\boldsymbol{r})$ is the single particle wavefunction.

The usual decomposition on the spherical harmonics

$$\psi(\boldsymbol{r}) = \sum_{\ell,m} \frac{f_l(r)}{r} Y_\ell^m(\Omega) \tag{4}$$

removes the angular variables. We are left with radial second-order differential equations depending on the value of the angular momentum ℓ:

$$f_\ell''(\lambda, E, r) = \left(\frac{2m}{\hbar^2}(E + \lambda W(r)) + \frac{\ell(\ell+1)}{r^2}\right) f_\ell(\lambda, E, r) \tag{5}$$

where a prime denotes a derivative with respect to the variable r.

In this section we study the transition from zero to one bound state, which corresponds to the 'critical' value $\lambda = \lambda_c$ [5]. Actually, since $|W(r)|$ is assumed to decrease faster than $1/r^2$ at infinity the Bargmann inequality [2] applies:

$$n_\ell \leqslant -\frac{1}{2\ell+1}\frac{2m}{\hbar^2}\lambda\int_0^{+\infty} rW^a(r)\,\mathrm{d}r \tag{6}$$

where n_ℓ is the number of bound states of the potential, involving only the attractive part, W^a, of the potential W. In the case of interest here, $n_\ell = 1$, it gives

$$-\frac{2m}{\hbar^2}\lambda\int_0^{+\infty} rW^a(r)\,\mathrm{d}r \geqslant 2\ell + 1. \tag{7}$$

For the existence of one bound state, this condition is necessary but not sufficient. It is saturated for shell-delta potential. An upper bound for λ_c would be very helpful, since for every $\lambda > \lambda_c$ the potential has at least one bound state. Note that the Calogero sufficiency condition [3] yields also an upper bound, but in a quite different way.

As shown in [5], the 'critical' value, λ_c, corresponds to a bound state of zero energy. For simplicity, we assume the potential $W(r)$ to be purely attractive and put

$$V^+(r) = -\frac{2m}{\hbar^2}W(r) \tag{8}$$

the function V^+ being positive definite.

2.1. $\ell = 0$

We start with the $\ell = 0$ case. Looking for λ_c, we search for the value of λ, such that

$$f_0''(\lambda, r) + \lambda V^+(r) f_0(\lambda, r) = 0 \tag{9}$$

with the following constraints: $f_0(\lambda, r)$ vanishes at $r = 0$, is constant asymptotically, and has no node ($f_0(\lambda, r) \geqslant 0$).

For every positive value of λ, asymptotically, equation (9) admits two solutions: 1 and r. Using Lagrange's method of 'variation of constants', the Schrödinger equation with the boundary condition $\lim_{r\to\infty} f_0(\lambda, r) = 1$ induces the Volterra integral equation:

$$f_0(\lambda, r) = 1 - \lambda \int_r^{+\infty} (r' - r) V^+(r') f_0(\lambda, r')\, \mathrm{d}r'. \tag{10}$$

Writing $f_0(\lambda, r)$ as a series expansion

$$f_0(\lambda, r) = \sum_{n=0}^{+\infty} f_0^n(\lambda, r) \tag{11}$$

allows us to solve (10) by iteration:

$$\begin{aligned} &f_0^0(\lambda, r) = 1 \\ &f_0^n(\lambda, r) = -\lambda \int_r^{+\infty} (r' - r) V^+(r') f_0^{n-1}(\lambda, r')\, \mathrm{d}r'. \end{aligned} \tag{12}$$

Since

$$|f_0^n(\lambda, r)| \leqslant \lambda^n \left(\int_0^{+\infty} r' V^+(r')\, \mathrm{d}r' \right)^n \Big/ n!$$

the series expansion (11) is normally convergent with respect to r.

By construction, the function $f_0(\lambda, r)$ corresponds at infinity to an s-wave bound state wavefunction at zero energy. The second condition is its vanishing at $r = 0$. For this purpose, we write

$$f_0(\lambda, 0) = \sum_{n=0}^{+\infty} (-)^n a_n \lambda^n \tag{13}$$

where

$$\begin{aligned} &a_0 = 1 \\ &a_1 = \int_0^{+\infty} r_1 V^+(r_1)\, \mathrm{d}r_1 \\ &a_2 = \int_0^{+\infty} r_1 V^+(r_1)\, \mathrm{d}r_1 \int_{r_1}^{+\infty} (r_2 - r_1) V^+(r_2)\, \mathrm{d}r_2 \\ &\ldots \end{aligned}$$

etc, and in general

$$\begin{aligned} a_n = \int_0^{+\infty} r_1 V^+(r_1)\, \mathrm{d}r_1 \int_{r_1}^{+\infty} (r_2 - r_1) V^+(r_2)\, \mathrm{d}r_2 \ldots \\ \ldots \int_{r_{n-2}}^{+\infty} (r_{n-1} - r_{n-2}) V^+(r_{n-1})\, \mathrm{d}r_{n-1} \int_{r_{n-1}}^{+\infty} (r_n - r_{n-1}) V^+(r_n)\, \mathrm{d}r_n. \end{aligned} \tag{14}$$

For attractive potentials $W(r)$, the a_n's are positive and therefore the series equation (13) is alternating. Furthermore, in appendix A, we show that

$$a_n \leqslant \frac{a_{n-1}}{2} \int_0^{+\infty} rV^+(r)\,\mathrm{d}r \tag{15}$$

for $n \geqslant 2$. This inequality ensures that for every $\lambda \leqslant 2/M_1$, where we have put $M_1 = \int_0^{+\infty} rV^+(r)\,\mathrm{d}r$, we know the sign of the nth-order remainder $\mathcal{R}_n$ for $n \geqslant 1$, namely

$$(\forall p \geqslant 1) \qquad \mathcal{R}_{2p}(\lambda) = \sum_{n=2p}^{+\infty} (-)^n a_n \lambda^n \geqslant 0 \tag{16}$$

$$(\forall p) \qquad \mathcal{R}_{2p+1}(\lambda) = \sum_{n=2p+1}^{+\infty} (-)^n a_n \lambda^n \leqslant 0. \tag{17}$$

For every $\lambda < 1/M_1$, $f_0(\lambda, 0)$ is positive. Indeed, taking the first two terms of (13), $a_0 - a_1\lambda = 1 - \lambda M_1 > 0$, we are left with $\mathcal{R}_2 \geqslant 0$.

At the next order, we look for the solutions of the equation

$$1 - M_1\lambda + a_2\lambda^2 = 0. \tag{18}$$

The lowest root reads

$$\lambda_2 = \frac{M_1 - \sqrt{M_1^2 - 4a_2}}{2a_2} \qquad (a_2 > 0).$$

It leads to

$$\lambda_2 = \frac{2}{M_1 + \sqrt{M_1^2 - 4a_2}} \leqslant \frac{2}{M_1} \tag{19}$$

for $a_2 \geqslant 0$, provided that $M_1^2 - 4a_2$ is positive, which is assumed. The bound λ_2 is dominated by $2/M_1$. The remainder $\mathcal{R}_3$ is negative or zero. Consequently, $f_0(\lambda_2, 0) \leqslant 0$ and the 'critical' value is situated in the interval

$$\frac{1}{M_1} \leqslant \lambda_c \leqslant \lambda_2 \tag{20}$$

or equivalently

$$1 \leqslant \lambda_c M_1 \leqslant \frac{2}{1 + \sqrt{1 - 4a_2/M_1^2}} \leqslant 2. \tag{21}$$

If the discriminant $M_1^2 - 4a_2$ is negative, we look for the lowest solution, λ_4, of

$$1 - M_1\lambda + a_2\lambda^2 - a_3\lambda^3 + a_4\lambda^4 = 0. \tag{22}$$

Again, if λ_4 exists and satisfies $\lambda_4 \leqslant 2/M_1$, the remainder $\mathcal{R}_5$ is negative or zero and therefore $f_0(\lambda_4, 0)$ is negative. We then have

$$1 \leqslant \lambda_c M_1 \leqslant \lambda_4 M_1 \leqslant 2. \tag{23}$$

Note that since the remainders satisfy inequalities (16), (17), we have

$$(\forall p \geqslant 1) \qquad \sum_{n=0}^{2p-1} a_n \lambda^n \leqslant f_0(\lambda, 0) \leqslant \sum_{n=0}^{2p} a_n \lambda^n \tag{24}$$

for $\lambda < 2/M_1$. On the other hand the term

$$1 - M_1\lambda + \lambda^2 a_2 - a_3\lambda^3 + a_4\lambda^4$$

is positive for $\lambda \leqslant 1/M_1$ and negative for $\lambda = \lambda_2$ (if λ_2 exists) therefore $\lambda_4 \leqslant \lambda_2$. Moreover, if λ_3 is the lowest solution of the equation

$$1 - M_1\lambda + a_2\lambda^2 - a_3\lambda^3 = 0 \tag{25}$$

for every $\lambda \leqslant \lambda_3$, $f_0(\lambda, 0)$ is positive provided that $\lambda_3 \leqslant 2/M_1$. In this case, $\lambda_c \geqslant \lambda_3$ and since the polynomial is positive for $\lambda \leqslant 1/M_1$, we have

$$\frac{1}{M_1} \leqslant \lambda_3 \leqslant \lambda_c \leqslant \lambda_4 \leqslant \lambda_2. \tag{26}$$

It follows from this relationship and the above discussion that an upper bound to λ_c can be obtained, provided that $\lambda_c M_1 < 2$. The first-order estimate, λ_2, is rather easy to calculate. It can be systematically improved by considering higher-order approximations.

It would be interesting to determine the class of potentials such that $M_1^2 - 4a_2 \geqslant 0$ ensuring the existence of λ_2, which is always bounded by $2/M_1$ (see (19)). Unfortunately, we have not found a simple criterion. A necessary condition, however, can be expressed as an inequality, which we now consider.

By definition, a_2 is given by

$$a_2 = \int_0^{+\infty} r_1 V^+(r_1)\,\mathrm{d}r_1 \int_{r_1}^{+\infty} (r_2 - r_1) V^+(r_2)\,\mathrm{d}r_2 = \frac{M_1^2}{2} - b_2 \tag{27}$$

where

$$b_2 = \int_0^{+\infty} r_1^2 V^+(r_1)\,\mathrm{d}r_1 \int_{r_1}^{+\infty} V^+(r_2)\,\mathrm{d}r_2. \tag{28}$$

With this new notation λ_2 reads

$$\lambda_2 = \frac{2}{M_1 + \sqrt{4b_2 - M_1^2}}. \tag{29}$$

The condition for a positive discriminant becomes

$$b_2 \geqslant \frac{M_1^2}{4} \tag{30}$$

or equivalently

$$\int_0^{+\infty} r^2 V^+(r)\,\mathrm{d}r \int_r^{+\infty} V^+(r')\,\mathrm{d}r' \geqslant \frac{M_1^2}{4}. \tag{31}$$

An equivalent expression can be found by defining

$$F(r) = \int_r^{+\infty} V^+(r')\,\mathrm{d}r'. \tag{32}$$

Inequality (31) is obtained when the function $\log F$ is concave, and $\lim_{r\to+\infty} rF(r) = 0$. This can be shown by integrating with respect to r and r' on both sides of the equation

$$(\forall r \geqslant 0)\ (\forall r' \geqslant 0) \qquad F^2\left(\frac{r + r'}{2}\right) \geqslant F(r)F(r') \tag{33}$$

derived for the concavity condition of $\log F$. It is equivalent to

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2} \log F(r) = \frac{FF'' - (F')^2}{F^2} \leqslant 0 \tag{34}$$

which means $FF'' - (F')^2 = -F(V^+)' - (V^+)^2 \leqslant 0$. Therefore condition (31) enters the category of convexity inequalities. It is satisfied by the Woods–Saxon, the Gaussian and the exponential potentials. Note that the latter is a limiting case where $\mathrm{d}^2/\mathrm{d}r^2 \log F(r)$ is zero corresponding to $\lambda_2 = 2/M_1$.

It is simple enough to evaluate the bound λ_2, so that for potentials not satisfying $4b_2 \geqslant M_1^2$, it is very tempting to circumvent this difficulty by calculating $\lambda_2(U)$ for an attractive comparison potential, U, satisfying (31), chosen in such a way that $\lambda_c(U) \geqslant \lambda_c(W)$. The intuitively simplest possibility is to consider

$$U(r) = W(r)\theta(r - r_0)\theta(R - r)$$

where θ is the Heaviside function. In this case,

$$\lambda_c M_1 \leqslant \inf_{(r_0,R)\in\mathcal{D}_1} \frac{2M_1}{M_1(r_0, R) + \sqrt{4b_2(r_0, R) - M_1^2(r_0, R)}} \tag{35}$$

where $\mathcal{D}_1$ is the set of values (r_0, R) such that $r_0 < R$ and $4b_2(r_0, R) - M_1^2(r_0, R) \geqslant 0$. However, this bound is not satisfactory numerically.

We found a better approximation by acting on the function $F(r)$. Consider two attractive potentials, W_1 and W_2, satisfying the usual integrability conditions. By defining V_1^+ and V_2^+ as before (see equation (8)), let us first show that $F_{V_1^+} \leqslant F_{V_2^+}$ implies $\lambda_c(W_2) \leqslant \lambda_c(W_1)$.

The Schrödinger equations at the 'critical' values read

$$f''_{W_1}(r) - \frac{2m}{\hbar^2}\lambda_c(W_1)W_1 f_{W_1}(r) = 0$$
$$f''_{W_2}(r) - \frac{2m}{\hbar^2}\lambda_c(W_2)W_2 f_{W_2}(r) = 0.$$

f_{W_1} and f_{W_2} having the characteristic behaviour of 1s-state wavefunctions (no nodes). Since $F_{V_i^+}(r) = \int_r^{+\infty} V_i^+(r')\,\mathrm{d}r'$, $i = 1, 2$, the Wronskian $\mathcal{W}[f_{W_1}, f_{W_2}]_{r_0}^R$, $r_0 < R$ is equal to

$$\begin{aligned}\mathcal{W}[f_{W_1}, f_{W_2}]_{r_0}^R = {} & [f_{W_1}(r) f_{W_2}(r)(\lambda_c(W_2)F_{V_2^+}(r) - \lambda_c(W_1)F_{V_1^+}(r))]_{r_0}^R \\ & -\lambda_c(W_2)\int_{r_0}^R (f_{W_2} f_{W_1})'(r)[F_{V_2^+}(r) - F_{V_1^+}(r)]\,\mathrm{d}r \\ & +[\lambda_c(W_1) - \lambda_c(W_2)]\int_{r_0}^R (f_{W_2} f_{W_1})'(r) F_{V_1^+}(r)\,\mathrm{d}r.\end{aligned} \tag{36}$$

If $F_{V_1^+}$ and $F_{V_2^+}$ are such that $\lim_{r\to 0} r F_{V_i^+}(r) = 0$, for $i = 1, 2$, the term in square brackets in (36) vanishes when $r_0 \to 0$ and $R \to +\infty$. Since the Wronskian tends to zero when $r_0 \to 0$ and $R \to +\infty$, the sum of the two last terms on the r.h.s. tends to zero. Assume $F_{V_1^+} \leqslant F_{V_2^+}$. As W_1 and W_2 are attractive the derivatives $f'_{W_i}, i = 1, 2$ decrease and since they are zero at infinity both are positive. Therefore $(f_{W_1} f_{W_2})'$ is positive, and consequently $\lambda_c(W_2) \leqslant \lambda_c(W_1)$.

According to this, we have introduced a comparison function $F_C(r)$, under the following constraints: $r \mapsto F_C(r)$ decreases (the corresponding potential must be attractive) and $(\forall r) F_c(r) \leqslant F(r)$. This can proceed in various ways. The following prescription, although not unique, has been found useful:

$$\begin{aligned} & F_C(r) = F(r_0) && r \leqslant r_0 \\ & F_C(r) = F(r) && r_0 \leqslant r \leqslant R \\ & F_C(r) = F(R)\left(1 - \frac{r - R}{\epsilon}\right) && R \leqslant r \leqslant R + \epsilon \\ & F_C(r) = 0 && r \geqslant R + \epsilon. \end{aligned} \tag{37}$$

It is easy to verify that $F_C(r)$ satisfies the stated conditions for sufficiently small ϵ and we obtain, in the limit $\epsilon \to 0$,

$$\lambda_c M_1 \leqslant \inf_{(r_0,R)\in\mathcal{D}_2} \frac{2M_1}{\tilde{M}_1(r_0,R) + \sqrt{4\tilde{b}_2(r_0,R) - \tilde{M}_1^2(r_0,R)}} = \lambda_2^F M_1 \tag{38}$$

where

$$\begin{aligned} \tilde{M}_1(r_0,R) &= RF(R) + \int_{r_0}^{R} rV^+(r)\,\mathrm{d}r \\ \tilde{b}_2(r_0,R) &= \frac{R^2F(R)^2}{2} + \int_{r_0}^{R} r^2V^+(r)\,\mathrm{d}r \int_r^{+\infty} V^+(r')\,\mathrm{d}r'. \end{aligned} \tag{39}$$

The domain $\mathcal{D}_2$ is the set of values (r_0, R), $r_0 < R$ such that the discriminant exists.

Among other possibilities which we have investigated numerically, the best phenomenological bound we have found consists in calculating M_1 and b_2 on a finite interval $[r_0, R]$, while keeping $F(r)$ at its original value, remembering that $b_2 = \int_0^{+\infty} r^2V^+(r)F(r)\,\mathrm{d}r$. In this case, we are left with

$$\lambda_c M_1 \leqslant \inf_{(r_0,R)\in\mathcal{D}_3} \frac{2M_1}{M_1(r_0,R) + \sqrt{4b_2^*(r_0,R) - M_1^2(r_0,R)}} = \lambda^{\mathrm{ph}} M_1 \tag{40}$$

where $\mathcal{D}_3$ is the set $(r_0, R), r_0 < R$ which satisfies $4b_2^*(r_0,R) - M_1^2(r_0,R) \geqslant 0$ and

$$\begin{aligned} M_1(r_0,R) &= \int_{r_0}^{R} rV^+(r)\,\mathrm{d}r \\ b_2^*(r_0,R) &= \int_{r_0}^{R} r^2V^+(r)F(r)\,\mathrm{d}r. \end{aligned} \tag{41}$$

This prescription has no further justification.

We shall end this section with two remarks. The above bounds, λ^b, require $\lambda^b M_1 \leqslant 2$. For cases such that $\lambda_c M_1 > 2$, there is no other solution to finding a positive function U such that $(\forall r)U(r) \leqslant V^+(r)$ and satisfying $\lambda^b(U)M_1(U) \leqslant 2$. It leads to

$$\lambda_c M_1 \leqslant \lambda^b(U)M_1.$$

Secondly, for potentials having a repulsive part $r \leqslant a$, the upper bounds are obtained by solving the equation for $f_0(\lambda, a) = 0$. This is more or less obvious since for a repulsive hard core, the condition $f_0(\lambda, 0) = 0$ is equivalent to $f_0(\lambda, a) = 0$. This is nothing but solving the Schrödinger equation for the translated potential $(\forall r)\ W^a(r) = W(r+a)$.

Indeed, if we put $f_0^a(\lambda, r) = f_0(\lambda, a+r)$ equation (10) reads

$$\begin{aligned} f_0^a(\lambda,r) &= 1 - \lambda \int_{r+a}^{+\infty} (r'-r-a)V^+(r')f_0^a(\lambda, r'-a)\,\mathrm{d}r' \\ &\equiv 1 - \lambda \int_r^{+\infty} (r'-r)V^+(r'+a)f_0^a(\lambda,r')\,\mathrm{d}r'. \end{aligned}$$

2.2. $\ell \neq 0$

As far as the critical zero energy bound state is concerned, the Schrödinger equation for waves of angular momentum $\ell \neq 0$ reduces to an s-wave problem. In order to show it, we start from the radial wave equation

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2} f_\ell(\lambda,r) + \left(\lambda V^+(r) - \frac{\ell(\ell+1)}{r^2}\right) f_\ell(\lambda,r) = 0. \tag{42}$$

The transformation

$$r = x^{1/(2\ell+1)}$$
$$f_\ell(r) = r^{-\ell}\phi_\ell(x) \tag{43}$$

yields

$$\frac{d^2}{dx^2}\phi_\ell(\lambda, x) + \frac{\lambda}{(2\ell+1)^2} V^+(x^{1/(2\ell+1)}) x^{-4\ell/(2\ell+1)}\phi_\ell(\lambda, x) = 0 \tag{44}$$

which is equivalent to an s-wave equation. Consequently the results of the preceding section can be applied to $\phi_\ell(\lambda, x)$. For instance, by using transformation (43), searching for λ_c for the Gaussian potential at $\ell = \frac{1}{2}$, is equivalent to searching for the critical value in the $\ell = 0$ Yukawa case.

Note that for regular potentials, this transformation introduces a singularity at the origin which never exceeds $1/x^2$. In the case of singular potentials behaving like $r^{-\alpha}$, $\alpha < 2$ at the origin, the transformed potential is still singular at the origin, where it behaves like $x^{-(\alpha+4\ell)/(2\ell+1)}$. Thus, its singularity is strictly less than x^{-2}. At $x \to +\infty$ the transformed potential decreases as $x^{-(\alpha+4\ell)/(2\ell+1)}$, when $\lim_{r\to+\infty} r^\alpha V^+(r) = 0$, $(\alpha > 2)$. Thus it decreases faster than x^{-2}.

Note also that the concavity of the transformed V^+, according to (32) and (34), is decreasing with increasing angular momentum ℓ. Thus, it becomes more and more difficult to get any bound $\lambda_2^{(\ell)}$ when the angular momentum increases.

The coefficients M_1 and b_2, introduced for $\ell = 0$, depend on ℓ according to

$$M_1 \mapsto (2\ell+1)\int_0^{+\infty} rV^+(r)\,dr = (2\ell+1)M_1$$
$$b_2 \mapsto (2\ell+1)^2\int_0^{+\infty} r^{2\ell+2}V^+(r)\,dr\int_r^{+\infty} r'^{-2\ell}V^+(r')\,dr' = (2\ell+1)^2 b_2^{(\ell)}. \tag{45}$$

In r-space, the expansion of the radial wavefunction becomes

$$\varphi_\ell(\lambda, r) = \sum_{n=0}^{+\infty}\varphi_\ell^{(n)}(\lambda, r) \tag{46}$$

where $\varphi_\ell(\lambda, r) = r^\ell f_\ell(\lambda, r)$. The values of $\varphi_\ell^{(n)}$ are given by

$$\varphi_\ell^{(0)}(\lambda, r) = 1$$
$$\varphi_\ell^{(n)}(\lambda, r) = -\frac{\lambda}{2\ell+1}\int_r^{+\infty}\left(r' - \left(\frac{r}{r'}\right)^{2\ell} r\right)\varphi_\ell^{(n-1)}(\lambda, r')V^+(r')\,dr'. \tag{47}$$

Note that (46) and (47) can be extracted from the Volterra integral equation obtained from the two solutions $r^{\ell+1}$ and $r^{-\ell}$, combined with the asymptotic condition $\lim_{r\to+\infty} r^\ell f_\ell(\lambda, r) = 1$.

At the origin

$$\lim_{r\to0^+}\varphi_\ell(\lambda, r) = \sum_{n=0}^{+\infty}(-)^n a_n^{(\ell)}\left(\frac{\lambda}{2\ell+1}\right)^n \tag{48}$$

where $a_0^{(\ell)} = 1$, $a_1^{(\ell)} = M_1$, $a_2^{(\ell)} = M_1^2/2 - b_2^{(\ell)}$ and

$$a_n^\ell = \int_0^{+\infty} r_1V^+(r_1)\,dr_1\int_{r_1}^{+\infty}\left(r_2 - r_1\left(\frac{r_1}{r_2}\right)^{2\ell}\right)V^+(r_2)\,dr_2\ldots$$

$$\ldots \int_{r_{n-2}}^{+\infty} \left(r_{n-1} - r_{n-2} \left(\frac{r_{n-2}}{r_{n-1}} \right)^{2\ell} \right) V^+(r_{n-1})\, \mathrm{d}r_{n-1}$$
$$\times \int_{r_{n-1}}^{+\infty} \left(r_n - r_{n-1} \left(\frac{r_{n-1}}{r_n} \right)^{2\ell} \right) V^+(r_n)\, \mathrm{d}r_n. \qquad (49)$$

Therefore the new series becomes an expansion of the variable $\lambda/(2\ell+1)$. Applying the previous results we find that when $\lambda/(2\ell+1) < 1/M_1$ no bound state exists, in agreement with the Bargmann inequality.

The bound λ_2 becomes

$$\frac{\lambda_2^{(\ell)}}{2\ell+1} M_1 = \frac{2}{1+\sqrt{4b_2^{(\ell)}/M_1^2 - 1}} \qquad (50)$$

and exists when $b_2^{(\ell)} \geqslant M_1^2/4$. This convexity inequality is satisfied when the second derivative of $\log(\int_{r^{1/(2\ell+1)}}^{+\infty} V^+(r') r'^{-2\ell}\, \mathrm{d}r')$ is negative or zero. It should be noted that the bound $\lambda_2^{(\ell)}$ is dominated by $2(2\ell+1)/M_1$ and we have

$$1 \leqslant \frac{\lambda_c^{(\ell)} M_1}{2\ell+1} \leqslant \frac{\lambda_2^{(\ell)} M_1}{2\ell+1} \leqslant 2. \qquad (51)$$

Due to reasons stated above, concerning the concavity (34) which decreases with ℓ increasing, the extraction of $\lambda_2^{(\ell)}$ faces rapidly increasing difficulties. In this case we use the variational approach of equation (38) or (40), where $\tilde{b}_2(r_0, R), b_2^*(r_0, R)$ have to be transformed in $\tilde{b}_2^{(\ell)}(r_0, R), b_2^{*(\ell)}(r_0, R)$ according to (45). Reciprocally, the concavity increases for ℓ decreasing and for values $\ell > -\frac{1}{2}$ close to $-\frac{1}{2}$, the coefficient $b_2^{(\ell)}$ tends to $M_1^2/2$. Then equation (31) is satisfied, and $\lambda_2^{(\ell)}$ always exists for ℓ close enough to $-\frac{1}{2}$.

3. Checking the bounds on some common potentials

In order to see if the bounds we are advocating are of practical interest, numerical tests have been performed for a set of common, relevant potentials. Unless specified, we consider the s-wave. The bounds are compared with the exact values λ_c. The results are displayed in table 1, where the quoted quantities are $\gamma_i = \lambda_i M_1/(2\ell+1)$, $i = 2$–4 and $\gamma_c = \lambda_c M_1/(2\ell+1)$.

Table 1. Second- to fourth-order approximations of the critical value λ_c. The symbol γ refers to the relevant variable $\lambda M_1/(2\ell+1)$ (see text). Lower and upper bounds are denoted by (−) and (+), respectively.

Potentials	γ_2 (+)	γ_3 (−)	γ_4 (+)	γ_c
Square well	1.267 95	1.232 29	1.233 74	$\pi^2/8 \simeq 1.233\,70$
Gaussian	1.453 18	1.336 15	1.342 26	1.3418
Exponential	2	1.429 99	1.446 78	$(r_1^2/4)$[a] $\simeq 1.445\,80$
Hulthén	—	1.579 67	1.652 38	$\pi^2/6 \simeq 1.644\,93$
Yukawa	—	1.600 78	1.689 85	1.6798
Square well $\ell = 1$	—	1.579 67	1.652 38	$\pi^2/6 \simeq 1.644\,93$

[a] r_1 denotes the first zero of the derivative of the zeroth order Bessel function.

Because of the scaling property, which does not affect the value of $\lambda_c M_1$, all the length constants appearing in the potentials have been set to unity. The variable r is thus dimensionless.

For the shell-delta potential, $V^+(r) = \delta(r-1)$, the series reduces to $1 - \lambda M_1$. Then $\lambda M_1 \equiv 1$. This means that the bound λ_2 gives the exact value in this case.

For the square well, $V^+(r) = \theta(1-r)$, the series equation (11) reads

$$f_0(\lambda, 0) = \sum_{n=0}^{+\infty} \frac{(-)^n}{(2n)!} \lambda^n \qquad \ell = 0$$

$$f_1(\lambda, 0) = \sum_{n=0}^{+\infty} \frac{(-)^n}{(2n+1)!} \lambda^n \qquad \ell = 1.$$

As can be seen from table 1, γ_2 constitutes a very good approximation to the exact value for $\ell = 0$. The case $\ell = 1$ is typical in that γ_2 does not exist. On the other hand, the fourth order γ_4 is very close to γ_c.

For the exponential, $V^+(r) = \mathrm{e}^{-r}$, (11) becomes

$$f_0(\lambda, 0) = \sum_{n=0}^{+\infty} \frac{(-)^n}{n!n!} \lambda^n. \tag{52}$$

This case is situated at the limit $\lambda_2 M_1 = 2$. The second-order bound is quite large and the results are sensibly improved at the fourth order.

For the Hulthén potential, $V^+(r) = (\mathrm{e}^r - 1)^{-1}$, we have the expansion

$$f(\lambda, 0) = \sum_{n=0}^{+\infty} \frac{(-)^n}{(2n+1)!} \pi^{2n} \lambda^n. \tag{53}$$

Up to the π^{2n} factor, this is the same as for the square well with $\ell = 1$. Thus, renormalizing by the volume integral leads to identical results.

For the following potentials, λ_c cannot be extracted analytically.

For the Gaussian potential, $V^+(r) = \mathrm{e}^{-r^2}$, (11) is approximated up to the fourth order by

$$\begin{aligned} f_0(\lambda, 0) = 1 - \frac{1}{2}\lambda + \frac{1}{16}(4-\pi)\lambda^2 - \left(\frac{1}{8} - \frac{\pi}{32} + \frac{3\arctan(\sqrt{2})}{8\sqrt{2}} - \frac{\pi}{8\sqrt{2}}\right)\lambda^3 \\ + \left(\frac{1}{16} + \frac{3\arctan(\sqrt{2})}{16\sqrt{2}} - \frac{\pi}{16\sqrt{2}} - \frac{\pi}{32\sqrt{3}} + \frac{\pi^2}{1536}\right)\lambda^4 + \mathrm{O}(\lambda^5). \end{aligned} \tag{54}$$

The second-order approximation, γ_2, approaches the exact value within 10%. The fourth order, evaluated using the property $a_3 = M_1^3/6 - b_2 M_1 + 2b_3$ (b_3 is introduced in appendix B) and by integrating a_4 by parts, gives almost the exact value.

For the Yukawa potential $V^+(r) = \mathrm{e}^{-r}/r$,

$$\begin{aligned} f_0(\lambda, 0) = 1 - \lambda + (1 - \log(2))\lambda^2 - (1 + \log(2) - \tfrac{3}{2}\log(3))\lambda^3 \\ + (1 - 4\log(2) + \tfrac{3}{2}\log(3) - Li_2(-1/2) + Li_2(-1) \\ + Li_2(-2) - Li_2(-3))\lambda^4 + \mathrm{O}(\lambda^5) \end{aligned} \tag{55}$$

where $Li_2(x)$ is the function [7]

$$Li_2(x) = -\int_0^x \frac{\log(1-y)}{y}\,\mathrm{d}y.$$

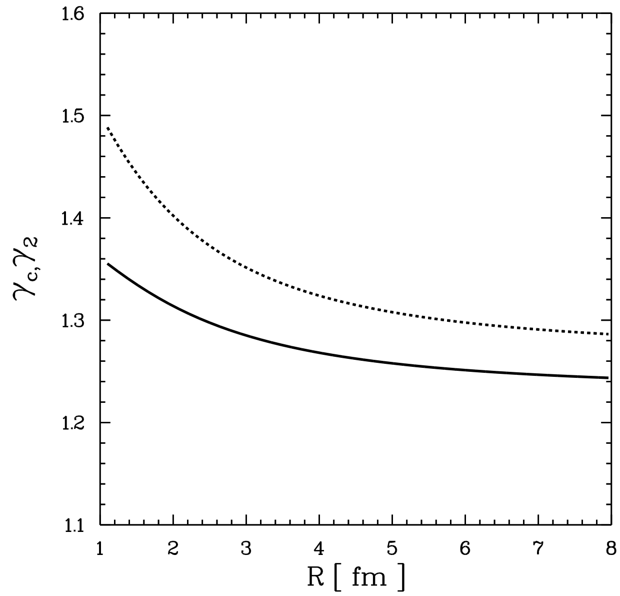

Figure 1. Full curve: variation of the critical parameter $\gamma_c = \lambda_c M_1/(2\ell + 1)$ as a function of R for the Woods–Saxon potential, equation (56). Broken curve: R-dependence of the second-order approximation to λ_c, equation (19), renormalized by $M_1/(2\ell + 1)$. Note that γ_4 would be indistinguishable from the γ_c curve (see text).

The bound γ_2 cannot be calculated whereas γ_4 is quite satisfactory. We notice that the Yukawa potential has a γ_c very close to that of the Hulthén potential. Both potentials behave in a similar way at the origin and infinity, suggesting that the behaviours at both extremes are of key importance for the value of λ_c.

The Woods–Saxon potential is

$$V^+(r) = \frac{1}{1 + \exp((r - R)/0.5)}. \tag{56}$$

The curve $R \mapsto \lambda_c M_1$ is drawn in figure 1. For R infinite the Woods–Saxon potential resembles a square well potential and we found a value γ_c similar to that of the square well. The upper bound γ_2 (broken curve) is a good approximation, better accuracy than 10% at low R; it gradually improves as R increases up to the square well results as $R \to +\infty$. We have verified that γ_4 approximates γ_c to better accuracy than 0.1%.

For the whole set of potentials considered, we display in table 1 the value of the lower bound γ_3. It proves to be rather efficient. In the worst case, among quoted values, it approaches γ_c within 5% for the Yukawa potential.

We complete this practical study of bounds by checking γ^{F} (38) and γ^{ph} (40) against γ_c, where $\gamma^{\mathrm{F,ph}} = \lambda^{\mathrm{F,ph}} M_1/(2\ell + 1)$. Although these bounds are essentially designed to overcome the problem encountered when γ_2 does not exist, it is instructive to verify their performance in cases where γ_2 can also be calculated.

The results are displayed in table 2. They are also compared with the lower bound of Glaser *et al* [4] and the upper bound of Calogero [3]. In all cases, the variational method provides a good estimate of γ_c. Except for the case $\ell = 10$ (for the square well potential $\ell = 10$ we have calculated the upper bound by truncating the potential in the vicinity of zero as explained above), γ^{F} is systematically better than the Calogero's bound. A substantial

Table 2. A comparison of different approaches of the critical value λ_c. The lower bound was derived by Glaser *et al* [4] (for the Hulthén potential, (2) is used for $p = \frac{3}{2}$), the upper bound was derived by Calogero [3], and the two semi-phenomenological bounds which we proposed: γ_2^{F} (an upper bound), (38) and γ_2^{ph}, (40). The symbol γ refers to the relevant variable $\lambda M_1/(2\ell+1)$ (see text). Lower and upper bounds are denoted by (−) and (+), respectively.

Potentials	γ^* (−) [4]	γ^{**} (+) [3]	γ_2^{F} (+)	γ_2^{ph}	γ_c
Square well	1.179	1.333	1.268	1.243	1.234
Gaussian	1.330	1.519	1.413	1.363	1.342
Exponential	1.438	1.692	1.567	1.489	1.446
Hulthén	$(p = \frac{3}{2})$ 1.616	2.000	1.875	1.733	1.645
Yukawa	1.664	2.067	1.932	1.777	1.680
Square well $\ell = 1$	1.520	1.969	1.861	1.726	1.645
Square well $\ell = 10$	2.908	6.914	6.933	5.840	4.611

improvement is obtained with γ^{ph}, nevertheless less satisfactory than γ_4.

Finally, we remark that for the lower bounds, γ_3 yields a result closer to γ_c than the value of Glaser *et al* [4] when γ_2 exists. The opposite is true otherwise, even for the exponential. It suggests that in this latter case γ_5 would bring a sizeable improvement over γ_3.

4. Conclusions

In the present work, we have established simple bounds to λ_c, the 'critical' value of the coupling constant ensuring the existence of at least one bound state for $\lambda \geqslant \lambda_c$ in the case of finite range or similar potentials [5]. The method is based on a formal resolution of the Schrödinger equation for the zero energy state, which allows us to determine λ_c.

For this particular case of zero energy states, a change of variable reduces the $\ell \neq 0$ equation into a form similar to the s-wave equation. It allows us to easily calculate bounds to λ_c for $\ell \neq 0$, except that, as ℓ increases, the condition to obtain low-order bounds, linked to the concavity condition (34), is satisfied with increasing difficulty.

We distinguish among two kinds of bounds. The first kind are derived from a systematic expansion of the Schrödinger equation solution. In principle, it yields λ_c to any desired accuracy. In practice however, only equations involving the lowest-order contributions are retained. The calculations are already quite involved at the fourth order, higher orders becoming tedious.

The second set is obtained in a semi-phenomenological way, introducing comparison functions $0 \leqslant U(r) \leqslant V^+(r)$ or $F_C(r) \leqslant F(r)$, so that the bounds result from the solution of a quadratic equation, together with a minimization procedure. Although it contains some arbitrariness, the prescription is found to be efficient, and yields results which compare well with the exact values.

Finally, by comparing our results with the bounds proposed by Glaser *et al* [4] and Calogero [3], the present method is found to be quite satisfactory.

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Appendix A

Let us expand the function $f_0(\lambda, r)$ as

$$f_0(\lambda, r) = \sum_{n=0}^{+\infty} (-)^n a_n(r) \lambda^n \tag{A1}$$

where, setting $r_0 = r$,

$$a_n(r) = \int_{(R^+)^n} \prod_{i=1}^{n} (r_i - r_{i-1}) \theta(r_i - r_{i-1}) V^+(r_i)\, \mathrm{d}r_i \qquad a_0 = 1. \tag{A2}$$

Introducing the explicit expression for the last two terms, we get, for $n \geqslant 2$:

$$\begin{aligned} a_n(r) = \int_{(R^+)^{n-2}} &\prod_{i=1}^{n-2} (r_i - r_{i-1}) \theta(r_i - r_{i-1}) V^+(r_i)\, \mathrm{d}r_i \\ &\times \int_{r_{n-2}}^{+\infty} (r_{n-1} - r_{n-2}) V^+(r_{n-1})\, \mathrm{d}r_{n-1} \int_{r_{n-1}}^{+\infty} (r_n - r_{n-1}) V^+(r_n)\, \mathrm{d}r_n \end{aligned} \tag{A3}$$

with the convention $\prod_{i=1}^{n-2} \equiv 1$ for $n = 2$. Here, $r_n - r_{n-1}$ is dominated by $r_n - r_{n-2}$, since $r_{n-2} \leqslant r_{n-1}$, and we get, because V^+ is positive

$$\begin{aligned} a_n(r) \leqslant \tfrac{1}{2} \int_{(R^+)^{n-2}} &\prod_{i=1}^{n-2} (r_i - r_{i-1}) \theta(r_i - r_{i-1}) V^+(r_i)\, \mathrm{d}r_i \\ &\times \left(\int_{r_{n-2}}^{+\infty} (r_{n-1} - r_{n-2}) V^+(r_{n-1})\, \mathrm{d}r_{n-1} \right)^2 \end{aligned} \tag{A4}$$

since the function $(r_n - r_{n-2})(r_{n-1} - r_{n-2}) V^+(r_n) V^+(r_{n-1})$ is symmetrical in the variables r_{n-1}, r_n. Moreover, taking into account that

$$\left(\int_{r_{n-2}}^{+\infty} (r_{n-1} - r_{n-2}) V^+(r_{n-1})\, \mathrm{d}r_{n-1} \right)^2$$

is dominated by

$$\int_{r}^{+\infty} (r' - r) V^+(r')\, \mathrm{d}r' \int_{r_{n-2}}^{+\infty} (r_{n-1} - r_{n-2}) V^+(r_{n-1})\, \mathrm{d}r_{n-1}$$

since $r_{n-2} \geqslant r_0 \equiv r$, we obtain:

$$a_n(r) \leqslant \tfrac{1}{2} \int_{r}^{+\infty} (r' - r) V^+(r')\, \mathrm{d}r' \int_{(R^+)^{n-1}} \prod_{i=1}^{n-1} (r_i - r_{i-1}) \theta(r_i - r_{i-1}) V^+(r_i)\, \mathrm{d}r_i. \tag{A5}$$

In other words

$$a_n(r) \leqslant \frac{a_{n-1}(r)}{2} \int_{r}^{+\infty} (r' - r) V^+(r')\, \mathrm{d}r'. \tag{A6}$$

This inequality holds for every positive r and $n \geqslant 2$ and in particular for $r = 0$ where $a_n(r)$ is equal to a_n.

The series $\sum_{n=0}^{+\infty} (-)^n a_n \lambda^n$ is alternating and satisfies $a_n \leqslant (M_1/2) a_{n-1}$. Provided that $\lambda \leqslant 2/M_1$, the nth-order remainder, $\mathcal{R}_n$, is positive or negative according to the parity of n. Indeed:

$$\mathcal{R}_{2p}(\lambda) = \sum_{n=p}^{+\infty} \lambda^{2n} (a_{2n} - \lambda a_{2n+1}) \tag{A7}$$

and

$$\mathcal{R}_{2p+1}(\lambda) = -\sum_{n=p}^{+\infty} \lambda^{2n+1}(a_{2n+1} - \lambda a_{2n+2}) \tag{A8}$$

all terms involved in (A7) ($p \geqslant 1$) and (A8) being positive.

Appendix B

In this appendix, we define b_3 and give its connection to a_3.

We recall the definition of a_3:

$$a_3 = \int_0^{+\infty} rV^+(r)\,\mathrm{d}r \int_r^{+\infty} (r'-r)V^+(r')\,\mathrm{d}r' \int_{r'}^{+\infty} (r''-r')V^+(r'')\,\mathrm{d}r''. \tag{B1}$$

Expanding the product $r(r'-r)(r''-r')$ we get

$$\begin{aligned} a_3 = \frac{M_1^3}{6} &- \int_0^{+\infty} r^2V^+(r)\,\mathrm{d}r \int_r^{+\infty} V^+(r')\,\mathrm{d}r' \int_{r'}^{+\infty} r''V^+(r'')\,\mathrm{d}r'' \\ &- \int_0^{+\infty} rV^+(r)\,\mathrm{d}r \int_r^{+\infty} r'^2V^+(r')\,\mathrm{d}r' \int_{r'}^{+\infty} V^+(r'')\,\mathrm{d}r'' \\ &+ \int_0^{+\infty} r^2V^+(r)\,\mathrm{d}r \int_r^{+\infty} r'V^+(r')\,\mathrm{d}r' \int_{r'}^{+\infty} V^+(r'')\,\mathrm{d}r'' \end{aligned} \tag{B2}$$

where

$$M_1^3/6 = \int_0^{+\infty} rV^+(r)\,\mathrm{d}r \int_r^{+\infty} r'V^+(r')\,\mathrm{d}r' \int_{r'}^{+\infty} r''V^+(r'')\,\mathrm{d}r''.$$

After a modification of the integration order, which is allowed since V^+ is positive, adding the second and the third integral leads to

$$\begin{aligned} &- \int_0^{+\infty} r^2V^+(r)\,\mathrm{d}r \int_r^{+\infty} r'V^+(r')\,\mathrm{d}r' \int_r^{r'} V^+(r'')\,\mathrm{d}r'' \\ &- \int_0^{+\infty} r^2V^+(r)\,\mathrm{d}r \int_0^{r} r'V^+(r')\,\mathrm{d}r' \int_r^{+\infty} V^+(r'')\,\mathrm{d}r'' \end{aligned}$$

which is equivalent to

$$\begin{aligned} &- \int_0^{+\infty} r^2V^+(r)\,\mathrm{d}r \int_r^{+\infty} r'V^+(r')\,\mathrm{d}r' \left(\int_r^{+\infty} V^+(r'')\,\mathrm{d}r'' - \int_{r'}^{+\infty} V^+(r'')\,\mathrm{d}r'' \right) \\ &- \int_0^{+\infty} r^2V^+(r)\,\mathrm{d}r \left(M_1 \int_r^{+\infty} V^+(r'')\,\mathrm{d}r'' - \int_r^{+\infty} r'V^+(r')\,\mathrm{d}r' \int_r^{+\infty} V^+(r'')\,\mathrm{d}r'' \right). \end{aligned}$$

Consequently the sum of the second and the third integral leads to $b_3 - M_1b_2$, where we have introduced

$$b_3 = \int_0^{+\infty} r^2V^+(r)\,\mathrm{d}r \int_r^{+\infty} r'V^+(r')\,\mathrm{d}r' \int_{r'}^{+\infty} V^+(r'')\,\mathrm{d}r'' \tag{B3}$$

and using the definition of b_2, (28). We find finally

$$a_3 = \frac{M_1^3}{6} - b_2M_1 + 2b_3. \tag{B4}$$

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