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New bounds on the number of bound states

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Abstract. We present methods for binding the number of bound states which allow us to take into account oscillations of the potential. Previous results for a particular angular momentum and for levels below a certain energy are also improved.

1. Introduction

There now exist many kinds of estimates on the number of bound states for a given potential with and without spherical symmetry (Bargmann 1952, Birman 1961, 1966, Schwinger 1961, Glaser *et al* 1976, Chadan 1976, Chadan and Martin 1977, Rosenblum 1972, Cwickel 1977, Lieb 1976, 1979, Ghirardi and Rimini 1965), as well as sufficient conditions for the existence of such states (Calogero 1965, Chadan and Martin 1980, Chadan 1980). In these estimates usually either the attractive part of the potential or its absolute value enters.

In § 2 we formulate the problem in such a way as to take into account oscillations of the potential, something which has not been done so far. For this purpose we introduce the following integral of the potential for the spherically symmetric case:

$$W_\sigma(r) = -\int_r^\infty \mathrm{d}t\, \sigma^2(t) V(t) \tag{1}$$

where $\sigma(t)$ will be chosen in a suitable way and $W_\sigma(r)$ for $\sigma = 1$ has already been used in scattering theory (Baeteman and Chadan 1976), as well as for the bound state problem. Then, by making a special transformation, we arrive at an equivalent problem, as far as the number of bound states is concerned (i.e. the number of nodes of the zero-energy wavefunctions), such that the new potential turns out to be everywhere attractive, whatever the sign of the starting potential may be. We then see that one can apply all estimates mentioned above, some of which are rather good, to this equivalent potential. In a simple example we shall see that our estimates give a large improvement over old results.

In the third part we transform the Schrödinger equation into an integral equation with a symmetric kernel. Applying standard Birman–Schwinger techniques allows us to improve known results in two cases. On the one hand, an estimate on the number of bound states for a particular angular momentum also suitable for oscillating potentials is derived; on the other hand, states below a certain energy are estimated.

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2. Bounds for oscillating potentials

Let us start with the Schrödinger equation for a spherically symmetric potential; the reduced wavefunction for a bound state with energy $-\gamma^2$ and angular momentum l satisfies

$$\left(-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+\gamma^2+V(r)\right)\varphi(r)=0 \qquad \varphi(0)=0 \tag{2}$$

where $V(r)$ should be such that $W_\sigma(r)$ defined in (1) satisfies, for $\sigma=1$,

$$W(r)=W_{\sigma=1}(r)\in L^1([0,\infty)) \qquad rW(r)|_{r=0,\infty}=0. \tag{3}$$

It has been shown (Baeteman and Chadan 1976) that the whole of scattering theory (including the bound state problem), which works under the old Bargmann–Jost–Kohn–Levinson condition

$$rV(r)\in L^1([0,\infty)) \tag{4}$$

also works under the more general requirements (3). However, in this paper we shall keep (4) and leave the more general case for a future publication. Next we introduce

$$U_\sigma(r)=\int_r^\infty dt\,\sigma^{-2}(t)W_\sigma(t) \tag{5}$$

and make the following change of variables:

$$z(r)=\int_0^r dt\,\sigma^{-2}(t)\exp(2U_\sigma(t)) \qquad \psi_\sigma(z)=[\sigma^{-1}(r)\exp(U_\sigma(r))\varphi(r)]|_{r=r(z)} \tag{6}$$

where we take $\sigma(r)$ to be the solution of

$$\left(-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+\gamma^2\right)\sigma(r)=0 \qquad \gamma\geqslant 0,\quad \sigma(r)\neq 0 \tag{7}$$

i.e.,

$$\sigma(r)=\mathrm{i}\exp(\mathrm{i}\pi l)(\tfrac{1}{2}\pi\mathrm{i}\gamma r)^{1/2}(\mathrm{i}\gamma)^l H^{(1)}_{l+\frac{1}{2}}(\mathrm{i}\gamma r) \tag{8}$$

where $H^{(1)}_\nu$ is the Hankel function (Erdelyi 1953). Indeed, it is known that $\sigma(r)$ is real and does not vanish for $r\geqslant 0$, $\gamma\geqslant 0$, $l>-\frac{1}{2}$ (Erdelyi 1953, see p 62), and we have

$$\begin{aligned}\sigma(r)&=(-1)^l[(2l-1)!!]r^{-l} && \gamma\to 0\\ \sigma(r)&=\exp(-\gamma r) && l\to 0.\end{aligned} \tag{9}$$

Note also that $|\sigma(r)|$ is a decreasing function of r (it is infinite at the origin and zero at $r=\infty$) as can be seen from the definition of the Hankel function for $l=1,2,\ldots$ (Erdelyi 1953).

Under (6), equation (2) transforms into

$$\left(-\frac{d^2}{dz^2}+\tilde V_\sigma(z)\right)\psi_\sigma(z)=0 \qquad \tilde V_\sigma(z)=-[W_\sigma^2(r)\exp(-4U_\sigma(r))]|_{r=r(z)}. \tag{10}$$

Notice, first of all, that the change of variables from r to z is a C^2 bijection and maps the interval $[0,\infty)$ to $[0,\infty)$. Furthermore, it follows from the definition of $\psi_\sigma(z)$ (equation (6)) that the nodes of $\psi_\sigma(z)$ and of $\varphi(r)$ correspond to each other. Therefore the number of bound states below energy $-\gamma^2$ of the original problem is equal to the number of nodes of $\psi_\sigma(z)$.

However, the surprising feature of equation (10) is that the new potential $\tilde{V}_\sigma(z)$ which enters is purely attractive. Moreover, using the monotonicity of $|\sigma(r)|$ as a function of r mentioned above, one can prove (see the appendix) that condition (4), that is to say finiteness of the integral

$$I=\int_0^\infty \mathrm{d}r\, r|V(r)|<\infty, \tag{11}$$

implies finiteness of the integral

$$J=\int_0^\infty \mathrm{d}z\, z|\tilde{V}_\sigma(z)|<\infty. \tag{12}$$

This means that (10) is a good radial Schrödinger equation in z for the s wave at zero energy with a purely attractive potential satisfying the Bargmann condition. This makes it clear that we can apply old results to (10) (and therefore to (2)) without being forced to throw out the repulsive part of the potential. So, for instance, we have the bounds on the number of bound states $n_l(\gamma)$ for angular momentum l below energy $-\gamma^2$ (Glaser *et al* 1976):

$$\begin{aligned} &n_l(\gamma)\leqslant C_p\int_0^\infty \frac{\mathrm{d}z}{z}(z^2|\tilde{V}_\sigma(z)|)^p \qquad \forall p\geqslant 1\\ &C_p=\frac{(p-1)^{p-1}\Gamma(2p)}{p^p\Gamma^2(p)}\end{aligned} \tag{13}$$

where $\sigma(r)$ entering in the transformation (6) is given by (8).

To check the improvement over old results, we examine an example for $\gamma=0$, $l=0$ which means $\sigma(r)=1$.

Example. Two δ-function potentials. Let

$$V(r)=\alpha\delta(r-r_1)+\beta\delta(r-r_2) \qquad r_1=1,\quad r_2=2. \tag{14}$$

Then it is trivial to obtain regions in the (α,β) plane for which we have no bound states (respectively, one or two states). In order to apply (13), we have to calculate the new potential and work out the change of variables from r to z; we obtain

$$\tilde{V}_\sigma(z)=\begin{cases} -\dfrac{1}{4(z-K_{\alpha,\beta})^2} & 0\leqslant z\leqslant C_{\alpha,\beta}+\dfrac{\exp(-2\beta)}{2\beta}\\[2ex] -\dfrac{1}{4(z-C_{\alpha,\beta})^2} & C_{\alpha,\beta}+\dfrac{\exp(-2\beta)}{2\beta}\leqslant z\leqslant C_{\alpha,\beta}+\dfrac{1}{2\beta}\\[2ex] 0 & C_{\alpha,\beta}+1/2\beta\leqslant z\end{cases} \tag{15}$$

where the constants are given by

$$K_{\alpha,\beta}=-\frac{\exp(-2\alpha-4\beta)}{2(\alpha+\beta)} \qquad C_{\alpha,\beta}=K_{\alpha,\beta}-\frac{\exp(-2\beta)\alpha}{2\beta(\alpha+\beta)}. \tag{16}$$

The new variable clearly becomes asymptotically equal to r:

$$z(r)=\begin{cases} K_{\alpha,\beta}(1-\exp[2(\alpha+\beta)r]) & 0\leqslant r\leqslant 1\\[1ex] C_{\alpha,\beta}+\dfrac{\exp[-2\beta(2-r)]}{2\beta} & 1\leqslant r\leqslant 2\\[2ex] r-2+C_{\alpha,\beta}+1/2\beta & 2\leqslant r.\end{cases} \tag{17}$$

In table 1 (respectively, table 2) we compare the naive estimate by taking

$$|V(r)|_- = \theta(-V(r))|V(r)| \tag{18}$$

and using the Bargmann bound ($p = 1$ in equation (13)) with results obtained with the help of $\tilde{V}_\sigma(z)$ and taking $p = 1$ or $\frac{3}{2}$. First, we fix α (respectively, β) such that the first bound state appears. Then, using equation (13), we have determined bounds on β (respectively, α) such that the number of bound states is zero. As expected, we obtain a large improvement over the naive estimates; the difference between our bounds and the exact results is of the order of a few per cent.

Table 1. The question of excluding bound states for the potential of equation (14) is studied. We fix α and determine the exact value of β such that there is a zero-energy resonance (β_{exact}). Next we determine a bound on β excluding bound states, by taking the naive estimate of equation (18) and using Bargmann's result ($p = 1$ in equation (13)). These β_{nb} are compared with the improved bounds β_{ib} by using $\tilde{V}_\sigma(z)$ from equation (15) and taking $p = 1$ or $\frac{3}{2}$ in equation (13).

α	β_{exact}	β_{nb}	β_{ib}	p
−0.50	−0.333	−0.250	−0.310	1
−0.25	−0.429	−0.375	−0.408	1
0.25	−0.556	−0.500	−0.544	1
0.50	−0.600	−0.500	−0.590	1
0.75	−0.636	−0.500	−0.624	1
1.00	−0.667	−0.500	−0.646	1

Table 2. The same as in table 1 but β is fixed first and α values are determined.

β	α_{exact}	α_{nb}	α_{ib}	p
−0.25	−0.667	−0.5	−0.622	1
0.25	−1.200	−1.0	−1.158	1
0.50	−1.333	−1.0	−1.270	1
0.75	−1.429	−1.0	−1.368	$\frac{3}{2}$
1.00	−1.500	−1.0	−1.411	$\frac{3}{2}$

Remark. Clearly the transformation (6) can be applied to the energy functional; one obtains

$$E(\psi_\sigma) = \frac{\int_0^\infty dz\{(d\psi_\sigma/dz)^2 - [\sigma^4(r)\exp(-4U_\sigma(r))W_\sigma^2(r)]|_{r=r(z)}|\psi_\sigma(z)|^2\}}{\int_0^\infty dz[\sigma^4(r)\exp(-4U_\sigma(r))]|_{r=r(z)}|\psi_\sigma(z)|^2}. \tag{19}$$

Only in the case where $|\sigma(r)\exp(-U_\sigma(r))|_{r=r(z)} \leq 1$ is there a relation between the eigenvalues of the old problem and the eigenvalues of the operator

$$-d^2/dz^2 + \tilde{V}_\sigma(z) \qquad \text{on } L^2([0,\infty)). \tag{20}$$

3. Bounds for angular momentum states below some energy

In this section we shall show how to generalise to higher angular momentum and to negative energy some necessary conditions (Chadan 1976, Chadan and Martin 1977), as well as sufficient ones (Chadan 1980), found previously. To this end, we start from the equation

$$-\left(\frac{\mathrm{d}}{\mathrm{d}r}+\omega(r)\right)\sigma^2(r)\left(\frac{\mathrm{d}}{\mathrm{d}r}-\omega(r)\right)u(r)=\sigma^2(r)\mu(r)u(r) \qquad u(0)=0 \tag{21}$$

where $\omega(r)$ and $\mu(r)$ will be chosen later and $u(r)$ will be related to the solution of the Schrödinger equation (27). If we now define

$$\sigma(r)\left(\frac{\mathrm{d}}{\mathrm{d}r}-\omega(r)\right)u(r)=w(r) \tag{22}$$

we can easily invert equation (22) and get

$$u(r)=\int_0^r \mathrm{d}t\,\sigma^{-1}(t)w(t)\exp\left(\int_t^r \mathrm{d}s\omega(s)\right). \tag{23}$$

Using (23) we can transform the differential equation (21) into the integral equation

$$w(r)=\int_0^\infty \mathrm{d}s\,K^{(1)}(r,s)w(s) \tag{24}$$

with a symmetric kernel

$$K^{(1)}(r,s)=\int_0^\infty \mathrm{d}t\,\theta(t-r)\theta(t-s)\frac{\sigma^2(t)\mu(t)}{\sigma(r)\sigma(s)}\exp\left(\int_s^t \mathrm{d}x\,\omega(x)+\int_r^t \mathrm{d}x\,\omega(x)\right). \tag{25}$$

It is also easily seen that if $\mu(t)\geqslant 0$ this kernel $K^{(1)}$ is positive definite.

Let us now specify σ, ω and μ to particular cases. To do so we take σ from equation (8). Under the substitution

$$u(r)=\sigma^{-1}(r)\phi(r) \tag{26}$$

the differential equation (21) becomes a Schrödinger equation for energy $-\gamma^2$ and angular momentum l:

$$\left(-\frac{\mathrm{d}}{\mathrm{d}r^2}+\frac{l(l+1)}{r^2}+\gamma^2+\omega'+\omega^2+\frac{2\sigma'}{\sigma}\omega-\mu\right)\phi(r)=0. \tag{27}$$

Let $\mu(r)=-V(r)$ and take ω to be a solution of

$$\omega'+\omega^2+\frac{2\sigma'}{\sigma}\omega=0 \qquad \omega^{-1}(r)=\sigma^2(r)\int^r \mathrm{d}t\,\sigma^{-2}(t). \tag{28}$$

In the case when V is purely attractive, we now apply the Birman–Schwinger argument to equation (24) and obtain a bound on the number of bound states with angular momentum l below the energy $-\gamma^2$, $n_l(\gamma)$, of the form

$$n_l(\gamma)\leqslant \mathrm{Tr}\,K^{(1)}=\int_0^\infty \mathrm{d}r\;V(r)\sigma^2(r)\int_0^r \mathrm{d}t\,\sigma^{-2}(t)\exp\left(2\int_t^r \mathrm{d}s\,\omega(s)\right). \tag{29}$$

In the case where V has no definite sign, we can iterate (24) once and use this iterated kernel $K^{(2)}$ which is now positive to get

$$n_l(\gamma)\leqslant \mathrm{Tr}\,K^{(2)}. \tag{30}$$

According to the Birman–Schwinger principle (Thirring 1981) $n_l(\gamma)$ is given by the number of characteristic values g_i of K which are smaller than one. For purely attractive potentials one observes that the condition

$$\mathrm{Tr}\,K^{(2)} \geqslant \mathrm{Tr}\,K^{(1)} \Leftrightarrow \sum_i g_i^{-2} \geqslant \sum_i g_i^{-1} \qquad g_i > 0 \tag{31}$$

implies the existence of at least one such value less than one; therefore (31) is a sufficient condition for the existence of bound states (Chadan 1980). If V changes sign $K^{(1)}$ need not be positive, so we have to use

$$\mathrm{Tr}\,K^{(4)} \geqslant \mathrm{Tr}\,K^{(2)}. \tag{32}$$

Let us quote two particularly interesting cases of the bounds given above.

(a) For $l = 0$, $\sigma(r) = \exp(-\gamma r)$, we get $\omega(r) = 2\gamma$

$$n_0(\gamma) \leqslant \mathrm{Tr}\,K^{(1)} = \int_0^\infty \mathrm{d}r\, \exp(2\gamma r) W_\gamma(r) \qquad W_\gamma(r) = -\int_r^\infty \mathrm{d}s\, \exp(-2\gamma s) V(s) \tag{33}$$

a result which is well known and due to Schwinger (1961). The next iteration gives

$$n_0(\gamma) \leqslant \mathrm{Tr}\,K^{(2)} = \int_0^\infty \mathrm{d}r\, \exp(2\gamma r) \frac{\exp(2\gamma r) - 1}{\gamma} W_\gamma^2(r). \tag{34}$$

(b) Choose $\gamma = 0$ and $\sigma(r) = \text{constant} \times r^{-1}$, then $\omega(r) = (2l+1)/r$; we obtain first

$$n_l(0) \leqslant \int_0^\infty \mathrm{d}r \frac{W_l(r)}{(2l+1)} r^{2l} \qquad W_l(r) = -\int_r^\infty \mathrm{d}s\, s^{-2l} V(s). \tag{35}$$

The second iteration improves a result of Chadan and Martin (1980):

$$n_l(0) \leqslant \frac{2}{2l+1} \int_0^\infty \mathrm{d}r\, r^{4l+1} W_l^2(r). \tag{36}$$

Remark. It is interesting to note that the choice $\mu = \omega^2$ with ω being a solution of

$$\omega' + \frac{2\sigma'}{\sigma}\omega = V \qquad \sigma^2(r)\omega(r) = -\int_r^\infty \mathrm{d}t\, V(t)\sigma^2(t) \tag{37}$$

in equation (27) also leads to the Schrödinger equation for angular momentum l and energy $-\gamma^2$. This time $\mathrm{Tr}\,K^{(1)}$ turns out to be identical to the Bargmann bound ($p = 1$ of equation (13)), although the Birman–Schwinger technique is not applicable directly because $K^{(1)}$ does not depend linearly on V.

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Appendix

Assuming that the integral I defined in equation (11) is finite, we show first that $U_\sigma(r)$ given by equation (5) is bounded for all r by $2I$. From the definitions we get

$$|U_\sigma(r)| \leqslant \int_r^\infty \mathrm{d}t\, \sigma^{-2}(t) \int_t^\infty \mathrm{d}u\, \sigma^2(u) |V(u)|. \tag{A1}$$

Then using the fact that $|\sigma(u)|$ is monotonically decreasing gives

$$|U_\sigma(r)| \leqslant \int_r^\infty \mathrm{d}r \int_t^\infty \mathrm{d}u |V(u)|. \tag{A2}$$

Exchanging integrations and binding r by u gives the result we are seeking:

$$|U_\sigma(r)| \leqslant 2 \int_r^\infty \mathrm{d}u\, u |V(u)| \leqslant 2I. \tag{A3}$$

Next we would like to prove the finiteness of the integral J defined in equation (12). Inserting all definitions gives

$$J = \int_0^\infty \mathrm{d}r \exp(-2U_\sigma(r))\sigma^{-2}(r) \int_0^r \mathrm{d}t \exp(2U_\sigma(t))\sigma^{-2}(t)\left(\int_r^\infty \mathrm{d}u\, \sigma^2(u) V(u)\right)^2. \tag{A4}$$

Using (A3) and also the monotonicity of $|\sigma(r)|$ allows us to get rid of all the σ dependence:

$$J \leqslant \exp(4I) \int_0^\infty \mathrm{d}r\, r \int_r^\infty \mathrm{d}u\ V(u) \int_r^\infty \mathrm{d}v\ V(v). \tag{A5}$$

Exchanging integrations and performing the r integration leads finally to the inequality

$$J \leqslant \exp(4I) I^2 \tag{A6}$$

which implies finiteness of J if I is finite.

Note added in proof. D B Pearson (1979 *Helv. Phys. Acta* **52** 541) has performed related work on a different, but connected, class of potential. There is, in fact, some similarity between Pearson's approach for scattering and our approach for bound states.

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