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Estimates of the number of quantal bound states in one and three dimensions

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Abstract. Using the relation between the number of bound states and the number of zeros of the radial eigen-function $\psi(r)$, or equivalently, that of $\phi(r) = r\psi(r)$ in the range $0 \leqslant r \leqslant \infty$, the upper bounds on the number of bound states generated by potential $V(r)$ in different angular momentum channels are obtained in three dimension. Using a similar procedure, the upper bound on the number of bound states in one dimension is also deduced. The analysis is restricted to a class of potentials for which $E = 0$ is the threshold. By taking a number of specific examples, it is demonstrated that both in one and three dimensions, the estimate of the upper bound obtained by this procedure is very close to or equal to the exact number of bound states. The correlation of the present method with the Levison's theorem and WKB approximation is discussed.

Keywords. Bound on number of states; zeros of wave-function; Schrödinger equation; *s*-wave; effective potential; number of gaps between consecutive minima points of the potential.

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1. Introduction

The problem of estimating the number of quantal bound states which can be generated by a potential in the Schrödinger equation is of much interest in various bound state and scattering problems in atomic physics, nuclear physics etc. In $3D$, the standard upper bound on the number of bound states n_l that can be generated by a potential $V(r)$ in the lth partial wave is given by the well-known Bargmann inequality (BI) (Bargmann 1952; Newton 1966; p. 357, 377):

$$B_l = (2l+1)^{-1} \int_0^\infty r|V(r)|\,dr \geqslant n_l. \tag{1}$$

A large number of reports in connection with the number of bound states for a potential under different conditions are reported based on various approaches (Birman 1961, 1966; Schwinger 1961; Titchmarsh 1962; Calegaro 1965; Martin 1972; Tamura 1974; Rozenbljum 1972; Lieb 1976; Cwikel 1977; Ronveaux *et al* 1977; Glaser *et al* 1978; Simon 1976a; Shastry and Marwadi 1976; Newton 1983; Li and Yau 1983; Blanchard 1987; Requardt 1985). The review work by Simon (1976b) summarizes most of the results obtained till 1976. Klaus (1977) found a Bargmann type inequality (BTI) in $1D$ for a class of potentials, given by

$$N_1(V) \leqslant 1 + \int_{-\infty}^{\infty} |x||V(x)|\,dx. \tag{2}$$

In this paper, we deduce expressions for estimating upper bounds on the number of bound states having eigen-values less than or equal to certain energy $E \leqslant 0$ both in $3D$ and $1D$. We verify that these bounds are quite close to the actual number of bound states for a number of potentials in $3D$ and $1D$.

The main idea behind our method can be stated as follows: It is well-known that the nth state s-wave eigenfunction $\psi(k_n, r) = \phi(k_n, r)/r$ for a spherically symmetric potential $V(r)$, corresponding to eigenenergy $E_n = -k_n^2 \leqslant 0$ ($n = 1$ corresponds to ground state both in $1D$ and $3D$) of the radial Schrödinger equation in $3D$, has n zeros in the interval $0 \leqslant r \leqslant \infty$ and as a consequence $\phi(k_n, r)$ has $(n+1) = n'$ zeros in the same interval. Similarly, the nth eigenstate $\phi(k_n, x)$ in the case of $1D$ has $(n+1) = n'$ zeros in the interval $0 \leqslant |x| \leqslant \infty$. Hence, in both the cases of $3D$ and $1D$ the actual number of bound states having eigenvalues below or equal to a certain energy $E \leqslant 0$ such that E_n is the highest energy level less than or equal to E, is given by $n = n' - 1$ (see Theorem 1·5 Simon 1976b, p. 307). We, therefore, obtain a procedure to find an upper bound for the total number of zeros or nodes of the appropriate eigenfunction having the eigenvalue closest to but less than or equal to a given energy $E \leqslant 0$. The basic idea of this 'node counting' approach has been used in different problems for finding eigenvalues with appropriate modifications. In case of $3D$, this method is generalized for $l \geqslant 0$ by noting that the radial Schrödinger equation satisfied by $\phi(k_n, r)$ for potential $V(r)$ for $l > 0$, is similar to the corresponding s-wave radial Schrödinger equation for the effective potential $V_{\text{eff}}(l, r) = V(r) + l(l+1)/r^2$. This procedure is valid for potentials with some constraints specified later.

We describe in §2 the detail of the derivation of the bounds on the number of bound states of Schrödinger equation in $3D$ and $1D$. In §3, we demonstrate the usefulness of the bounds obtained in this paper in the case of a number of potentials both in $3D$ and $1D$ and compare them with the corresponding results obtained by using BI and BTI respectively. The concluding §4 relates the present procedure with Levinson's theorem and the WKB method.

2. Estimates of upper bounds on the number of bound states in one and three dimensions

We first consider the formulation for the s-wave Schrödinger equation for $E \leqslant 0$, for the spherically symmetric potential $V(r)$ in $3D$:

$$\frac{d^2\phi}{dr^2} - (V(r) + k^2)\phi = 0, \tag{3}$$

where $k^2 = -E$, in the system of units in which $\hbar = 2m = 1$. The radial solution is $\psi(r) = \phi(r)/r$ and $\psi(0) \neq 0$. We assume that

(i) $V(r)$ is less singular than r^{-2} at $r = 0$,
(ii) as $r \to \infty$, $V(r) \to 0$ $(r^{-1-\delta})$, $\delta \geqslant 0$,
(iii) $V(r)$ is finite and integrable in the interval $0 \leqslant r \leqslant \infty$, and that the bound state energies are less than or equal to the threshold ($E = 0$) and greater than the absolute minima $V_{\min}$ of the potential $V(r)$. It is known that (Kato 1951) local potentials which go to zero as $r^{-1-\delta}$ ($\delta > 0$) as $r \to \infty$, do not generate bound states in the continuum. Let E be a particular energy below or at the threshold ($E \leqslant 0$) and E_n be the highest eigen-energy which is less than or equal to E, E_n denoting the energy in the nth state,

$n = 1$ corresponding to the ground state. That is, the number of s-wave bound states $N(l = 0, E)$ generated by the potential $V(r)$, with energy eigen-values less than or equal to E, is equal to n. The eigen-function $\phi(k_n, r)$, corresponding to energy E_n, has $(n + 1)$ zeros in the interval $0 \leqslant r \leqslant \infty$ including the zeros at $r = 0$ and $r = \infty$. Hence, if we can get a bound on the number of zeros of $\phi(k_n, r)$, that would lead to a bound on the number of s-wave bound states generated by $V(r)$ in the range $(V_{\min}, E)$.

To elaborate the procedure of estimating this, let us first consider a continuous potential $V(r)$ having only one minimum below $E = 0$, such that

$$\begin{aligned} V(r) &< E_n, \quad a < r < b, \\ &\geqslant E_n, \quad r \leqslant a, r \geqslant b. \end{aligned} \tag{4}$$

As a result, one can write the radial Schrödinger equation as

$$\frac{d^2\phi(k_n, r)}{dr^2} + (E_n - V(r))\phi(k_n, r) = 0, \quad a < r < b, \tag{5}$$

$$\frac{d^2\phi(k_n, r)}{dr^2} - (V(r) - E_n)\phi(k_n, r) = 0, \quad r \leqslant a \text{ or } r \geqslant b. \tag{6}$$

To obtain the number of zeros of $\phi(K_n, r)$ in the regions $r \leqslant a$ and $r \geqslant b$, we use the following theorem (Ross 1964):

Theorem If $f(x)$ is continuous and $f(x) < 0$ throughout a range $x_1 \leqslant x \leqslant x_2$, then no non-trivial solution of $d^2y/dx^2 + f(x)y = 0$ can have more than one zero in the region $x_1 \leqslant x \leqslant x_2$.

In the case $V(r) > E_n$, applying the above theorem for (6) in the region $r \leqslant a$ and $r \geqslant b$ and noting that $\phi(k_n, 0) = \phi(k_n, \infty) = 0$, we find that $\phi(k_n, r)$ has no zero other than $r = 0$ and $r = \infty$ in the regions $0 \leqslant r \leqslant a$ and $b \leqslant r \leqslant \infty$ respectively. The same conclusion can be made in case of $V(r) = E_n$, since in this case (6) becomes $d^2\phi(k_n, r)/dr^2 = 0$ and the general solution is of the form $\phi(k_n, r) = Ar + B$ (A and B are constants), which also can have no more than one zero in each of the regions $0 \leqslant r \leqslant a$ and $b \leqslant r \leqslant \infty$.

In fact, there can be no more than one zero in each of the intervals $r \leqslant a$ and $b \leqslant r \leqslant \infty$ where $V(r) \geqslant E_n$. Physically speaking, it can be seen that the presence of more than one zero in either of these intervals leads to the unphysical conclusion that a non-attractive potential can generate a bound state. Hence, the only zeros of $\phi(k_n, r)$ in $0 \leqslant r \leqslant a$ and $b \leqslant r \leqslant \infty$ for $V(r) \geqslant E_n$ are at $r = 0$ and $r = \infty$.

This conclusion is also consistent with the fact that the eigen-function corresponding to eigen-value E_n does not oscillate in the classically inaccessible region of the potential. Now, we proceed to estimate the number of zeros of $\phi(k_n, r)$ in the region $a < r < b$.

In order to accomplish this, we split the interval $a < r < b$ into p equal non-overlapping consecutive intervals $a_{i-1} < r < a_i$, $i = 1, 2, \ldots, p$, such that $a_0 = a$, $a_p = b$ and $a_i - a_{i-1} = \Delta_i = \Delta$. Further, we construct an enclosing potential $V_{SQ}(r) \leqslant V(r)$ in the interval $a < r < b$ defined as follows:

$$V_{SQ}(r) = V_i < 0, \quad a_{i-1} < r < a_i, \tag{7}$$

with

$$|V_i| = \max(|V(r = a_{i-1})|, \quad |V(r = a_i)|), \tag{8}$$

$$i = 1, 2, \ldots, p$$

It is clear that as $p \to \infty$, $\Delta \to 0$, the difference $[V(r) - V_{SQ}(r)] \to 0$. That is, $V_{SQ}(r)$ represented by (7) encloses $V(r)$ in the region $a < r < b$ and merges with $V(r)$ in the limit of large p and infinitesimally small Δ. Since, $|V_{SQ}(r)| \geqslant |V(r)|$, the number of zeros $Z^{SQ}_{a,b}(E_n)$ of the wave-function ϕ of the Schrödinger eq (5) in the range $a < r < b$ with $V(r)$ replaced by $V_{SQ}(r)$ is a bound for the number of zeros $Z_{a,b}(E_n)$ of $\phi(k_n, r)$ corresponding to $V(r)$ in the same region (see Theorem 1·6, Simon 1976b). In order to get a bound for the former we proceed as follows:

The s-wave radial Schrödinger equation for $V_{SQ}(r)$ in a typical interval like $a_{i-1} \leqslant r \leqslant a_i$ is

$$\frac{d^2\phi_i}{dr^2} + k_i^2 \phi_i = 0, \tag{9}$$

where $k_i^2 = E_n - V_i > 0$. The general solution ϕ_i is given by

$$\phi_i(r) = A_i \sin(k_i r + \alpha_i), \tag{10}$$

where, A_i and α_i are constants satisfying the usual continuity conditions (matching of ϕ and its derivative ϕ' at the boundaries) at $r = a_i$ and $r = a_{i-1}$. The boundary conditions at $r = a_p = b$ show that

$$\alpha_p = -k_p a_p + \gamma, \tag{11}$$

where, $\tan\gamma = k_p \phi(r = b)/\phi'(r = b)$. It follows that

$$\phi_p(r = b) = A_p \sin\gamma. \tag{12}$$

Specifying that γ is the phase of $\phi(r)$ at $r = b$, we proceed to estimate the accumulation of additional phase as r varies from b to a. This is done by successive applications of the boundary conditions at the boundaries $r = a_{p-1}, a_{p-2}, \ldots, a_1$. The algebraic relations resulting from the application of boundary conditions upto $r = a_i$ give

$$\alpha_i = \gamma - k_i a_i - \sum_{q=i+1}^{p} k_p \Delta - \sum_{q=i+1}^{p} \frac{\Delta k_i}{2k_q} \sin\left(2 \sum_{j=q}^{p} k_j \Delta\right) \tag{13}$$

where, $\Delta k_i = k_i - k_{i-1}$, $i = 1, 2, \ldots, p-1$. It should be noted that Δ is always positive whereas Δk_i may be positive or negative or zero. Using (13) we get

$$\phi(r = a_0 = a) = A_1 \sin(k_1 a + \alpha_1) \tag{14}$$

where

$$\alpha_1 = \gamma - k_1 a_1 - \sum_{q=2}^{p} k_q \Delta - \sum_{q=2}^{p} \frac{\Delta k_1}{2k_q} \sin\left(2 \sum_{j=q}^{p} k_j \Delta\right). \tag{15}$$

Obviously, in the range $a < r < b$ the wave-function $\phi_i(r)$ will have zeros as many times as $\sin(k_i r + \alpha_i)$ becomes equal to zero in the same range. Hence,

$$\begin{aligned} Z^{SQ}_{a,b}(E_n) &\leqslant \frac{1}{\pi}[\text{phase of } \phi(r = b) - \text{phase of } \phi(r = a)] \\ &\leqslant \frac{1}{\pi}\left[\sum_{q=1}^{p} k_q \Delta + \sum_{q=2}^{p} \frac{\Delta k_1}{2k_q} \sin\left(2 \sum_{j=q}^{p} k_j \Delta\right)\right]. \end{aligned} \tag{16}$$

As $p \to \infty$ and $\Delta \to 0$, inequality (16) will correspond to the original potential $V(r)$ which was enclosed by $V_{SQ}(r)$:

$$Z_{a,b}(E_n) \leqslant Z_{a,b}^{SQ}(E_n) \leqslant \frac{1}{\pi} \int_a^b [E_n - V(r)]^{1/2} \, dr + \varepsilon(E_n), \tag{17}$$

where,

$$\varepsilon(E_n) = \frac{1}{\pi} \lim_{\Delta \to 0} \sum_{q=2}^{\infty} \frac{\Delta k_1}{2k_q} \sin\left(2 \sum_{j=q}^{\infty} k_j \Delta\right). \tag{18}$$

We can expect $\varepsilon(E_n)$ to be very small. This expectation will be shown to be supported by the illustrations in §3 for a number of well-behaved potentials.

Therefore, the total number of zeros $Z(l=0, E_n)$ of s-wave radial eigen-function $\phi(k_n, r)$ for $V(r)$ in the interval $0 \leqslant r \leqslant \infty$ satisfies the inequality

$$Z(l=0, E_n) \leqslant \frac{1}{\pi} \int_a^b [E_n - V(r)]^{1/2} \, dr + 2 + \varepsilon(E_n). \tag{19}$$

Hence, the bound on the number of s-wave bound states $N(l=0, E)$ with energy eigenvalues less than or equal to energy E is given by

$$N(l=0, E) \leqslant \frac{1}{\pi} \int_a^b [E_n - V(r)]^{1/2} \, dr + 1 + \varepsilon(E_n) \tag{20}$$

$$\leqslant \frac{1}{\pi} \int_0^{\infty} |V_a^0(E_n, r)|^{1/2} \, dr + 1 + \varepsilon(E_n), \tag{21}$$

where,

$$V_a^0(E_n, r) = V(r) - E_n, \quad \text{when } V(r) < E_n,$$
$$= 0, \quad \text{when } V(r) \geqslant E_n. \tag{22}$$

Obviously, the integral in (21) corresponds to the region where the potential $V(r)$ is below the energy level E_n. $V_a^0(E, r)$ is as defined by (22) with E_n replaced by E and since $|V_a^0(E, r)| \geqslant |V_a^0(E_n, r)|$, therefore, the bound given by (23) can also be written as

$$N(l=0, E) \leqslant \frac{1}{\pi} \int_0^{\infty} |V_a^0(E, r)|^{1/2} \, dr + 1 + \varepsilon(E_n). \tag{23}$$

We now generalize the above method in case of (i) the s-wave problem with a more general potential $V(r)$, satisfying the conditions specified in the beginning of this section and having a finite number of minima in general and (ii) the corresponding lth partial wave problem with $l = 0, 1, 2, \ldots$ and apply a similar procedure to find upper bound on the number of bound states in case of $1D$.

2.1 *Estimate of upper bound on the number of s-wave bound states for* $V(r)$

Let us assume that

$$V(r) < E_n, \quad a_j < r < b_j,$$
$$\geqslant E_n, \quad b_j \geqslant r \geqslant a_{j+1}, \tag{24}$$

where $j = 1, 2, \ldots, s$. Figure 1 illustrates a typical potential of this type.

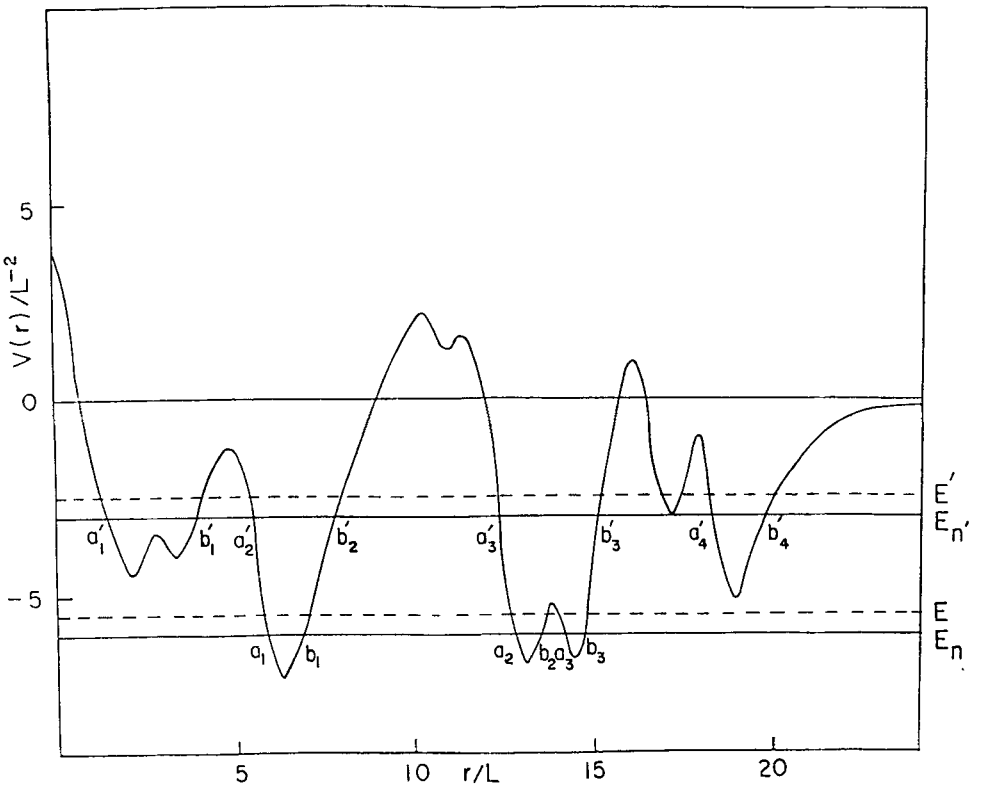

Figure 1. Partitioning of a typical potential $V(r)$ into effectively attractive and non-attractive regions for two cases at energies E and E'. E_n and $E_{n'}$ denote the eigenvalues closest to but less than or equal to E and E' respectively. Corresponding to E and E', $n_f(E_n)=2$ and $n_f(E_{n'})=3$ respectively, where, $n_f(E_p)$ denotes the number of gaps between non-overlapping consecutive regions of $V(r)$ below E_p. However, N_F, the number of finite gaps between consecutive minima of $V(r)$ below $E=0$, is 6 in both cases. L denotes any suitable unit of length pertaining to the problem of interest.

Following the procedure used to deduce inequality (17), we find that the number of zeros of $\phi(k_n, r)$ in the $l=0$ state in a typical interval like $a_j < r < b_j$ satisfies the inequality

$$Z_{a_j,b_j}(l=0, E_n) \leqslant \frac{1}{\pi}\int_{a_j}^{b_j} [E_n - V(r)]^{1/2}\,\mathrm{d}r + \varepsilon_j(E_n), \tag{25}$$

where, $\varepsilon_j(E_n)$ for this interval is as defined in (18). Hence, the total number of zeros of $\phi(k_n, r)$ in the $l=0$ state in all such intervals where $V(r) < E_n$, has the bound given by

$$\sum_{j=1}^{s} Z_{a_j,b_j}(l=0, E_n) \leqslant \frac{1}{\pi}\sum_{j=1}^{s}\int_{a_j}^{b_j} [E_n - V(r)]^{1/2}\,\mathrm{d}r + \varepsilon_{3T}(E_n), \tag{26}$$

where,

$$\varepsilon_{3T}(E_n) = \sum_{j=1}^{s} \varepsilon_j(E_n)$$

and is small. In a typical interval like $b_j \geqslant r \geqslant a_{j+1}$, where $V(r) \geqslant E_n$, the s-wave radial Schrödinger equation is of the form given in (6). Hence, using the theorem and the procedure described earlier, we conclude that in each interval like $b_j \geqslant r \geqslant a_{j+1}$, there can be no more than one zero of $\phi(k_n, r)$. Since $\phi(k_n, r) = 0$ at $r = 0$ and $r = \infty$ any such interval which includes either $r = 0$ or $r = \infty$ cannot have any other zero. Hence, the total number of zeros of s-wave eigen-function $\phi(k_n, r)$ including the two zeros at $r = 0$ and $r = \infty$ satisfies the inequality

$$Z(l=0, E_n) \leqslant \sum_{j=1}^{s} \int_{a_j}^{b_j} [E_n - V(r)]^{1/2} \, dr + 2 + n_f(E_n) + \varepsilon_{3T}(E_n) \tag{27}$$

where, $n_f(E_n)$ denotes the number of finite sections between any two consecutive non-overlapping sections of the potential $V(r)$ below the energy level E_n. This is illustrated in figure 1. Hence, a bound on the number of s-wave bound states $N(l=0, E)$ with energies less than or equal to the energy $E \leqslant 0$, generated by $V(r)$ is given by

$$\begin{aligned} N(l=0, E) &\leqslant \frac{1}{\pi} \sum_j \int_{a_j}^{b_j} [E_n - V(r)]^{1/2} \, dr + n_f(E_n) + 1 + \varepsilon_{3T}(E_n) \\ &\leqslant \frac{1}{\pi} \int_0^{\infty} |V_a^0(E_n, r)|^{1/2} \, dr + n_f(E_n) + 1 + \varepsilon_{3T}(E_n) \end{aligned} \tag{28}$$

where $V_a^0(E_n, r)$ is as defined in (22). We can replace $V_a^0(E_n, r)$ by $V_a^0(E, r)$ since $|V_a^0(E_n, r)| \leqslant |V_a^0(E, r)|$. Also, in the case of some potentials, $n_f(E_n)$ may be practically inconvenient to estimate (may be due to ignorance about the value of E_n). For such cases, we can replace $n_f(E_n)$ by N_F for all E, where, N_F denotes the number of finite gaps between two consecutive minima points of the potential below threshold. Obviously, $N_F \geqslant n_f(E_n)$ in general. It may be noted that in the case of most of the commonly used potentials discussed in § 3, $n_f(E_n) = N_F$. In figure 1, we have indicated a possibility when N_F is larger than $n_f(E_n)$ for some energies. The bound now is as follows:

$$N(l=0, E) \leqslant \frac{1}{\pi} \int_0^{\infty} |V_a^0(E, r)|^{1/2} \, dr + N_F + 1 + \varepsilon_{3T}(E_n). \tag{29}$$

2.2 *Estimate of upper bound on the number of bound states for* $V(r)$ for $l \geqslant 0$.

The radial Schrödinger equation for E_{nl}(E_{nl} denoting the highest energy level in the lth partial wave less than or equal to E) is,

$$\frac{d^2\phi(l, k_{nl}, r)}{dr^2} - \left(V(r) + \frac{l(l+1)}{r^2} \right) \phi(l, k_{nl}, r) - k_{nl}^2 \phi(l, k_{nl}, r) = 0, \tag{30}$$

where, $k_{nl}^2 = -E_{nl} \geqslant 0$.

This is similar to the s-wave radial Schrödinger equation for the effective potential

$$V_{\text{eff}}(l, r) = V(r) + \frac{l(l+1)}{r^2}. \tag{31}$$

In order to estimate the number of bound states for $l > 0$, we can treat (30) as an

effective s-wave problem. However, one should note that $V_{\text{eff}}(l,r)$ is repulsive and behaves like r^{-2} near $r=0$ since $V(r)$ is assumed to be less singular than r^{-2} at $r=0$. Hence, in the interval $(0,r_0)$, where r_0 is the point closest to $r=0$ such that $V_{\text{eff}}(l,r_0)=0$, $V_{\text{eff}}(l,r)$ is repulsive. Therefore, in this interval, $\phi(l,k_{nl},r)$ is zero only at $r=0$. Apart from this feature, the analysis is similar to that in the s-wave case. Therefore, using the earlier procedure, the bound on the number of bound states generated by $V(r)$ in the lth partial wave with energy below or equal to $E\leqslant 0$, can be written as

$$N(l,E)\leqslant \frac{1}{\pi}\int_0^\infty |V_a^l(E,r)|^{1/2}\,\mathrm{d}r + N_F + 1 + \varepsilon_{3T}(E_{nl}) \tag{32}$$

where,

$$\begin{aligned} V_a^l(E,r) &= V_{\text{eff}}(l,r) - E \quad \text{when } V_{\text{eff}}(l,r) < E \\ &= 0 \quad \text{when } V_{\text{eff}}(l,r) \geqslant E. \end{aligned} \tag{33}$$

A bound on the total number of bound states generated by $V(r)$ in the lth partial wave can be written by setting $E=0$ in (32):

$$N(l,0)\leqslant \frac{1}{\pi}\int_0^\infty |V_a^l(0,r)|^{1/2}\,\mathrm{d}r + 1 + N_F + \varepsilon_{3T}(E_{nl}).$$

Clearly, the integration corresponds to the regions of the potential where $V_{\text{eff}}(l,r)$ is effectively attractive.

The estimate of the upper bound on the number of lth partial wave bound states of energies less than or equal to energy E (in the range of the energy spectrum) in $3D$ given by (32) with $\varepsilon_{3T}(E_{nl})=0$ will be referred to as $B3D$.

2.3 *Estimate of upper bound on the number of bound states in* $1D$

The problem of bound state in $1D$ differs from the case in $3D$ in several respects. It is well-known that an arbitrarily weak attractive potential in $1D$ can generate a bound state (Blankenbecler *et al* 1977; Klaus 1977; Sahu *et al* 1989). It has been shown that (Simon 1976a; Klaus 1977) for a potential $V(x)$ the bound state $E<0$ exists whenever $\int V(x)\,\mathrm{d}x \leqslant 0$ and $\int(1+|x|)|V(x)|\mathrm{d}x < \infty$ and under such conditions the upper bound on the number of bound states is given by

$$N_1(V)\leqslant 1 + \int |x||V(x)|\,\mathrm{d}x. \tag{34}$$

This is similar to the Bargmann inequality in $3D$ except for the fact that it indicates the possibility of existence of bound state even for very weak attractive potentials.

An estimate of the upper bound on the number of bound states in $1D$ can also be made using a similar procedure described in the analysis of radial Schrödinger equation in $3D$. The Schrödinger equation for a negative or zero energy $E=-k^2\leqslant 0$ for potential $V(x)$ is given by

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} - (k^2 + V(x))\phi = 0. \tag{35}$$

The boundary conditions for bound states require that $\phi(x) \to 0$ as $|x| \to \infty$ such that $\int_{-\infty}^{\infty} |\phi(x)|^2 \, dx < \infty$. We assume that $V(x)$ is continuous and finite in the interval $|x| < \infty$ and $V(x) \to 0$ as $x \to \infty$ on $x \to -\infty$ on $x \to \pm \infty$ and that the bound state energies are less than or equal to the threshould energy $E = 0$ and greater than the absolute minimum $V_{\min}$ of $V(x)$.

Let E_n denote the highest energy level less than or equal to an energy $E \leqslant 0$. Then following the similar procedure as in the case of $3D$, we can write the bound on the number of bound states $N(E)$ with energy equal to or less than the energy, E, generated by $V(x)$ as

$$N(E) \leqslant \frac{1}{\pi} \int_{-\infty}^{\infty} |V_a(E, x)|^{1/2} \, dx + n_f(E_n) + 1 + \varepsilon_{1T}(E_n) \tag{36}$$

where,

$$\begin{aligned} V_a(E_n, x) &= V(x) - E_n \quad \text{when } V(x) < E_n \\ &= 0 \quad \text{when } V(x) \geqslant E_n \end{aligned} \tag{37}$$

and $n_f(E_n)$ denotes the number of finite sections of $V(x)$ between two consecutive non-overlapping sections of $V(x)$ below the energy level E_n. ε_{1T} is similar to ε_{3T} in case of $3D$ and can be expected to be small. As before, we replace $|V_a(E_n, x)|$ by $|V_a(E, x)|$ where $V_a(E, x)$ is as defined in (37) with E_n replaced by E. Further, $n_f(E_n)$ can also be replaced by N_F for all E, where, N_F denotes the number of finite gaps between two consecutive minima points of the potential $V(x)$ below threshold. In that case, the bound can be written as

$$N(E) \leqslant \frac{1}{\pi} \int_{-\infty}^{\infty} |V_a(E, x)|^{1/2} \, dx + N_F + 1 + \varepsilon_{1T}(E_n). \tag{38}$$

A bound on the total number of bound states can be obtained by setting $E = 0$ in (38):

$$N(0) \leqslant \frac{1}{\pi} \int_{-\infty}^{\infty} |V_a(0, x)|^{1/2} \, dx + N_F + 1 + \varepsilon_{1T}(E_n). \tag{39}$$

Clearly, the integral corresponds to the effectively attractive regions of the potential $V(x)$. The estimate of the upper bound on the number of bound states with energies less than or equal to energy $E \leqslant 0$ in $1D$, given by (38) with $\varepsilon_{1T}(E_n) = 0$ will be referred to as $B1D$.

3. Illustrative examples

In this section we illustrate using a number of examples, the usefulness of the formulae $B3D$ (eq (32) with $\varepsilon_{3T} = 0$) and $B1D$ (eq (38) with $\varepsilon_{1T} = 0$) in estimating bounds on the number of bound states for a number of potentials and compare them with the corresponding results obtained using other methods. In table 1, we summarize the results obtained for several well-known potentials in $3D$ and $1D$. The table lists both the analytical and numerical results for typical potential parameters. It may be noted that the values of the number of bound states and the upper bounds are taken to be the highest integers less than or equal to the values calculated using various

Table 1. Analytical and typical numerical estimates of the upper bounds on the total number of bound states $N(E=0)$ or $N(l, E=0)$ for various potentials in $1D$ and $3D$ and their comparison with the exact results and bounds obtained using BTI and BI respectively. $[x]$ denotes the highest integer less than or equal to x.

Potential ($1D$ or $3D$)	l	$N(E=0)$ or $N(l, E=0)$	Upper bound from $B1D$ or $B3D$	Upper bound from BTI or BI	Remarks
Square well ($1D$) $V(x) = -V_0, \lvert x\rvert < a$, $= 0, \lvert x\rvert > a, V_0 > 0$.		$N(0) \leqslant \left[\frac{2aV_0^{1/2}}{\pi} + 1\right]$	$\left[\frac{2aV_0^{1/2}}{\pi} + 1\right]$	$[a^2 V_0 + 1]$	The result for $N(E=0)$ is obtained using the eigen-value equation $\cot \alpha a = \alpha/\beta$ for even parity eigenfunction and $\cot \alpha a = -\beta/\alpha$ for odd parity eigenfunction, where, $\alpha^2 = V_0 - \beta^2, \beta^2 = -E$.
$V_0 = 2, a = 4$		$N(0) \leqslant 4$	4	33	
Morse ($1D$) $V(x) = V_0(e^{-2x/a} - 2e^{-x/a})$ $V_0 > 0, a > 0$		$[aV_0^{1/2} + \frac{1}{2}]$	$[aV_0^{1/2} + 1]$	∞	$N(E=0)$ is calculated from the number of solutions of the eigenvalue equation $E_n = -V_0\{1 - (n+\frac{1}{2})/a_0 V^{1/2}\}^2 \leqslant 0$, where $n = 0, 1, 2, \ldots$
$V_0 = 4, a = 1$		2	3	∞	
Hulthen ($3D$) $V(r) = -\frac{V_0 e^{-r/a}}{1 - e^{-r/a}}$,					
$V_0 > 0, a > 0$.	0	$[aV_0^{1/2}]$	$[aV_0^{1/2} + 1]$	$[\pi^2 a^2 V_0/6]$	$N(l=0, E=0)$ is estimated from the eigen-value expression $E_n = -((a^2 V_0 - n^2)/4a^2 n^2)$ $n = 1, 2, \ldots\ldots$ (Newton 1966, p. 422)
$V_0 = 4, a = 1$	0	2	3	6	
$V_0 = 1, a = 10$	0	10	11	164	
Exponential ($3D$) $V(r) = -V_0 e^{-r/a}$,					
$V_0 > 0, a > 0$	0	$[2aV_0^{1/2}/\pi]$	$[2aV_0^{1/2}/\pi + 1]$	$[a^2 V_0]$	$N(l=0, E=0)$ is estimated from the number of solutions of the eigenvalue equation $J_q(c) = 0$, where, $q^2 = -4Ea^2$, $c = 4V_0 a^2$, as E varies from $-V_0$ to 0. (Flügge 1974, p. 197)
$V_0 = 5, a = 1$	0	1	2	5	
$V_0 = 10, a = 1{\cdot}5$	0	3	4	22	

formulae. Since we have set $2m = 1$, $\hbar = 1$, the potential and energy have dimension L^{-2}. From table 1, it is clear that the estimates of bounds for *B3D* and *B1D* are equal to or very close to the exact number of bound states. In many cases, estimates from *B3D* and *B1D* are larger than the actual number of bound states only by unity. We have verified that equally good estimates can be obtained in case of several other typical potentials like modified Pöschl-Teller (1*D*), attractive square well (3*D*), Yukawa (3*D*), Wood-Saxon (3*D*), second Pöschl-Teller (3*D*) etc., but have not included in the table to maintain brievity. These results clearly indicate that the prescriptions *B3D* and *B1D* are powerful formulae and give estimates of bounds on the number of bound states which are superior to those given by BI and BTI respectively except when potential strength and range parameters are small. It may be noted that Calegaro's bound (Calegaro 1965) given by $n_0 \leqslant 2/\pi \int_0^\infty |V(r)|^{1/2}\,dr$ for the number of *s*-wave bound states gives approximately twice the estimate of the number of bound states obtained by *B3D* in the case of purely attractive potentials.

The case of sum of n delta-shell potential given by $V(r) = -\Sigma_{i=1}^{n} \lambda_i \delta(r - a_i)$ is somewhat special. In this case the bound from BI is $\Sigma_{i=1}^{n} \lambda_i a_i$. In order to estimate the bound from *B3D*, we can heuristically represent delta-function by $\delta(x) \simeq (\Delta/\pi)/(x^2 + \Delta^2)$, $\Delta \to 0$. One can show that

$$\int_{-a}^{a} \left[\frac{\Delta/\pi}{x^2 + \Delta^2}\right]^{1/2} dx$$

is of the order of $\Delta^{1/2} \ln \Delta$ for $\Delta \to 0$. In this sense, we can write $\int_{-\infty}^{\infty} |V(r)|^{1/2}\,dr = 0$. But, the number of gaps N_F between consecutive minima points of the potential below threshold is equal to $(n-1)$ in this case and hence the upper bound becomes equal to n, same as the total number of attractive delta shell potentials. This particular result can also be found in the work of Jain *et al* (1978). The case of n-delta function indicates that estimate *B3D* is likely to be applicable for all potentials for which $|V_a^l(E,r)|^{1/2}$ is integrable even when $|V_a^l(E,r)|^{1/2}$ have integrable singularities.

In §2 we had stated that the terms ε_{1T} and ε_{3T} can be expected to be small. The results listed in table 1 does not contradict this conclusion in the cases illustrated. Hence, *B3D* and *B1D* can be expected to be upper bounds on the number of bound states in the case of commonly used potentials. However, *B3D* and *B1D* (eq (38) and (32) with $\varepsilon_{3T} = 0$ and $\varepsilon_{1T} = 0$ respectively) can be considered as estimates of number of bound states because of the closeness of these upper bounds to the actual number of bound states. It may be noted that a lower bound on the number of bound states below energy E is given by Titchmarsh (1962) in case of 1*D*:

$$N(E) \geqslant \frac{1}{\pi} \int_0^X [E - V(x)]^{1/2}\,dx - 1,$$

where $V(X) = E$. This clearly shows why *B3D* and *B1D* can be taken as reasonable estimates of the number of bound states. In the next section, we will discuss other plausible arguments which also indicate that ε_{1T} and ε_{3T} are expected to be small in case of most of the commonly used potentials. It may be mentioned that recently Requardt (1985) has obtained the following bound on the number of bound states generated by $V(r)$ below energy E for $l \geqslant 0$:

$$N(l,E) \leqslant \left(1 - \frac{l(l+1)}{Z_E}\right) \int_0^\infty r(V(r) - E)\,dr, \tag{40}$$

where, $Z_E = \sup r^2(V(r)-E)_-$ and $-(V(r)-E)_-$ is the negative part of $(V(r)-E)$. Obviously,

$$-(V(r)-E)_- = V(r)-E, \quad \text{when } V(r) < E,$$
$$= 0, \quad \text{when } V(r) \geqslant E,$$

that is, $-(V(r)-E)_-$ is equivalent to $V_a^0(E,r)$ defined in §2. For example, for attractive coulomb potential $V(r) = -\lambda/r$, $\lambda > 0$, $N(l,E)$ is equal to the highest integer less than or equal to $[(\lambda/2|E|^{1/2}) - 1]$. The upper bound on $N(l,E)$ calculated by Requardt's formula (40) is the highest integer less than or equal to $[(\lambda^2/2|E|) - 2l(l+1)]$ whereas that calculated using *B3D* is the highest integer less than or equal to

$$\left[\frac{\lambda}{2|E|^{1/2}} - \{l(l+1)\}^{1/2} + 1\right].$$

It is clear that estimates by *B3D* are much superior to that given by (40) in these cases.

The conditions specified in the beginning of §2 have excluded confining potentials like harmonic oscillator, linear potential, infinite square well, logarithmic potential etc., in our analysis. These potentials generate infinite number of bound states and for then $E = 0$ is not the threshold of the continuum. However, we found that *B3D* and *B1D* for a given E in these cases also provide the estimates of the upper bounds which are greater than and quite close to the actual number of bound states with energies less than or equal to the specified energy E. For example, for 3*D* linear potential $V(r) = \lambda r$, $\lambda > 0$ and for $l = 0$, the bound on the number of bound states having energies equal to or below energy $E > 0$, is given by the highest integer less than or equal to $[2E^{3/2}/3\pi\lambda + 1]$ whereas the actual number of such bound states is given by the highest integer less than or equal to $[2E^{3/2}/3\pi\lambda + 1/4]$. Similarly close results are obtained for other confining potentials like harmonic oscillation, logarithmic, symmetric Pöschl-Teller etc. These indicate that the procedure and the results developed in §2 may be applicable for a larger class of potentials.

4. Discussion and conclusion

The formulation of the bounds on the number of bounds states deduced in §2, is based on the node counting method. Our final results appear to be similar to the asymptotic formulae given by Titchmarsh (1962). These also look akin to the WKB formulation for the bound state problem in some respects. For a single potential well, the leading order WKB expressions for obtaining the bound states are (Fröman and Fröman 1965)

$$\int_{x'(E)}^{x''(E)} |q(x)|\,dx \approx \left(s+\frac{1}{2}\right)\pi + \varepsilon_{1\text{WKB}}, \tag{41a}$$

in case of 1*D* and

$$\int_{r'(E)}^{r''(E)} |q(r)|\,dr \approx \left(s+\frac{1}{2}\right)\pi + \varepsilon_{3\text{WKB}}, \tag{41b}$$

in case of 3*D* ($s = 0, 1, 2, \ldots$).

Here, $q(x) = |V(x) - E|^{1/2}$ and x', x'' and r', r'' are the turning points in the potential well at energy E in $1D$ and $3D$ respectively. $\varepsilon_{1\text{WKB}}$ and $\varepsilon_{3\text{WKB}}$ are the corrections to the WKB formula. The eigenvalues for a potential well, within WKB approximation are obtained using (41a) and (41b) with the correction terms $\varepsilon_{1\text{WKB}}$ or $\varepsilon_{3\text{WKB}}$ set to zero. It may be noted that the WKB formalism provides the following estimates for the number of bound states for the single potential well in $1D$ and $3D$ (s-wave) respectively.

$$n \approx \frac{1}{\pi}\int_{x'(0)}^{x''(0)} |V(x)|^{1/2}\,\mathrm{d}x + \frac{1}{2}$$

$$= \frac{1}{\pi}\int_{-\infty}^{\infty} |V_a(x)|^{1/2}\,\mathrm{d}x + \frac{1}{2}, \tag{42a}$$

$$n \approx \frac{1}{\pi}\int_{r'(0)}^{r''(0)} |V(r)|^{1/2}\,\mathrm{d}r + \frac{1}{2}$$

$$= \frac{1}{\pi}\int_{0}^{\infty} |V_a(r)|^{1/2}\,\mathrm{d}r + \frac{1}{2}, \tag{42b}$$

where, $n = s + 1$. Clearly, in our estimates, the term 1/2 in (42a) and (42b) are replaced by 1. It is shown that for reasonably well-behaved potentials which have appropriate analytical continuation, the corrections $\varepsilon_{1\text{WKB}}$ and $\varepsilon_{3\text{WKB}}$ are quite small compared to unity (Fröman and Fröman 1965). In fact, Migdal (1977) has given an estimate of the correction $\varepsilon_{1\text{WKB}}$ or $\varepsilon_{3\text{WKB}}$ in the eigenvalue equations (41a, b) which is of the order of $(\pi n)^{-2}$, $n = 1, 2, \ldots\ldots$ Recently, Adhikari *et al* (1988), in a paper on higher order WKB approximation, have given an explicit expression for quantisation condition in WKB approximation up to several higher order terms in case of a $1D$ single well potential:

$$\left(s + \frac{1}{2}\right)\pi = \frac{\sqrt{2m}}{\hbar}\int_{x'(E)}^{x''(E)} (E - V(x))^{1/2}\,\mathrm{d}x - \frac{\hbar}{24\sqrt{2m}}\frac{\mathrm{d}}{\mathrm{d}E}$$
$$\times \int_{x'(E)}^{x''(E)} V''(x)(E - V(x))_{\mathrm{dx}}^{-1/2} + \frac{\hbar^3}{2880(2m)^{3/2}}\frac{\mathrm{d}^3}{\mathrm{d}E^3}$$
$$\times \int_{x'(E)}^{x''(E)} [7(V''(x))^2 - 5V'(x)\,V''(x)](E - V(x))_{\mathrm{dx}}^{-1/2} + \ldots. \tag{43}$$

This expression indicates that the next order correction is of the order of $o(\hbar^2)$ compared to the leading order term. Since, our estimates for number of bound states for a single attractive well potential is very similar to the leading order term in WKB approximation formula for bound states, we expect that the correction should be of the order of higher order term in the general WKB approximation formula. The above observation indicates that the correction term in the case of a single attractive well potential should be expected to be small. In the case of a more general well-behaved potential having a finite number of attractive and repulsive sections, ε_{1T} and ε_{3T} can be expected to be negligibly small. These show that the estimate of the total number of bound states by $B1D$ or $B3D$ obtained after neglecting ε_{1T} or ε_{3T} can be expected to hold true quite well. This is particularly so because the replacement of the term 1/2 of the WKB formula by unity in $B1D$ or $B3D$ can be

expected to compensate for the omission of ε_{1T} or ε_{3T} in obtaining *B1D* or *B3D* respectively for commonly used well behaved potentials.

Our procedure of estimating the number of bound states can be correlated to the Levinson's theorem in potential scattering (Newton 1966). This theorem relates the number of s-wave bound states N to the zero energy phase shift: $\delta(0) = (N-1)\pi$ if there is no zero energy bound state, $= (N-1/2)\pi$ if there is a zero energy bound state, where $N = 1, 2, 3, \ldots$. Here $\delta(0)$ is the magnitude of the total phase accumulated with respect to the corresponding solution of the free Schrödinger equation as the wave-function evolves from $r = 0$ to $r = \infty$. Hence, Levinson's theorem indicates that the number of s-wave bound states that can be generated is of the order of $N \approx \delta(0)/\pi + 1$, which is consistent with the estimate *B3D*. In fact, *B3D* accomplishes a bound on $\delta(0)$ by separating the potential into effectively attractive (< 0) and non-attractive ($\geqslant 0$) regions as described in §2.

In conclusion we find that the estimates *B1D* and *B3D* provide us with quite reliable and useful upper bounds on the number of bound states with energies less than or equal to an energy E in $1D$ and $3D$ respectively. Their usefulness is clearly demonstrated using a large number of potentials commonly used in physical problems. For long range potentials like the coulomb potential, the integral in *B3D* diverges, just like BI, indicating the possibility of existence of infinite number of bound states. For all potentials, specified in §2, for which the integral

$$\int_0^\infty |V_a^l(E,r)|^{1/2}\,\mathrm{d}r \quad \text{or} \quad \int_{-\infty}^\infty |V_a(E,x)|^{1/2}\,\mathrm{d}x$$

exists, the formula *B3D* or *B1D* can be profitably utilised to get a close estimate of the bound on the number of bound states.

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