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APPROXIMATE CENTRIFUGAL BARRIERS AND CRITICAL ANGULAR MOMENTUM

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In the $D = 3$ dimensional space, some potentials admit analytical solution of the Schrödinger equation for the $\ell = 0$ states. To extend the analytical results to levels of higher angular momentum, the centrifugal barrier is often approximated by a repulsive term having the radial dependence as the original potential. These approximations are valid for well bound states. They become dubious as ℓ approaches a critical value ℓ_c above which the states of higher angular momentum are unbound by the original potential. The present work proposes a way to determine an upper bound ℓ_c^+ to ℓ_c. The derived formula is tested against four typical potentials. The excellent agreement found between ℓ_c^+ and ℓ_c in these case proves the present upper bound to be a useful approximation.

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1. INTRODUCTION

In the $D = 3$ dimensional space, few short range potentials are known, which admit analytical solutions to the Schrödinger equation for the states of $\ell = 0$ angular momentum. Let us mention the Hulthén, Morse, Manning-Rosen and Pöschl-Teller potentials. None of them, however, leads to exact solutions for $\ell \neq 0$. To overcome this situation, an approximation is often used, which simulate the $1/r^2$ dependence of the centrifugal barrier by a repulsive shape identical to the original potential. This is equivalent to a short range potential with a strength depending on ℓ. In order to take into account the long range effect of the centrifugal barrier tail, a constant term proportional to $\ell(\ell+1)$ is often added.

A typical example of such a procedure is given in the textbook by Flügge for the Morse potential [1]. In this case, the centrifugal barrier is approximated by

$$\frac{\ell(\ell+1)}{r^2} \approx \frac{\ell(\ell+1)}{\gamma^2}\left(C_0 + C_1 e^{-\alpha r} + C_2 e^{-2\alpha r}\right), \tag{1}$$

where γ, C_0, C_1, C_2 and α are constants. Examples and applications can be found in recent work [2–5].

Approximations of this type are valid, and even accurate, as long as the calculated ℓ-state is well bound. However, they break down as soon as ℓ gets large and comes close to the critical value ℓ_c. We recall the reader that short range potentials possess at the most a finite number of bound states, and that for each angular momentum ℓ a critical value of the potential strength (or coupling constant) exists below which the ℓ-state is unbound. Consequently, for a given strength, a critical value of the angular momentum ℓ_c exists, such that for $\ell > \ell_c$ the states are unbound. In the approximated expression (1), the constant term proportional to $\ell(\ell+1)$ acts as a confining barrier. It bounds ℓ states which are unbound by the actual potential.

For this reason, it is important to fix the limit up to which the effective centrifugal barrier can be used with confidence. Obviously, for a given potential, it amounts to know ℓ_c, namely the highest angular momentum for which a bound state exists.

To our knowledge, this problem has never been touched. It the purpose of the present work to propose a simple criterion, and to check its validity on few examples.

The paper is organized as follows. A general criterion is derived in section 2, leading to an upper bound to ℓ_c. A few typical examples are worked out in section 3. Conclusions are drawn in section 4.

2. A GENERAL CRITERION

The starting point is the reduced radial Schrödinger equation in the $D = 3$ dimensional space, assuming spherical symmetry of the potential. In the units $\hbar = 2m = 1$, we are left with

$$\left[-\frac{d^2}{dr^2} - \lambda V(r) + \frac{\ell(\ell+1)}{r^2}\right]\psi_{n\ell}(r) = E_{n\ell}\psi_{n\ell}. \tag{2}$$

Here, $-\lambda V(r)$ is a short range potential, defined as not too singular near the origin and decreasing faster than $1/r^2$ at large distances. Note that according to the convention used here, λ is positive definite, and the positive part of $V(r)$ corresponds to an attractive potential.

The question of the minimal value of λ needed to get a bound state has been discussed since a long time. It is connected to the number of bound state produced by a given potential, which is discussed in many textbooks (see for instance [6, 7]. Sufficient conditions has been derived by Calogero [8] in 1965, and more recently by two of us [9].

Consider the effective potential

$$V_{eff}(r) = -\lambda V(r) + \frac{\ell(\ell+1)}{r^2}. \tag{3}$$

In order for an ℓ-state to be bound, V_{eff} needs not necessarily to have a negative part, but at least a minimum. It means that besides bound states of negative energy, we also consider confined state of positive energy.

For the sake of simplicity, we assume here that $V(r)$ is either a monotonic decreasing function or it possesses a single maximum, below which it decreases monotonically.

The minimum of V_{eff} is solution of

$$\lambda V'(r_0)r_0^3 + 2\ell(\ell+1) = 0, \tag{4}$$

where the prime denotes the derivative with respect to r. This equation has either 2, 1 or zero solutions. In case that two solutions exist, the most exterior one is chosen, because it corresponds to a minimum in the attractive part of the potential. By comparison, the interior zero reflects the geometry of the repulsive part.

Two further conditions can be invoked to determine r_0 according to the kind of bound states which are considered. In the case of bound states of negative energy $V_{eff}(r)$ must have a negative part.

Consequently a bound can be establish by setting $V_{eff}(r_0) = 0$. This leads to

$$r_0 = -2\frac{V(r_0)}{V'(r_0)}. \tag{5}$$

On the other hand, the definition of bound states can be extended to levels of positive energy confined inside the potential well created by $V_{eff}(r)$ with its minimum at $r = r_0$. Such states have a finite lifetime, which may be long enough the corresponding width to be negligible. The disappearance of these quasi-bound states is connected with the disappearance of the minimum. Thus, the second condition is the vanishing of the second derivative, namely $V''_{eff}(r'_0) = 0$.

This leads to

$$r'_0 = -3\frac{V'(r'_0)}{V''(r'_0)}. \tag{6}$$

Both determinations are not sufficient conditions to ensure a ℓ-state to be unbound. This is due to the fact that in $D = 3$, a minimal strength of the potential is required a given state to be bound.

Consequently, the above criteria determine upper bounds ℓ_c^+ to the critical angular momentum ℓ_c.

Because the main interest is in the bound states of negative energy, we shall merely work with the first condition and take r_0 from (5).

The upper limit is obtained from

$$\ell_c^+(\ell_c^+ + 1) = -\frac{r_0^3}{2}\lambda V'(r_0). \tag{7}$$

The angular momentum being a positive integer, we retain for ℓ_c^+ the integer part of the positive solution, namely

$$\ell_c^+ = \text{Int}\left\{\frac{1}{2}\left[-1+\sqrt{1-2\lambda r_0^3 V'(r_0)}\right]\right\}. \tag{8}$$

It is interesting to note that the value of r_0 determined from (5) is not dependent on the strength λ but only on the geometry of the potential. The same remark holds for r_0' obtained from (6). Furthermore, the limit for large ℓ_c^+ is given by

$$\ell_c^+ \approx \sqrt{\frac{-r_0^3 V'(r_0)}{2}}\sqrt{\lambda}. \tag{9}$$

This asymptotic behavior can be compared to predictions from inequalities estimating the number of bound states n_ℓ for short range potentials. Indeed, it was shown by Calogero [10] that the number of bound states increases proportionally to the square root of the potential strength (see also the work of Chadan [11]). Consequently, the present estimate corroborates his result and yields a good bound to the critical strength needed to bind a ℓ-state, namely

$$\lambda_c \geq \ell(\ell+1)\frac{2}{-r_0^3 V'(r_0)}. \tag{10}$$

3. A FEW TYPICAL EXAMPLES.

The present work establishes an upper bound to ℓ_c. The remaining question is to verify that it constitutes a useful approximation, *i.e.* that it yields values close to the actual ℓ_c. In order to check the efficiency of the bound ℓ_c^+, calculations have been performed for a few potentials, and compared to the ℓ_c values determined numerically. The following potentials have been considered:

The Hulthén potential :

$$V_H(r) = \frac{1}{e^r-1}, \tag{11}$$

the Morse potential

$$V_M(r) = -2e^{-2r}+e^{-r}, \tag{12}$$

the Pöschl-Teller potential

$$V_{PT}(r) = \frac{1}{\cosh^2(r)} \tag{13}$$

and a power-law decreasing potential

$$V_{pl}(r) = \frac{1}{1+r^4}. \tag{14}$$

The three first potentials have a decreasing exponential tail. A power-law potential has been added to check a possible dependence on the shape of the potential tail.

Table 1.

The values of r_0 and the proportionality factors to $\sqrt{\lambda}$ according to (9) and the numerical estimates.

potential	r_0	$\sqrt{-r_0^3 V'(r_0)/2}$	num. slope
V_H	1.594	0.805	0.804
V_M	2.493	0.655	0.654
V_{PT}	1.200	0.663	0.661
V_{pl}	1.000	0.707	0.704

The values of ℓ_c^+ obtained from (5) and (8) have been checked against the numerical determinations of ℓ_c up to $\ell = 20$. The results are summarized in table 1. For each of the four potentials, the values of r_0 and the coefficients $\sqrt{-r_0^3 V'(r_0)/2}$ are given. This last quantity is compared to the numerical estimate of the slope of the line

$$\ell_c = a + b\sqrt{\lambda}. \tag{15}$$

The agreement between the two values is better than 1 %. It means that the present approach is a sound method to evaluate ℓ_c.

Note that, in the case of the Morse potential, two solutions exist for r_0. As stated above, the lowest one is due to the repulsive part of the potential, and is irrelevant for the binding of the ℓ-states. The second (larger) root has to be retained.

For the sake of comparison, the values of r_0' and $\sqrt{(-r_0')^3 V'(r_0)}$ are displayed in table 2. They correspond to quasi bound states, *i.e.* possible bound state of positive energy. As expected the r_0' are sensibly greater than r_0, and the corresponding ℓ_c^+ about 10 % larger.

This could also be tested numerically. However, it requires sophisticated numerical techniques, and it goes beyond the aim of the present work to get involved in this problem.

Table 2.

The value of r_0' and $\sqrt{-(r_0')^3 V'(r_0)}$ for the four considered potentials.

potential	r_0'	$\sqrt{-(r_0')^3 V'(r_0')/2}$
V_H	2.577	0.873
V_M	3.486	0.754
V_{PT}	1.718	0.756
V_{pl}	1.136	0.778

4. CONCLUSIONS

Approximations to the centrifugal barrier are used in the $D = 3$ dimensional space to obtain approximated but analytical solution of the Schrödinger equation in the case of short range potential being solvable for the $\ell = 0$ states. These approximations are valid for well bound states, but necessarily wrong for angular momentum close to or above the critical ℓ_c. These state are unbound by the original potential. Consequently it is important to have at least an estimate of ℓ_c.

The present work provides us with an upper bound ℓ_c^+, which agrees remarkably with ℓ_c as far as we have been able to check. That the increase of ℓ_c is proportional to $\sqrt{\lambda}$ is well established. The agreement of the proportionality factors obtained from (9) and the numerical values is impressive. This result is even somewhat surprising because of the values of r_0 are obtained from the condition $V_{eff}(r_0)$ = 0. In $D = 3$, we know that a minimal negative part of $V_{eff}(r)$ is needed to get a bound state.

The present results suggests that for $\ell \neq 0$ the reduced radial Schrödinger equation behaves very much like in the $D = 1$ dimensional space. In this case an infinitely small but negative part $V_{eff}(r)$ would admit a bound state. In other words, the critical strength $\lambda_c(\ell)$ needed to bind an ℓ state represents the necessary strength of the short range potential required for $V_{eff}(r)$ to have a negative part. We expect the same kind of situation to occur in the $D = 2$ dimensional space. It would be interesting to test the case of higher dimensional space.

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REFERENCES

1. S. Flügge, *Practical Quantum Mechanics* (New York, Heidelberg, Berlin, Springer-Verlag, second printing, 1994).
2. W. Qiang, K. Li and W. Chen, Chem. J. Phys. A Math. Theor. **42**, 205306 (2009).
3. S. M. Ikhdair, Eur. Phys. J. A **39**, 307 (2009).
4. C. S. Jia, J. Y. Liu and P. Q. Wang, Phys. Lett. A **372**, 4779 (2008).
5. A. Diaf and A. Chouchaoui, Physica Scripta **84**, 015004 (2011) doi:10.1088/0031-8949/84/01/015004.
6. A. Galindo and P. Pascual, *Quantum Mechanics I* (2nd edn., Berlin, Springer, 1991).
7. R. G. Newton, *Scattering theory of waves and particles* (2nd edn., New York, Springer, 1982).
8. F. Calogero, J. Math. Phys **6** 161 and 1105 (1965).
9. M. Lassaut and R. J. Lombard, J. Phys. A : Math. Gen. **30**, 2467 (1997).
10. F. Calogero, *Variable Phase Approach to Potential Scattering* (Acad. Press, New York, 1967).
11. K. Chadan, Nuovo Cimento A **58**, 191 (1968).