Necessary and sufficient conditions for existence of bound states in a central potential

2003 J. Phys. A: Math. Gen. 36 9907

(http://iopscience.iop.org/0305-4470/36/38/308)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **36** (2003) 9907–9913 PII: S0305-4470(03)64381-7

Necessary and sufficient conditions for existence of bound states in a central potential

Fabian Brau

Service de Physique Générale et de Physique des Particules Elémentaires, Groupe de Physique Nucléaire Théorique, Université de Mons-Hainaut, Mons, Belgium

E-mail: fabian.brau@umh.ac.be

Received 4 June 2003
Published 10 September 2003
Online at stacks.iop.org/JPhysA/36/9907

Abstract

We obtain, using the Birman–Schwinger method, a series of necessary conditions for the existence of at least one bound state applicable to arbitrary central potentials in the context of nonrelativistic quantum mechanics. These conditions yield a monotonic series of lower limits on the 'critical' value of the strength of the potential (for which a first bound state appears) which converges to the exact critical strength. We also obtain a sufficient condition for the existence of bound states in a central monotonic potential which yield an upper limit on the critical strength of the potential.

PACS numbers: 03.65.−w, 03.65.Ge

1. Introduction

The problem of finding upper and lower limits on the number of bound states of a given potential has become a classical problem since the pioneer works of Jost and Pais in 1951 [1] and Bargmann in 1952 [2]. They obtained, for the first time, a necessary condition for the existence of bound states in a central potential which can be obtained from the following upper limit on the number of ℓ-wave bound states (setting N_ℓ to 1):

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

In this inequality, $V^-(r)$ is the negative part of the potential obtained by setting its positive part to zero and ℓ is the angular momentum. Note that we use the standard quantum-mechanical units such as $\hbar = 2m = 1$, where m is the mass of the particle. This upper limit (1), called the Bargmann–Schwinger upper limit in the literature, was the starting point of intensive studies and a fairly large number of upper and lower limits on the number of bound states for various classes of potentials was found, see for example [3–21].

0305-4470/03/389907+07$30.00

An important theorem for classifying these results was found by Chadan [8] and gives the asymptotic behaviour of the number of bound states as the strength, g, of the central potential goes to infinity:

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

where the symbol $\approx$ means asymptotic equality and $V^-(r) = -gv(r)$. This result implies that any upper and lower limit which could yield cogent results should behave asymptotically as $g^{1/2}$. More importantly, relation (2) gives the functional of the potential, that is to say the coefficient in front of $g^{1/2}$, that appears in the asymptotic behaviour. The upper limit (1) is proportional to g instead of $g^{1/2}$ and is not very stringent for strong potentials. Upper and lower limits featuring the correct $g^{1/2}$ dependence were first obtained in [7]. Upper and lower limits featuring the correct asymptotic behaviour (2) were first derived in [19, 20]. 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 and in particular upper and lower limits on the 'critical' value of the strength of the potential, g_c, for which a first bound state appears. In this case, there is no theorem to know in advance which limit yields the most stringent restriction on g_c. It is then of interest to obtain various limits, since the limit yielding the most stringent restriction changes from one potential to another.

In section 2, we obtain a series of necessary conditions for the existence of at least one bound state, applicable to arbitrary central potentials, which converges to the exact critical strength. In section 3, we present a sufficient condition for the existence of bound states in a central monotonic potential. In section 4, we perform several tests of the cogency of the limits presented in this paper and we compare them to some previously known results and to the exact results.

2. Necessary conditions

The necessary conditions for the existence of bound states derived in this section are obtained with the help of a simple extension of the Birman–Schwinger method. Birman [3] and Schwinger [4] have shown how to obtain an upper limit on the number of bound states once the Green function of the kinetic energy operator of a wave equation is known. We recall briefly the main line of the method applied to the radial Schrödinger equation for completeness; for more details see the original articles [3, 4].

The Schrödinger equation for a central potential $V(r)$ reads

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\ell(\ell+1)}{r^2}\right) u_\ell(r) = (E - V(r))u_\ell(r). \tag{3}$$

The zero-energy Schrödinger equation can be written in the form of the following integral equation:

$$u_\ell(r) = -\int_0^\infty \mathrm{d}r'\, g_\ell(r, r')V(r')u_\ell(r') \tag{4}$$

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

$$g_\ell(r, r') = \frac{1}{2\ell+1} r_<^{\ell+1} r_>^{-\ell} \tag{5}$$

where $r_< = \min[r, r']$ and $r_> = \max[r, r']$. Since the purpose of the method is to obtain an upper limit on the number of bound states, we can replace $V(r)$ by $-|V^-(r)|$ where $V^-(r)$

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

We now introduce, to obtain a symmetrical kernel, a new wavefunction as

$$\phi_\ell(r) = |V^-(r)|^{1/2} u_\ell(r). \tag{6}$$

Equation (4) becomes

$$\lambda^{-1}\phi_\ell(r) = \int_0^\infty \mathrm{d}r'\, K_\ell(r, r')\phi_\ell(r') \tag{7}$$

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

$$K_\ell(r, r') = |V^-(r)|^{1/2} g_\ell(r, r')|V^-(r')|^{1/2}. \tag{8}$$

The kernel being positive, we have $0 < \lambda_1 < \lambda_2 < \cdots < \lambda_N \leqslant 1$ and $0 < \lambda_k < \infty$ (λ_k denotes each eigenvalue of (7)). It is well known that the trace of the iterated kernels equals the sum of the eigenvalues of the integral equation (7) as follows:

$$\sum_{k=1}^{\infty} \frac{1}{(\lambda_k)^n} = \int_0^\infty \mathrm{d}r\, K_\ell^{(n)}(r, r) \tag{9}$$

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

$$K_\ell^{(n)}(s, t) = \int_0^\infty \mathrm{d}u\, K_\ell(s, u) K_\ell^{(n-1)}(u, t) \tag{10}$$

with

$$K_\ell^{(1)}(s, t) \equiv K_\ell(s, t) \tag{11}$$

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

$$\sum_{k=1}^{\infty} \frac{1}{(\lambda_k)^n} \geqslant \sum_{k=1}^{N_\ell} \frac{1}{(\lambda_k)^n} > N_\ell \tag{12}$$

where N_ℓ is the number of ℓ-wave bound states. From (9)–(12) we find that an upper limit on the number of ℓ-wave bound states of the Schrödinger equation is given by

$$N_\ell < \int_0^\infty \mathrm{d}r\, K_\ell^{(n)}(r, r). \tag{13}$$

In his article, Schwinger considers only the case $n = 1$ for equation (13) which yields the Bargmann–Schwinger upper limit (1). Indeed, greater values of n would yield upper limits which possess a worse dependence on the strength of the potential g than the upper limit (1) and which would be very poor for strong potentials. But it appears that, as described in section 4, the larger the value n the better the lower limit on the critical value of strength of the potential.

The necessary conditions for the existence of ℓ-wave bound states obtained from (13) read, respectively, for $n = 1, 2, 3$:

$$\frac{1}{2\ell + 1} \int_0^\infty \mathrm{d}r\, r\, |V^-(r)| \geqslant 1 \tag{14}$$

$$\frac{2}{(2\ell+1)^2}\int_0^\infty \mathrm{d}r_1\, r_1^{-2\ell}|V^-(r_1)|\int_0^{r_1}\mathrm{d}r_2\, r_2^{2\ell+2}|V^-(r_2)| \geqslant 1 \tag{15}$$

$$\frac{6}{(2\ell+1)^3}\int_0^\infty \mathrm{d}r_1\, r_1^{-2\ell}|V^-(r_1)|\int_0^{r_1}\mathrm{d}r_2\, r_2|V^-(r_2)|\int_0^{r_2}\mathrm{d}r_3\, r_3^{2\ell+2}|V^-(r_3)| \geqslant 1 \tag{16}$$

The improvements of the lower limits on g_c implied by relations (15) and (16) over the lower limit inferred from the well-known relation (14) are described in section 4 for a square-well potential and an exponential potential.

Let us end this section by noting that the procedure employed here also yields a necessary condition for the existence of bound states analogous to the condition obtained by Glaser *et al* [10]

$$\frac{(p-1)^{p-1}\Gamma(2p)}{(2\ell+1)^{2p-1}p^p\Gamma^2(p)}\int_0^\infty \mathrm{d}r\, r^{2p-1}|V^-(r)|^p \geqslant 1 \tag{17}$$

where $p > 1$ must be chosen to optimize the result. Indeed, for $\ell > 0$, we can use the n times the Hölder inequality in relation (13) and taking n going to infinity (see [22] for more details) we obtain

$$\left[\frac{(2\ell+1)p(p-1)}{p^2(\ell+2)(\ell-1)+3p-1}\right]^{p-1}\int_0^\infty \mathrm{d}r\, r^{2p-1}|V^-(r)|^p \geqslant 1. \tag{18}$$

The constant in front of the integral is unfortunately always greater than the constant appearing in the necessary condition (17), and relation (18) is thus always less stringent.

3. Sufficient condition

The sufficient condition is obtained with the help of a generalization of the comparison theorem proved recently and where the comparison potentials intersect (theorem 7 of [23]). The new theorem reads

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

(i) $V_1(r) < V_2(r)$ *for* $0 < r < r_1$ *and*

(ii) $\displaystyle\int_0^{r_2}\mathrm{d}y\,[V_1(y) - V_2(y)]y^2 \leqslant 0$

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

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

$$V_2(r) = -V_0\theta(R-r) \tag{19}$$

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

$$V_1(r) = -gs^{-2}v(r/s, k) \tag{20}$$

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

$$g_c^{\mathrm{up}} = \frac{\pi^2}{12}\frac{\alpha}{\int_0^\alpha \mathrm{d}y\, y^2 v(y,k)} \tag{21}$$

Table 1. Comparison between the exact values of the critical coupling constant g_c of a square-well potential for various values of ℓ and the lower limits, $g_c^{lo} \leqslant g_c$, obtained with relations (25)–(27), the lower limit obtained with relation (13) with $n = 4$ and $N_\ell = 1$ (calculated numerically) and the lower limit obtained with formula (17) (with the optimal value of p).

ℓ	$n = 1$	$n = 2$	$n = 3$	$n = 4$	Equation (17)	Exact
0	2	2.4495	2.4662	2.4672	2.3593	2.4674
1	6	9.4868	9.8132	9.8592	9.1220	9.8696
2	10	18.708	19.895	20.120	18.454	20.191
3	14	29.699	32.383	32.981	30.245	33.217
4	18	42.214	47.064	48.272	44.425	48.831
5	22	56.089	63.788	65.868	60.947	66.954

where $\alpha = R/s$. The best restriction is obviously obtained with the value of α minimizing the right-hand side of (21). The upper limit can thus be written as

$$g_c^{up} = \frac{\pi^2}{12} \frac{1}{\alpha^2 v(\alpha, k)} \tag{22}$$

where α is the unique solution of

$$\int_0^\alpha \mathrm{d}y\, y^2 v(y, k) = \alpha^3 v(\alpha, k). \tag{23}$$

Definition (23) of α has a simple geometric significance which implies that $\alpha > \max[y^2 v(y, k)]$.

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

4. Tests

The first potential we consider to test the limits presented in the previous sections is a square-well potential that we write in the convenient form

$$V(r) = -gR^{-2}\theta(1 - r/R). \tag{24}$$

The sufficient condition (22)–(23), applicable only for $\ell = 0$, is saturated for this potential (with $\alpha = 1$) and thus leads to the exact result. The necessary conditions (14)–(16) give the following lower limits:

$$g_c^{lo} = 2(2\ell + 1) \tag{25}$$

$$g_c^{lo} = (2\ell + 1)[2(2\ell + 3)]^{1/2} \tag{26}$$

$$g_c^{lo} = (2\ell + 1)[(2\ell + 3)(2\ell + 5)]^{1/3}. \tag{27}$$

The comparison between the new lower limits on g_c, the limit (17) and the exact results is reported in table 1 and shows that the new limits are quite cogent and converge quickly to the exact result especially for small values of ℓ.

The last test is performed with an exponential potential written as

$$V(r) = -gR^{-2} \exp(-r/R). \tag{28}$$

Table 2. Comparison between the exact values of the critical coupling constant g_c of an exponential potential for various value of ℓ and the lower limits, $g_c^{lo} \leqslant g_c$, obtained with relations (25)–(27), the lower limit obtained with relation (13) with $n = 4$ and $N_\ell = 1$ (calculated numerically) and the lower limit obtained with formula (17) (with the optimal value of p).

ℓ	$n = 1$	$n = 2$	$n = 3$	$n = 4$	Equation (17)	Exact
0	1	1.4142	1.4422	1.4453	1.4383	1.4458
1	3	6.2700	6.8546	6.9913	7.0232	7.0491
2	5	13.145	15.257	15.804	16.277	16.313
3	7	21.593	26.265	27.364	29.218	29.259
4	9	31.363	39.616	41.296	45.849	45.893
5	11	42.297	55.120	57.480	66.173	66.219

For $\ell = 0$, the sufficient condition (22)–(23) leads to $g_c^{up} = 2.118$ while the exact result is given by $g_c = z_0^2/4 \cong 1.4458$ ($z_0 = 2.4048$ is the first zero of the Bessel function $J_0(x)$). The upper limit is not very stringent for this potential because the comparison potential that we choose (a square well) is very different from an exponential potential. The upper limit yields more cogent results, for example, for a Wood–Saxon potential. For an exponential potential a better upper limit can be obtained with the Calogero lower bound [5]: $g_c^{up} = 1.677$.

The comparison between the new lower limits on g_c, the limit (17) and the exact result is reported in table 2. The new lower limits on g_c are quite cogent and converge quickly to the exact results especially for small values of ℓ, but this convergence is slower than in the case of a square-well potential.

Acknowledgment

We would like to thank the FNRS for financial support (FNRS Postdoctoral Researcher position).

References

[1] Jost R and Pais A 1951 *Phys. Rev.* **82** 840
[2] Bargmann V 1952 *Proc. Natl Acad. Sci. USA* **38** 961
[3] Birman S 1961 *Math. Sb.* **55** 124
Birman S 1966 *Am. Math. Soc. Transl.* **53** 23
[4] Schwinger J 1961 *Proc. Natl Acad. Sci. USA* **47** 122
[5] Calogero F 1965 *Commun. Math. Phys.* **1** 80
[6] Calogero F 1965 *J. Math. Phys.* **6** 161
[7] Calogero F 1965 *Nuovo Cimento* **36** 199
[8] Chadan K 1968 *Nuovo Cimento* A **58** 191
[9] Martin A 1972 *Helv. Phys. Acta* **45** 140
[10] Glaser V, Grosse H, Martin A and Thirring W 1976 *Studies in Mathematical Physics—Essays in Honor of Valentine Bargmann* (Princeton, NJ: Princeton University Press) p 169
[11] Simon B 1976 *Studies in Mathematical Physics—Essays in Honor of Valentine Bargmann* (Princeton, NJ: Princeton University Press) p 305
[12] Martin A 1977 *Commun. Math. Phys.* **55** 293
[13] Lieb E H 1980 *Proc. Am. Math. Soc.* **36** 241
[14] Chadan K, Martin A and Stubbe J 1995 *J. Math. Phys.* **36** 1616
[15] Chadan K, Martin A and Stubbe J 1995 *Lett. Math. Phys.* **35** 213
[16] Chadan K, Kobayashi R, Martin A and Stubbe J 1996 *J. Math. Phys.* **37** 1106
[17] Blanchard Ph and Stubbe J 1996 *Rev. Math. Phys.* **8** 503

[18] Lassaut M L and Lombard R J 1997 *J. Phys. A: Math. Gen.* **30** 2467
[19] Brau F and Calogero F 2003 *J. Math. Phys.* **44** 1554
[20] Brau F and Calogero F *J. Phys. A: Math. Gen.* submitted
[21] Brau F and Calogero F 2003 *Phys. Lett.* A **312** 16
[22] Brau F 2003 *Phys. Lett.* A **313** 363
[23] Hall R L and Katatbeh Q D 2002 *J. Phys. A: Math. Gen.* **35** 8727