

CHALLENGES FROM SOME KNOWN RESULTS IN QUANTUM MECHANICS

V. Gupta, Departamento de Física Aplicada, CINVESTAV – Unidad Mérida, Yucatán, México

ABSTRACT

Generalization of some known results for the Schrödinger equation still need rigorous proofs which provide a challenge to the practitioners of quantum mechanics.

The discovery of quark-antiquark ($q\bar{q}$) atoms like charmonium ($c\bar{c}$) and bottonium ($b\bar{b}$) led to general investigations of the Schrödinger equation with a central potential $V(r)$ representing the ($q\bar{q}$) potential. The motivation was to prove results based on general properties of $V(r)$, like its shape, since its precise form was (and still is) not known. Some questions of interest were, for example, the ordering of bound state energy levels [1] and the dependence of the value of the S-state wave function at the origin ($r = 0$) on the reduced mass m [2] and the principal quantum number n [3]. This knowledge was of practical use in predicting decay rates and understanding quarkonium spectra.

Some of the results I will mention have been around for a long time. For some reason they are not as widely as they should be to students and teachers of quantum mechanics. Rigorous proofs of the generalizations of these results still provide a theoretical challenge.

For a central potential $V(r)$, the reduced radial equation for bound states is ($u' = du/dr$ etc.):

$$-\frac{\hbar^2}{2m} u'' + \frac{\hbar^2 l(l+1)}{2mr^2} u + V(r)u = Eu \quad (1)$$

where $u = u_{nl}$ and the radial wave function $R_{nl} = 1/ru_{nl}$ with the normalization:

$$\int_0^{\infty} R_{nl}^2(r)r^2 dr = \int_0^{\infty} u_{nl}^2(r) dr = 1 \quad (2)$$

Multiplying equation (1) by $r^q u'_{nl}(r)$ (q integer) and integrating over r from 0 to ∞ leads to various interesting results through simple manipulations like integration by parts. These give recursion relations between expectation values of $V(r)$ and its derivatives, $V'(r) = dV/dr$, $V''(r)$, etc.

The most well known of these results is the Virial Theorem obtained for $q = 1$. However, the results obtained for $q = 0$ are very interesting and for some reason are not common knowledge. Applying $\int_0^{\infty} dr u'_{nl}(r)$ to both sides of equation (1) one obtains:

$$-\frac{\hbar^2}{2m} (u'_{nl}(r)) \Big|_0^{\infty} + (W_l(r)u_{nl}^2(r)) \Big|_0^{\infty}$$

$$\int_0^{\infty} W_l' u_{nl}^2 dr - E_{nl} u_{nl}^2 \Big|_0^{\infty} = 0 \quad (3)$$

where the effective potential:

$$W_l(r) = \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) \quad (4)$$

Since u_{nl} represents a bound-state there is no contribution for $r = \infty$. One has to be careful about the contribution for $r = 0$.

For the potentials which satisfy $\lim_{r \rightarrow 0} r^2 V(r) = 0$ one has the general result $u_{nl} \sim r^{l+1}$ as $r \rightarrow 0$. This means that for all $l = 0, 1, 2, \dots$, the second and fourth terms of equation (3) give no contribution. The first term contributes only for $l = 0$ since $u_{nl}'(0) = R_{nl}(0)$. For S-wave states one has:

$$R_{n0}^2(0) = \frac{2m}{\hbar^2} \langle V'(r) \rangle_{n0} > 0 \quad (5)$$

This is a very interesting result which we use below. Historically, no one knows who derived it first but it is safe to attribute it to Fermi. For $l \neq 0$ [4], the first term vanishes giving:

$$\langle W_l' \rangle_{nl} = 0$$

or

$$\langle V' \rangle_{nl} = \frac{\hbar^2 l(l+1)}{2m} \langle 1/r^3 \rangle_{nl} \quad (6)$$

In the first form it states average of the effective force in $l \neq 0$ states is zero. In the second form it connects $\langle V' \rangle$ with $\langle 1/r^3 \rangle$ for a large class of functions $V(r)$. For power law potentials it gives simple relations. For example, it checks for the Coulomb case.

Two useful results applied to quarkonium phenomenology which emerged for S-waves states, for potentials with definite curvature were [4]:

$$|R_{n+1,0}(0)| - |R_{n0}(0)| \underset{<}{\geq} 0 \quad V''(r) \underset{<}{\geq} 0 \quad \forall r,$$

and

$$\frac{\partial}{\partial m} (1/m(R_{n0}^2)) \underset{<}{\geq} 0 \quad V''(r) \underset{<}{\geq} 0 \quad \forall r. \quad (8)$$

These results for the lowest value $n = 1$ were proved [2,3] rigorously starting from the radial equation. The validity of eqs. (7) and (8) for arbitrary but large n , using the WKB approximation was proved [5] for a large class of potentials with finite $V(0)$, $V'(r) > 0$ for all r and which have definite curvature i.e. same sign for $V''(r)$ for all r .

Note that for a linear potential $V(r) \sim r$ ($V''(r) = 0$ for all r) results in eqs. (7) and (8) for all n follow immediately from equation (5)! Furthermore, exactly solvable potentials $-1/r$ ($V''(r) < 0$ for all r) and r^2 ($V''(r) > 0$ for all r) satisfy eqs. (7) and (8).

Thus the conjecture is that equations (7) and (8) are valid for all n . The challenge is to give a rigorous proof.

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