Some results for the wave function at the origin for S-wave levels.

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Abstract
Starting with the S-wave radial equation for an attractive central potential $V(r)$, we give results for the $n$ (principal quantum number) and the $\mu$ (reduced mass) dependence of $R_{n0}(0)$, the S-wave radial wavefunction at the origin, for potentials with definite curvature.

1 Introduction
Discovery of quark-antiquark atoms like charmonium in 1974 led to general investigations[1] of the Schrödinger equation with a central potential $V(r)$ representing the $q\bar{q}$-potential. The motivation was to obtain results based on general properties of $V(r)$ like its shape, since its precise form was then (and still is) unknown.

Some results were obtained for the S-wave ($\ell = 0$) bound state radial wave function $R_{n0}(r)$ [2]. Specifically, it was shown that $R_{20}(0)$ is larger (smaller) than $R_{10}(0)$ provided $V(r)$ was everywhere convex, $V''(r) > 0$ (concave, $V''(r) < 0$). Prime denotes derivative with respect to $r$. The variation of $R_{10}(0)$ with the reduced mass $\mu$ was also related to the curvature of the potential. This was directly proved from the radial equation for $n = 1$ [3]. Both types of results mentioned above were proved for large $n$ using the WKB approximation [4].

In this note we show that both types of results follow directly from the S-wave radial Schrödinger equation for all $n$. For notational simplicity, define

$$S_n(0) = [R_{n0}(0)]^2. \quad (1)$$

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We will prove that for \( n = 1, 2, \ldots \),

(a) if \( V'(r) > 0 \) and \( V''(r) = 0 \) for all \( r \) then

\[ S_n(0) - S_{n+1}(0) = 0 \quad \text{and} \quad \frac{\partial}{\partial \mu} \left[ \frac{1}{\mu} S_n(0) \right] = 0; \quad (2) \]

(b) if \( V'(r) > 0 \) and \( V''(r) < 0 \) for all \( r \) and \( V'(\infty) \) is finite then

\[ S_n(0) - S_{n+1}(0) > 0 \quad \text{and} \quad \frac{\partial}{\partial \mu} \left[ \frac{1}{\mu} S_n(0) \right] > 0; \quad (3) \]

(c) if \( V'(r) > 0 \) and \( V''(r) > 0 \) for all \( r \) and \( V'(0) \) is finite then

\[ S_n(0) - S_{n+1}(0) < 0 \quad \text{and} \quad \frac{\partial}{\partial \mu} \left[ \frac{1}{\mu} S_n(0) \right] < 0. \quad (4) \]

Case (a) corresponds to an attractive linear potential. This case is exactly solvable. Indeed, there are well known exactly solvable examples for the concave (Coulomb potential) and convex (harmonic oscillator) cases which satisfy the above inequalities. Explicit solutions of convex power law potentials \( r^k \) with \( k > 1 \) and the concave log(\( r \)) potential satisfy the above inequalities \([5]\). With all this evidence at hand we believe that the above inequalities are really theorems. In the next section we present a result for non-zero \( \ell \) followed by our arguments for the S-wave results. The concluding section contains some discussion.

2 Proof of the results

The radial equation, for a two-body system with reduced mass \( \mu \) in an attractive central potential \( V(r) \) for \( u_{n\ell}(r) = rR_{n\ell}(r) \) is

\[ -Hu''_{n\ell}(r) + [W_\ell(r) - E_n]u_{n\ell}(r) = 0, \quad (5) \]

where

\[ H = \frac{\hbar^2}{2\mu}, \quad (6) \]

and

\[ W_\ell(r) = V(r) + H \frac{\ell(\ell + 1)}{r^2}. \quad (7) \]

The radial wavefunction \( R_{n\ell}(r) \) for energy \( E_n \) is real so its modulus square is the same as its square. Consequently, the inequalities in the introduction are usually stated for the modulus square. The energy of the bound state
increases with principal quantum number, \( n \), thus \( E_1 < E_2 < E_3 \ldots \). The potential obeys the standard restrictions, namely, \( \lim_{r \to 0} r^2 V(r) = 0 \). Also, recall that \( R_{n\ell}(r) \) behaves as \( r^\ell \) as \( r \) tends to zero. For an attractive force, the asymptotic behaviour \( (r \to \infty) \) of the radial wavefunction \( u(r) \) will be like \( \exp(-ar) \), \( a > 0 \).

Multiply the radial equation by \( u'_{n\ell} \) and integrate from zero to infinity. The term with \( E_n \) gives zero. One integration by parts gives

\[
H[u'_{n\ell}(0)]^2 \delta_{\ell 0} = \int_0^\infty W'_\ell(r)u^2_{n\ell}(r)dr. \tag{8}
\]

The term \( W'_\ell(r)u^2_{n\ell}(r) \) from the partial integration does not contribute. This is obvious for the upper limit \( r = \infty \). One has to be careful at the lower limit \( r = 0 \). However, since \( V(r) \) is less singular than \( r^{-2} \) and \( u^2_{n\ell}(r) \sim r^{2(\ell+1)} \) as \( r \to 0 \), the lower limit also does not contribute. All this is well known.

Before specialising to S-wave it is interesting to consider the above equation for non-zero \( \ell \).

### 2.1 Result for non-zero \( \ell \)

In this case, since the l.h.s. of Eq(8) is zero, the equation simply says that the expectation value of the effective force \( W'_\ell(r) \) is zero. Alternatively, it implies that the expectation value of \( V'(r) \) for a general potential is related to that of \( r^{-3} \). Explicitly,

\[
\langle V'(r) \rangle_{n\ell} = 2H\ell(\ell + 1) \left\langle \frac{1}{r^3} \right\rangle_{n\ell}. \tag{9}
\]

This general result (probably known personally to many [6]) deserves to be better known. It is is very useful. For example, for a Coulomb potential it immediately gives the correct relation between the expectation values of \( r^{-2} \) and \( r^{-3} \).

### 2.2 S-wave relations

For \( \ell = 0 \), Eq(8) reduces to

\[
HS_n(0) = \int_0^\infty V'(r)u^2_{n0}(r)dr = \langle V'(r) \rangle_{n0}. \tag{10}
\]

This is a well-known result and provides the basis for the arguments leading to the proof of the results given in the introduction.
Case (a): \( V''(r) = 0 \) for all \( r \).
This is the case of the attractive linear potential \( V(r) = \lambda r \). So, \( V'(r) = \lambda \) is positive for all \( r \). In this case, Eq.(10) reduces to simply
\[
H S_n(0) = \lambda,
\]
(11)
since \( u_{n0}(r) \) is normalized, that is
\[
\int_0^\infty u_{n0}^2(r)dr = 1.
\]
(12)
Thus, in this case \( H S_n(0) \) is a constant (the potential strength) independent of \( \mu \) or \( n \) as required. It is well known that the linear potential is exactly solvable in terms of Airy functions. The above relation for \( H S_n(0) \) has been noted earlier using the explicit solutions [7].

Case (b). \( V''(r) < 0 \) and \( V'(r) > 0 \) for all \( r \), with \( V'(\infty) \) finite.
A well-known exactly solvable example of this case is the Coulomb potential. Perform an integration by parts in Eq(10) to obtain
\[
H S_n(0) = V'(\infty) - \int_0^\infty V''(r)f_{n0}(r)dr,
\]
(13)
where
\[
f_{n0}(r) = \int_0^r u_{n0}^2(r)dr.
\]
(14)
Note that \( f_{n0}(\infty) = 1 \) because the radial wavefunction is normalized. The term \( V'(r)f_{n0}(r) \), from the integration by parts at \( r = \infty \), gives \( V'(\infty) \) while that at \( r = 0 \) vanishes. This is because \( V(r) \) is less singular than \( r^{-2} \) as \( r \) tends to 0 while one expects \( f_{n0}(r) \sim r^3 \) as \( r \) tends to 0 because \( u_{n0}^2(r) \sim r^2 \). Physically, \( f_{n0}(r) \) represents the probability of finding the particle (two-body system) between 0 and \( r \). As \( n \) increases the energy \( E_n \) of the state increases. For a single well potential, the classical turning point \( E_n = V(r) \) will be at a larger value of \( r \) as \( n \) or energy increases (keep in mind the Coulomb potential). So, one expects \( f_{n0}(r) \) to be larger than \( f_{m0}(r) \) for \( n < m \) for small \( r \). Asymptotically, the states with larger energy may have a longer tail (true for the Coulomb case) with the result \( f_{n0}(r) - f_{m0}(r) \) is negative for large \( r \) for \( n < m \). However, the large \( r \) contribution will be damped out since for concave potential \( V''(r) \) decreases asymptotically. In fact, for power law potentials \( r^k \) with \( 1 > k > -2 \) with \( V'(r) > 0, V''(r) \) goes to zero as \( r \) tends to infinity and goes to infinity as \( r \) tends to zero.

Given the above physical reasoning, we expect that
\[
H[S_n(0) - S_m(0)] = -\int_0^\infty V''(r)[f_{n0}(r) - f_{m0}(r)]dr > 0 \quad \text{(15)}
\]
for \( n < m \) if \( V''(r) < 0 \) for all \( r \). This gives the first inequality in Eq(3).

For the variation with respect to the reduced mass, we note that with increasing \( \mu \), the system will shrink in size. So, physically one expects that \( f_{n0}(r) \) will increase, that is, \( \left. \frac{\partial}{\partial \mu} f_{n0}(r) \right| > 0 \). Thus, taking the derivative w.r.t. \( \mu \) of Eq(13), since \( V'(\infty) \) is a constant, gives the second inequality in Eq(3).

Case(c). \( V''(r) > 0 \) and \( V'(r) > 0 \) for all \( r \), with \( V'(0) \) finite.

An exactly solvable example for this case is harmonic oscillator potential \( r^2 \). In this case we perform a slightly different integration by parts in Eq(10) to obtain

\[
H S_n(0) = V'(0) + \int_0^\infty V''(r) g_{n0}(r) dr. \quad (16)
\]

where

\[
g_{n0}(r) = \int_r^\infty u^2_{n0}(r) dr = 1 - f_{n0}(r). \quad (17)
\]

The term \( V'(r)g_{n0}(r) \), from the integration by parts, gives \( V'(0) \) for \( r = 0 \). For the upper limit \( r \to \infty \) it vanishes because \( u_{n0}(r) \) represents a bound state. From the above two equations we obtain

\[
H[S_n(0) - S_m(0)] = \int_0^\infty V''(r)[g_{n0}(r) - g_{m0}(r)] dr \quad (18)
\]

Now, as \( n \) or \( E_n \) increases, \( g_{n0}(r) \) will increase so for a convex potential \( V''(r) > 0 \) for all \( r \), \( [S_n(0) - S_m(0)] > 0 \) for \( n > m \). For the variation with respect to the reduced mass \( \mu \), we obtain

\[
\frac{\partial}{\partial \mu} \left( \frac{1}{\mu} S_n(0) \right) < 0, \quad (19)
\]

since the variation with \( \mu \) of \( g_{n0}(r) \) is opposite in sign to that of \( f_{n0}(r) \). This concludes the proof of the S-wave results given in the introduction.

A justification for the behaviour of \( f_{n0}(r) \) or \( g_{n0}(r) \) w.r.t. \( n \) required above, in Eq(15) and Eq(18), for our proof is provided by the Virial theorem. For S-wave levels, it states

\[
E_{n0} = \langle U(r) \rangle_{n0}, U(r) = V(r) + \frac{1}{2} r V'(r). \quad (20)
\]

So, if \( U(\infty) \) is finite, then an integration by parts gives

\[
-[E_{n0} - E_{m0}] = \int_0^\infty U'(r)[f_{n0}(r) - f_{m0}(r)] dr > 0. \quad (21)
\]
For \( n < m \), the l.h.s. is always positive, it implies that the integral is always positive. If \( U'(r) > 0 \) for all \( r \), one can physically understand the positivity of the integral because of the expected behavior of \( f_{n0}(r) \) discussed prior to Eq(15).

For example, general power law potentials \( V(r) = -|\lambda|r^\alpha \) with \(-2 < \alpha < 0\) (which includes the Coulomb potential) satisfy all the conditions required for Case(b) and Eq(21). For these potentials the energy \( E_{n0} \) is always negative. Furthermore, the behaviour of \( U'(r) \sim r^{\alpha-1} \) is milder than that of \((-V''(r) \sim r^{\alpha-2}\) because of the extra derivative in the latter. In fact, \([(-rV''') - U'] = \frac{3}{2}\lambda|\alpha|r^{\alpha-1} \) which is positive for all \( r \). Thus, the positivity of the integral in Eq(21) implies the positivity of the integral in Eq(15) for \((-V''(r) > 0 \) for all \( r \).

Guided by the above discussion, for Case(b) the already stated conditions on the potential, perhaps need to be supplemented with the conditions \( U(\infty) \) finite and \( U'(r) > 0 \) for all \( r \).

For potentials with \( U(0) \) finite, an integration by parts of Eq(20) will give

\[
- [E_{n0} - E_{m0}] = - \int_0^\infty U'(r)[g_{n0}(r) - g_{m0}(r)]dr > 0, \quad (22)
\]

for \( n < m \). Thus, if \( U'(r) > 0 \) for all \( r \), the integral will be negative since \( g_{n0}(r) \) increases with \( n \) as noted earlier.

For example, power law potentials \( V(r) = |\lambda|r^\alpha \) with \( \alpha > 1 \), with all \( E_{n0} > 0 \), satisfy all the conditions needed for Eq(18) and Eq(22). Perhaps, for Case(c) we should require the potential to satisfy additional conditions, namely \( U(0) \) finite with \( U'(r) > 0 \) for all \( r \).

Even if the general conditions on the potential have to be supplemented (as per the above discussion) for the cases (b) and (c), the fact remains that the proof of the inequalities is for all \( n \) for a general class of potentials.

### 3 Concluding remarks

The proofs of the S-wave results presented above are not highly mathematical but rely on the physical meaning of the quantities involved and how they are expected to change physically with energy of the bound state (or \( n \)) and the reduced mass \( \mu \). All known soluble examples of attractive potentials with curvature of the same sign for all \( r \) support the results given in the introduction. Such potentials imply that the bound states lie in a single potential well. This is important for the physical arguments presented here. A potential with more than a single well cannot possibly have curvature of
the same sign everywhere. There are lot of solvable potentials for S-waves [9] without definite curvature for which the results given in the introduction may or may not hold. It would be an interesting challenge to find a counter example to the inequalities presented in the introduction.

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