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Sufficient conditions for the existence of bound states in a central potential

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Abstract

We show how a large class of sufficient conditions for the existence of bound states, in non-positive central potentials, can be constructed. These sufficient conditions yield upper limits on the critical value, $g_{\rm c}^{(\ell)}$, of the coupling constant (strength), g, and of the potential, $V(r) = -gv(r)$, for which a first ℓ-wave bound state appears. These upper limits are significantly more stringent than hitherto known results.

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1. Introduction

There exist in the literature several necessary conditions for the existence of at least one ℓ-wave bound state in a given central potential. These necessary conditions yield lower limits on the critical value, $g_{\rm c}^{(\ell)}$, of the coupling constant (strength), g, and of the potential, $V(r) = -gv(r)$, for which a first ℓ-wave bound state appears.

In 1976, Glaser *et al* obtained a strong necessary condition for the existence of bound states in an arbitrary central potential in three dimensions ($\hbar^2/(2m) = 1$) [1],

$$\frac{(p-1)^{p-1}\Gamma(2p)}{(2\ell+1)^{2p-1}p^p\Gamma^2(p)}\int_0^\infty \frac{\mathrm{d}r}{r}[r^2V^-(r)]^p \geqslant 1 \tag{1}$$

where $V^-(r) = \max(0, -V(r))$ is the negative part of the potential and with the restriction $p \geqslant 1$. This inequality is nontrivial provided 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)

$$\lim_{r\to 0}[r^{2-\varepsilon}V(r)] = 0 \tag{2}$$

$$\lim_{r\to\infty}[r^{2+\varepsilon}V(r)] = 0. \tag{3}$$

We assume throughout that the potentials satisfy relations (2) and (3) and that they are piecewise continuous for $r \in]0, \infty[$. The lower limit on $g_c^{(\ell)}$ obtained from (1) is actually very accurate as has been demonstrated in several examples (see for example [1–3] as well as section 3).

Recently other strong necessary conditions have also been obtained [3],

$$\frac{2}{(2\ell+1)^2}\int_0^\infty \mathrm{d}x\, x^{-2\ell}V^-(x)\int_0^x \mathrm{d}y\, y^{2\ell+2}V^-(y) \geqslant 1 \tag{4}$$

$$\frac{6}{(2\ell+1)^3}\int_0^\infty \mathrm{d}x\, x^{-2\ell}V^-(x)\int_0^x \mathrm{d}y\, yV^-(y)\int_0^y \mathrm{d}z\, z^{2\ell+2}V^-(z) \geqslant 1. \tag{5}$$

As shown in [3], these two inequalities, (4) and (5), are natural extensions of the Bargmann–Schwinger necessary condition [4, 5] (first obtained by Jost and Pais [6])

$$\frac{1}{2\ell+1}\int_0^\infty \mathrm{d}x\, xV^-(x) \geqslant 1. \tag{6}$$

Actually inequalities (6), (4) and (5) are the first members of a sequence of necessary conditions which yield a monotonic sequence of lower limits on the critical value of the strength of the potential, $g_c^{(\ell)}$, which converges to the exact critical strength [3]. This remark implies that inequality (5) yields stronger restriction than relation (4). The complexity of each member of this sequence of necessary conditions becomes rapidly important and only relations (4) and (5) can be easily used. It has been shown, with some test potentials, that relation (5) can be better than relation (1), especially for $\ell = 0$ (see tests performed in [3] and in section 3).

Other necessary conditions for the existence of bound states can be found in the literature (see for example [7, 8] and for reviews see [9–11]), but none, in general, yields stronger restrictions than (1) and (5).

Few sufficient conditions for the existence of an ℓ-wave bound state in a central potential, yielding upper limits on $g_c^{(\ell)}$, can be found in the literature. Let us mention two sufficient conditions found by Calogero in 1965 [12, 13]

$$\int_0^a \mathrm{d}r\, r|V(r)|(r/a)^{2\ell+1} + \int_a^\infty \mathrm{d}r\, r|V(r)|(r/a)^{-(2\ell+1)} > 2\ell+1 \tag{7}$$

and

$$a\int_0^\infty \mathrm{d}r|V(r)|[(r/a)^{2\ell} + (r/a)^{-2\ell}a^2|V(r)|]^{-1} > 1. \tag{8}$$

These two conditions apply provided the potential is nowhere positive, $V(r) = -|V(r)|$; in both of them a is an arbitrary positive constant, and of course the most restrictive conditions are obtained by minimizing the left-hand sides of (7) and (8) over all positive values of a.

Few other sufficient conditions for the existence of bound states can be found in the literature (see [2, 3, 14]), but they are either quite complicated or less stringent than (7) and (8).

In this paper, we obtain a strong sufficient condition for the existence of bound states yielding accurate restrictions on the critical strength $g_c^{(\ell)}$ which improve significantly the restrictions provided by relations (7) and (8).

2. Sufficient condition and upper limit on the critical strength

The idea used to derive the upper limit on $g_c^{(\ell)}$ is to transform the standard eigenvalue problem obtained with the time independent Schrödinger equation, where the eigenvalues are the eigenenergies, into an eigenvalue problem where the eigenvalues are the critical coupling constants. These critical values of the strength of the potential correspond to the occurrence of an eigenstate with vanishing energy.

Following Schwinger [5] (see also [15]), we consider the zero energy Schrödinger equation that we write in the form of an integral equation incorporating the boundary conditions

$$u_\ell(r) = -\int_0^\infty \mathrm{d}r'\, g_\ell(r,r')V(r')u_\ell(r') \tag{9}$$

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

$$g_\ell(r,r') = \frac{1}{2\ell+1} r_<^{\ell+1} r_>^{-\ell} \tag{10}$$

where $r_< = \min[r,r']$ and $r_> = \max[r,r']$. An important technical difficulty appears if the potential possesses some changes of sign (see relation (11)). This is overcome in the derivation of necessary conditions, or of upper bounds on the number of bound states, by considering the negative part of the potential instead of the potential itself ($V(r) \to V^-(r) = \max(0, -V(r))$). Indeed, the potential $V^-(r)$ is more negative than $V(r)$ and thus a necessary condition for the existence of an ℓ-wave bound state 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 $v(r) \geqslant 0$.

To obtain a symmetrical kernel we now introduce a new wavefunction as

$$\phi_\ell(r) = |V(r)|^{1/2} u_\ell(r). \tag{11}$$

Equation (9) becomes

$$\phi_\ell(r) = g\int_0^\infty \mathrm{d}r'\, K_\ell(r,r')\phi_\ell(r') \tag{12}$$

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

$$K_\ell(r,r') = v(r)^{1/2} g_\ell(r,r') v(r')^{1/2}. \tag{13}$$

Relation (12) is thus an eigenvalue problem and, for each value of ℓ, the smallest characteristic number is just the critical value $g_{\mathrm{c}}^{(\ell)}$. The other characteristic numbers correspond to the critical values of the strength for which second, third, ..., ℓ-wave bound states appear. The kernel (13) acting on the Hilbert space $L^2(\mathbb{R})$ is a Hilbert–Schmidt operator for the class of potentials defined by (2) and (3). Thus this kernel satisfies the inequality

$$\int_0^\infty \int_0^\infty \mathrm{d}x\,\mathrm{d}y\, K_\ell(x,y)K_\ell(x,y) < \infty. \tag{14}$$

Consequently the eigenvalue problem (12) always possesses at least one characteristic number [16, pp 102–6] (in general, this problem has an infinity of characteristic numbers). Note also that the kernel (13) is the so-called Birman–Schwinger kernel [5, 15].

Now we use the theorem (see for example [16, pp 118–9] which states that, for a symmetric (positive) Hilbert–Schmidt kernel, we have the variational principle

$$\max_\varphi \left[\int_0^\infty \int_0^\infty \mathrm{d}x\,\mathrm{d}y\, K_\ell(x,y)\varphi(x)\varphi(y)\right] = \frac{1}{g_{\mathrm{c}}^{(\ell)}} \tag{15}$$

for $\varphi(r)$ satisfying

$$\int_0^\infty \mathrm{d}r\, \varphi(r)^2 = 1. \tag{16}$$

The maximal value is reached for $\varphi(x) = \phi_\ell^{c}(x)$, where $\phi_\ell^{c}(x)$ is the eigenfunction associated with $g_c^{(\ell)}$. Consequently for an arbitrary normalized function, $f(x)$, we obtain the following upper limit on $g_c^{(\ell)}$:

$$g_c^{(\ell)} \leqslant \left[\int_0^\infty \int_0^\infty \mathrm{d}x\,\mathrm{d}y\, K_\ell(x,y) f(x) f(y)\right]^{-1}. \tag{17}$$

To apply the above theorem, we simply choose

$$f(r) = A[r^{2p-1} v(r)^p]^{1/2} \qquad p > 0 \tag{18}$$

where A is the normalization factor. With the choice (18), the upper limit (17) reads

$$g_c^{(\ell)} \leqslant \mathcal{L} \int_0^\infty \mathrm{d}x\, F(2p-1; x) \left[\int_0^\infty \mathrm{d}x\, F(p; x) x^{-\mathcal{L}} \int_0^x \mathrm{d}y\, F(p; y) y^{\mathcal{L}}\right]^{-1} \tag{19}$$

with $F(q; x) = x^q v(x)^{(q+1)/2}$ and $\mathcal{L} = \ell + 1/2$.

We do not consider other choices for the function $f(r)$ here since, as shown in section 3, relation (19) is already very accurate. We just mention that another possible choice for monotonic potentials is $f(r) = A[v(r)(v(0) - v(r))^p]^{1/2}$. We have verified with an exponential potential, see (22), that this choice yields a slight improvement.

Obviously, the sufficient condition for the existence of an ℓ-wave bound state, from which the upper limit (19) on $g_c^{(\ell)}$ is obtained, reads

$$\int_0^\infty \mathrm{d}x\, \tilde{F}(p; x) x^{-\mathcal{L}} \int_0^x \mathrm{d}y\, \tilde{F}(p; y) y^{\mathcal{L}} \left\{\mathcal{L} \int_0^\infty \mathrm{d}x\, \tilde{F}(2p-1; x)\right\}^{-1} \geqslant 1 \tag{20}$$

with $\tilde{F}(q; x) = x^q |V(x)|^{(q+1)/2}$, $\mathcal{L} = \ell + 1/2$ and $p > 0$.

3. Tests

In this section, we propose to test the accuracy of the upper limit (19) with four potentials: a square well potential

$$V(r) = -gR^{-2}\theta(1 - r/R) \tag{21}$$

an exponential potential

$$V(r) = -gR^{-2}\exp(-r/R) \tag{22}$$

a Yukawa potential

$$V(r) = -g(rR)^{-1}\exp(-r/R) \tag{23}$$

and the shifted truncated inverse square (STIS) potential

$$\begin{aligned} V(r) &= -g(R + r)^{-2} && \text{for} \quad 0 \leqslant r \leqslant \alpha R \\ &= 0 && \text{for} \quad r > \alpha R. \end{aligned} \tag{24}$$

In these potentials, the radius R is arbitrary (but positive) and α is an arbitrary positive number.

The minimization of the upper limit (19) over the positive values of p can be performed analytically only for the square well potential. We find

$$g_c^{(\ell)} \leqslant \mathcal{L}(\sqrt{\mathcal{L} + 1} + 1)^2. \tag{25}$$

Comparisons between the exact value of the critical coupling constants of the potentials, $g_c^{(\ell)}$, the previously known upper and lower limits reported in section 1 and the new upper limit (19) are given in tables 1, 2 and 3 for various values of ℓ and for the potentials (21)–(23). These comparisons clearly show that the new upper limit is very cogent as well as the lower

Table 1. Comparison between the exact values of the critical coupling constant $g_c^{(\ell)}$ of the square well potential (21) for various values of ℓ and the lower limits on $g_c^{(\ell)}$ obtained with relations (1), (5) and (6), called respectively $g_{\mathrm{GGMT}}^{(\ell)}$, $g_{\mathrm{B}}^{(\ell)}$ and $g_{\mathrm{BS}}^{(\ell)}$ and the upper limits obtained with the formulae, (7), (8) and (19), called respectively, $g_{\mathrm{C1}}^{(\ell)}$, $g_{\mathrm{C2}}^{(\ell)}$ and $g_{\mathrm{New}}^{(\ell)}$.

ℓ	$g_{\mathrm{BS}}^{(\ell)}$	$g_{\mathrm{B}}^{(\ell)}$	$g_{\mathrm{GGMT}}^{(\ell)}$	$g_{\mathrm{c}}^{(\ell)}$	$g_{\mathrm{New}}^{(\ell)}$	$g_{\mathrm{C1}}^{(\ell)}$	$g_{\mathrm{C2}}^{(\ell)}$
0	2	2.4662	2.3593	2.4674	2.4747	2.6667	4
1	6	9.8132	9.1220	9.8696	9.9934	11.719	10.068
2	10	19.895	18.454	20.191	20.604	25.413	20.895
3	14	32.383	30.245	33.217	34.099	43.570	35.424
4	18	47.064	44.425	48.831	50.357	66.089	53.519
5	22	63.788	60.947	66.954	69.295	92.909	75.114

Table 2. Same as for table 1 but for the exponential potential (22). In the column p, we report the values of the variational parameter p which optimize the upper limit (19).

ℓ	$g_{\mathrm{BS}}^{(\ell)}$	$g_{\mathrm{B}}^{(\ell)}$	$g_{\mathrm{GGMT}}^{(\ell)}$	$g_{\mathrm{c}}^{(\ell)}$	$g_{\mathrm{New}}^{(\ell)}$	$g_{\mathrm{C1}}^{(\ell)}$	$g_{\mathrm{C2}}^{(\ell)}$	p
0	1	1.4422	1.4383	1.4458	1.4467	1.6755	1.5442	1.4686
1	3	6.8546	7.0232	7.0491	7.0584	9.7188	7.7262	2.4313
2	5	15.257	16.277	16.313	16.334	24.724	19.794	3.4103
3	7	26.265	29.218	29.259	29.289	46.985	37.791	4.4015
4	9	39.616	45.849	45.893	45.932	76.586	61.758	5.3874
5	11	55.120	66.173	66.219	66.264	113.55	91.708	6.3804

Table 3. Same as for table 1 but for the Yukawa potential (23). In the column p, we report the values of the variational parameter p which optimize the upper limit (19).

ℓ	$g_{\mathrm{BS}}^{(\ell)}$	$g_{\mathrm{B}}^{(\ell)}$	$g_{\mathrm{GGMT}}^{(\ell)}$	$g_{\mathrm{c}}^{(\ell)}$	$g_{\mathrm{New}}^{(\ell)}$	$g_{\mathrm{C1}}^{(\ell)}$	$g_{\mathrm{C2}}^{(\ell)}$	p
0	1	1.6689	1.6643	1.6798	1.6826	2.0505	1.6810	1.7217
1	3	8.5999	9.0384	9.0820	9.1039	13.390	10.706	3.1281
2	5	19.553	21.839	21.895	21.937	35.255	28.374	4.5302
3	7	33.931	40.074	40.136	40.194	67.914	54.819	5.9344
4	9	51.368	63.744	63.809	63.880	111.42	90.071	7.3404
5	11	71.615	92.850	92.918	92.998	165.80	134.14	8.7481

Table 4. Same as for table 1 but for the STIS potential (24) and $\ell = 0$. In the column p, we report the values of the variational parameter p which optimize the upper limit (19).

α	$g_{\mathrm{BS}}^{(0)}$	$g_{\mathrm{B}}^{(0)}$	$g_{\mathrm{GGMT}}^{(0)}$	$g_{\mathrm{c}}^{(0)}$	$g_{\mathrm{New}}^{(0)}$	$g_{\mathrm{C1}}^{(0)}$	$g_{\mathrm{C2}}^{(0)}$	p
0.1	227.22	282.11	269.84	282.26	283.12	306.01	440.67	1.2329
0.5	13.864	17.613	16.842	17.626	17.683	19.311	24.664	1.2608
1	5.1774	6.7253	6.4307	6.7319	6.7550	7.4520	8.6588	1.2889
5	1.0434	1.4837	1.4214	1.4875	1.4939	1.7201	1.5799	1.4159
10	0.67168	1.0066	0.96638	1.0107	1.0156	1.1998	1.0304	1.5004
50	0.33882	0.58085	0.56233	0.58684	0.59085	0.74673	0.59855	1.7633

limit (1) obtained by Glaser *et al*. We have also performed other tests, that we do not report here, with nonmonotonic potentials and the results obtained are quite similar to those reported in these tables.

In table 4, we present the same comparison for the STIS potential but for $\ell = 0$. For this potential, the critical coupling constant depends on α. The value of $g_c^{(0)}$ is obtained, for given α, by solving the following equation [10],

$$\lambda \ln(1+\alpha) + 2\arctan(\lambda) = 2\pi \tag{26}$$

with $\lambda = \sqrt{4g_{\mathrm{c}}^{(0)} - 1}$. For all values of α the results obtained with the new upper limit are again very stringent compared to previously known limits.

4. Conclusions

The sufficient condition (20) proposed in this paper yields the upper limit (19) on $g_{\mathrm{c}}^{(\ell)}$ which is analogous to the lower limit obtained three decades ago by Glaser *et al* [1]. The upper limit applies provided that the potential is nowhere positive, is less singular than the inverse square radius at the origin and that it vanishes asymptotically faster than the inverse square radius. We could use the method proposed in [17] to consider potentials with some positive parts but the result would then be much less neat and less interesting.

The method we use to derive the upper limit on the critical strength $g_{\mathrm{c}}^{(\ell)}$ is quite general and other (possibly more complicated) families of upper limits yielding (possibly) stronger restrictions on $g_{\mathrm{c}}^{(\ell)}$ could also be obtained. Indeed, the method is based on a variational principle for which a trial zero energy wavefunction is needed. There is no limitation on the accuracy of such a trial function, which implies that there is, in principle, no limitation on the accuracy of the upper limit on $g_{\mathrm{c}}^{(\ell)}$ derived with this procedure. In this paper, we have proposed in section 2 a compromise between accuracy and simplicity of the final formula. The accuracy of the upper limit on $g_{\mathrm{c}}^{(\ell)}$ was then tested in section 3 with some typical potentials. Clearly, the upper limit (19) proposed in this paper improves significantly the restriction on the possible values of $g_{\mathrm{c}}^{(\ell)}$ obtained with previously known upper limits.

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