Hypervirial Theorem for Singular Potentials

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Using well-known methods we generalize (hyper)virial theorems to the case of a singular potential. We discuss themost general second order differential equation, which involves all physically interesting cases, such as Schrödinger and Klein-Gordon equations with singular potentials. Some physical consequences are also discussed.

Key words: Virial theorem, Schrodinger equation, Klein-Gordon equation, singular potential, bound states.

I. Introduction

Virial theorem has a wide application in the classical as well as in the quantum mechanics. This theorem connects average values of kinetic and potential energies for the systems confined in limited areas. Moreover it allows making definite conclusions about some interesting problems without solving equations of motion.

There are many generalizations of virial theorem, especially in relativistic quantum mechanics, for investigating bound states [1].

Recently much attention was devoted to singular potentials, namely, to potentials, behaving like $r^2V(r) \rightarrow -V_0$, $(V_0 > 0)$ at $r \rightarrow 0$ in the Schrödinger equation, and as $rV = -V_0$ for $r \rightarrow 0$ in the Klein-Gordon and Dirac equations.

So behaved potentials appear in large classes of physical problems. Particularly, in Calogero model [2], Coulomb or Hulthen potential in Klein-Gordon and Dirac equations [3], Black Hole theory [4] and etc. Virial like theorems can make things clear while studying such problems.

Therefore, it is natural attempts to generalize virial theorem to the case of such (singular) potentials too.

The most general methods for obtaining various virial like theorems were developed in [5] by C. Quigg for regular potentials in the Schrodinger equation. The general character of these methods allows us to carry over singular potentials as well. It appears that formally the theorem almost keeps the form familiar for regular potentials with obvious differences. But the main difference is additional solutions, whose existence is a specific property of singular potentials and is related to the necessity of self-adjoint extension (SAE).

This article is organized as follows:

First of all we remember the needed methods for deriving virial like theorems and apply them to general second order differential equation.

Consequences for regular potentials are reviewed and then the singular potentials are considered. It is shown, that there arise additional terms in the usual virial like theorems, which depend on the additional solution in the case of a singular potential. Some consequences of the new form of virial theorems are also considered.

After that the corresponding corrections to the Feynman-Hellmann theorem are discussed.

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II. Derivation of Hypervirial (generalized virial) Theorems

Let us consider the second order differential equation of the most general form (exclusion of the first derivative terms is always possible by using a suitable transformation [6])

$$u''(r) + L(r)u(r) = 0, \qquad (2.1)$$

where L(r) is an arbitrary function of r. Central potential in three-dimensions will be important for us in what follow. Exactly to equation (2.1) reduces the radial Schrodinger equation with $0 < r < \infty$. Even the one-dimensional case may be investigated on the same foot, as well, where $-\infty < x < \infty$. In the following some of physical requirements will be used to restrict this function, L(r).

Now we proceed to the methods of C.Quigg [5]. Let us multiply (2.1) by fu' and integrate in the interval $(0,\infty)$. (here f(r) is an arbitrary three-time differentiable function, which will be specified below). We derive

$$-\int_{0}^{\infty} fu'u''dr = \int_{0}^{\infty} fLuu'dr$$
(2.2)

Let us mention that using the following relations $u'u'' = \frac{1}{2}(u')^2$ and $uu' = \frac{1}{2}(u^2)'$, one can perform partial integration in (2.2).

$$-f[u']^{2}\Big|_{0}^{\infty} + \int_{0}^{\infty} f'[u']^{2} dr = fLu^{2}\Big|_{0}^{\infty} - \int_{0}^{\infty} f'Lu^{2} dr - \int_{0}^{\infty} fL'u^{2} dr$$
(2.3)

For bound states $u, u' \rightarrow 0$ at large distances and therefore one neglects contributions from the upper boundary in (2.3), if f and L are restricted as follows

$$\lim_{r \to \infty} fu'^2 \to 0; \qquad \lim_{r \to \infty} fLu^2 \to 0$$
(2.4)

(For scattering problems u, u' are not decreasing functions and the conditions (2.4) may not be satisfied, except the special choice of f).

Therefore there remain expressions in (2.3) only at lower boundary

$$fu'^{2}\Big|_{0} + \int_{0}^{\infty} f'u'^{2} dr = -fLu^{2}\Big|_{0} - \langle fL \rangle - \langle fL' \rangle, \qquad (2.5)$$

where < > denotes averaging by means of u function. For example,

$$\left\langle f\mathcal{L}\right\rangle = \int_{0}^{\infty} f\mathcal{L}u^{2}dr \tag{2.6}$$

Perform partial integration in the second term of RHS of eq. (2.5), using evident relation (uu')' = u'u' + uu''. It follows

$$I = \int_{0}^{\infty} f' u'^{2} dr = f' u u' \bigg|_{0}^{\infty} - \int_{0}^{\infty} f' u u'' dr - \int_{0}^{\infty} f'' u u' dr$$
(2.7)

For bound states the first term on RHS at the upper limit may be neglected, if

$$\lim_{r \to \infty} f' u u' \to 0 \tag{2.8}$$

Now let us integrate the last term on RHS of (2.7)

$$I_{1} = \int_{0}^{\infty} f'' u u' dr = \frac{1}{2} \int_{0}^{\infty} f'' (u^{2})' dr = \frac{1}{2} f'' u^{2} \Big|_{0}^{\infty} - \frac{1}{2} < f''' >$$
(2.9)

For bound states f must be restricted as follows

$$\lim_{n \to \infty} f'' u^2 \to 0 \tag{2.10}$$

Therefore, we have (taking into account the equation of motion (2.1))

$$I = -f' u u' \Big|_{0} + \langle f' L \rangle + \frac{1}{2} f'' u^{2} \Big|_{0} + \frac{1}{2} \langle f''' \rangle$$
(2.11)

Finally, from (2.5) and (2.11) we derive the following hypervirial theorem for bound states:

$$fu'^{2} - f'uu' + \frac{1}{2}f''u^{2} - fuu'' \bigg\}_{r=0} = -2 < f'L > - < fL' > -\frac{1}{2} < f''' >$$
(2.12)

For scattering states (2.4), (2.8) and (2.10) restrictions are not satisfied and instead of (2.12) we have

$$-\left\{fu'^{2} - f'uu' + \frac{1}{2}f''u^{2} - fuu''\right\}_{r=\infty} + \left\{fu'^{2} - f'uu' + \frac{1}{2}f''u^{2} - fuu''\right\}_{r=0} =$$

$$= -2 < f'L > - < fL' > -\frac{1}{2} < f''' >$$
(2.13)

After substitution here u function at infinity corresponding hypervirial theorem can be derived for scattering problems as well.

Now let us make some comments in connection which (2.12) about restrictions on f:

(a) Because < > means averaging by *u*-functions, *f* must be such, that corresponding integrals do exist.

(b) When $f = r^q (q \ge -2l)$, then (2.12) coincides with (2.27) of the paper [7], where only the Schrödinger equation is considered, i.e.

$$L = 2m \left[E - V - \frac{l(l+1)}{2mr^2} \right]$$
(2.14)

with regular V.

Let us note that the choice $f = r^q$ satisfies (2.4), (2.8) and (2.10) restrictions.

(c) The expression (2.12) for arbitrary f is derived in [8], but in that paper, as well as in [7], only the Schrodinger equation was considered.

III. Some Applications of Hypervirial Theorem

Choosing f, one can obtain several interesting expressions from (2.12). Let us consider some of them.

Consider a particular case for L(r) in (2.1)

$$L = A(r) - \frac{s(s+1)}{r^2}, \quad s \ge 0$$
(3.1)

i.e. we separate a centrifugal term.

We use here a general notation A(r) instead of (2.14) because a lot of physical equations reduce to the form, like (3.1), where potential participates in different manners.

It is necessary to make distinction between two cases: $\lim_{r \to 0} r^2 A(r) = 0$ (regular) and $\lim_{r \to 0} r^2 A(r) \neq 0$ (singular).

Consider each of them in detail:

(i) regular case, when

$$\lim_{r \to 0} r^2 A(r) = 0$$
 (3.2)

It is easy to guess, that only regular potentials

$$\lim_{r \to 0} r^2 V(r) = 0$$
 (3.3)

obey (3.2) in the case of the Schrödinger equation (if we take s = l; l = 0,1,2).

While, for example, for one- and two-particle Klein-Gordon equations (3.2) is satisfied if

$$\lim_{r \to 0} rV(r) = 0 \tag{3.4}$$

When (3.2) is satisfied it follows the following behavior of wave function at the origin

$$\underset{\to 0}{u} \approx a_s r^{s+1} + b_s r^{-s} \tag{3.5}$$

The second term in (3.5) does not obey the condition of hermitianity for Hamiltonian [9,10] and radial momentum operator $p_r = -i(\frac{\partial}{\partial r} + \frac{1}{r})[11]$, which is imposed on the wave function at the origin $\lim_{r \to \infty} r P_r(r) = \lim_{r \to \infty} w(r) = 0$.

$$\lim_{r \to 0} rR(r) = \lim_{r \to 0} u(r) = u(0) = 0$$
(3.6)

Therefore it is forbidden as a rule (see, any textbook in quantum mechanics). Then at small distances only the first term remains

$$u_s \approx a_s r^{s+1} \tag{3.7}$$

Substituting this into (2.12) one obtains

$$a_{s}^{2}\left\{r^{2s}\left[(s+1)f - (s+1)f'r + \frac{r^{2}}{2}f''\right]\right\}_{r=0} = -2 < f'A > - < fA' > +$$
(3.8)

 $+ 2s(s+1) < \frac{J}{r^2} - \frac{J}{r^3} > -\frac{1}{2} < f''' >$ necial form for f [5]

Now consider special form for f [5]

$$f = r^q \tag{3.9}$$

We have

$$\left\{ (s+1)(1-q) + \frac{1}{2}q(q-1) \right\} a_s^2 r^{q+2s} \Big|_{r=0} = -\langle 2qr^{q-1}A + r^q A' \rangle - \left[2s(s+1)(1-q) + \frac{1}{2}q(q-1)(q-2) \right] \langle r^{q-3} \rangle$$
(3.10)

In order the LHS of this expression not to be divergent at r = 0, we must require

$$q \ge -2s \tag{3.11}$$

Therefore, (3.10) becomes

$$(2s+1)^{2} a_{s}^{2} \delta_{q,-2s} = = -\langle 2qr^{q-1}A + r^{q}A' + \left[2s(s+1)(1-q) + \frac{1}{2}q(q-1)(q-2)\right]r^{q-3} \rangle$$
(3.12)

It must be noted that (3.12) is a generalization of the relation (2.30) from the paper [5] where only the Schrodinger equation was considered.

Let us now consider various interesting values of q in (3.12): a) q = 1

Then it follows from (3.12) that

$$\langle 2A + rA' \rangle = 0 \tag{3.13}$$

In case of Schrodinger equation, when

$$A = 2m(E - V) \tag{3.14}$$

we derive

$$E = \left\langle V + \frac{1}{2}rV' \right\rangle,\tag{3.15}$$

which is the usual virial theorem

$$\langle T \rangle = \frac{1}{2} \langle rV' \rangle$$
 (3.16)

b) q = -2l

Taking into account separability of the total wave function

$$\psi(r,\theta,\varphi) = R_{ne}(r)Y_{em}(\theta,\varphi) = \frac{u_{n,e}(r)}{r}Y_{em}(\theta,\varphi)$$
(3.17)

we derive

$$(2l+1)^2 \left| R_{n,e}^{(e)}(0) \right|^2 = (l!)^2 < 4l \frac{A}{r^{2l+1}} - \frac{A'}{r^{2l}} >_{n,e}$$
(3.18)

Here $R_{n,e}^{(e)}(0)$ is the lth order derivative of radial wave function at the origin. (3.18) generalizes eq. (1.4) of [7] for Schrodinger equation

$$(2l+1)^{2} \left| R_{n,e}^{(e)}(0) \right|^{2} = 2m(l!)^{2} \left[\left\langle \frac{1}{r^{l}} \frac{dV}{dr} \right\rangle_{l} + 4l \left\langle \frac{E-V}{r^{2l+1}} \right\rangle \right]$$
(3.19)

c) q=0, i.e. f = const

or

$$(l+1)a_l^2 r^{2l}\Big|_{r=0} = -\langle A'(r) \rangle - \left\langle \frac{2l(l+1)}{r^3} \right\rangle$$
(3.21)

If now we take l = 0, then

$$a_0^2 = (u_0)^{\prime 2}(0) = -\langle A'(r) \rangle$$
(3.22)

It generalizes eq. (39a) from [8] to the arbitrary A(r). When we take expression (3.14), then it follows from (3.22) the well-known relation

$$\left|\psi_{0}(0)\right|^{2} = \frac{m}{2\pi} \left\langle \frac{dV}{dr} \right\rangle$$
(3.23)

In the case of $l \neq 0$, the LHS of (3.21) is zero and therefore we obtain

$$2l(l+1)\left\langle\frac{1}{r^3}\right\rangle = -\left\langle A'\right\rangle \tag{3.24}$$

which generalizes the eq. (39b) from [8] derived for the particular case of A(r) given by the (3.14). The relations (3.22) and (3.24) are formulated in terms of A(r). Depending on equations of motion, the potential V(r) appears in various forms and one must take care, which restrictions arise on potential V(r).

d) $q \neq 0, 1, -2l$

In this case we have

$$<2qr^{q-1}A+r^{q}A'+\left[2l(l+1)(1-q)+\frac{1}{2}q(q-1)(q-2)\right]r^{q-3}>=0$$
 (3.25)

This expression allows us to connect average values of the various degrees of r. For example, in the Schrodinger equation case we have

$$2Eq\langle r^{q-1}\rangle - 2q\langle r^{q-1}V\rangle - \langle r^{q}V'\rangle + \frac{(q-1)}{m} \left[\frac{q}{4}(q-2) - l(l+1)\right]\langle r^{q-3}\rangle = 0$$
(3.26)

For the power-like potential, $V = V_0 r^n$ it follows from (3.26), that

$$2Eq\langle r^{q-1}\rangle - V_0(2q+n)\langle r^{q+n-1}\rangle + \frac{(q-1)}{m} \left[\frac{q}{4}(q-2) - l(l+1)\right]\langle r^{q-3}\rangle = 0$$
(3.27)

If n = -1, the well-known Kramer's formula [12] follows from (3.27) for the Coulomb potential

$$V = -\frac{\alpha}{r}, \quad (\text{i.e. } V_0 = -\alpha; \ q = s+1)$$
$$2E(s+1)\langle r^s \rangle + \alpha(2s+1)\langle r^{s-1} \rangle + \frac{s}{m} \left[\frac{s^2 - 1}{4} - l(l+1) \right] \langle r^{s-2} \rangle = 0 \tag{3.28}$$

For the particular case of n = 2, the relation for isotropic harmonic oscillator $V = \frac{1}{2}\omega^2 r^2$ is derived [13]

$$2E(s+1)\langle r^{s}\rangle - \omega^{2}(s+2)\langle r^{s+2}\rangle + \frac{s}{m}\left[\frac{s^{2}-1}{4} - l(l+1)\right]\langle r^{s-2}\rangle = 0$$
(3.29)

Also it is possible to derive recurrence like relations between different powers of r for various relativistic equations. Such relations have many applications in many physical problems [14].

ii) Singular case. Now

$$\lim_{r \to 0} r^2 A(r) = -V_0; (V_0 > 0)$$
(3.30)

Alt is shown in [15-16], for Schrodinger and two equal mass particles' Klein-Gordon equations, that besides the standard levels there exist additional levels as well, whose wave function behaves at small distances as

$$u_{st} \approx a_{st} r^{\frac{1}{2}+P}; \quad u_{add} \approx a_{add} r^{\frac{1}{2}-P}$$

$$(3.31)$$

where, for example, in the Schrodinger equation

$$P = \sqrt{(l+1/2)^2 - 2mV_0} > 0$$
 (3.32)

while in the Klein-Gordon equation for two equal mass particles

$$P = \sqrt{(l+1/2)^2 - V_0^2/4} > 0$$
 (3.33)

Likely it is possible to find P for given L for each relativistic equation. At the same time, as is indicated in [15-16], for the existence of additional levels following constraint must be satisfied $0 \le P \le 1/2$ (3.34)

which is expression of vanishing of the radial wave function
$$u(r)$$
 at the origin, $u(0) = 0$.
Now if we take the wave function at small distances as general form [15]

$$u = a_{st} r^{\frac{1}{2} + P} + a_{add} r^{\frac{1}{2} - P}$$
(3.35)

and use (3.9) for f, then (2.13) gives

$$(1-q)(1/2+P-q/2)a_{st}^{2}\delta_{q,1-2p} + (1-q)(1/2-P-q/2)a_{add}^{2}\delta_{q,1+2P} + [(q-1)^{2}-4P^{2}]a_{st}a_{add}\delta_{q,1} = -\left\langle 2qr^{q-1}A+r^{q}A' + \left[2l(l+1)(1-q)+\frac{q}{2}(q-1)(q-2)\right]\right\rangle \langle r^{q-3} \rangle$$

$$(3.36)$$

Here we must require that $q \ge 1 - 2P$. If $V_0 = 0$, i.e. if we return to the regular case (3.2), because the RHS of (3.36) remains unchanged, but the LHS transforms into the LHS of (3.12)

Let us consider various q-ss in (3.36) as above.

a) q = 1; $P \neq 0, 0 < P < 1/2$ Then from (3.36) it follows that

$$\left\langle 2A + rA' \right\rangle = 4P^2 a_{st} a_{add} \tag{3.37}$$

For the Schrodinger equation this means

$$E = \left\langle V + \frac{1}{2}rV' \right\rangle + \frac{P^2}{m}a_{st}a_{add}$$
(3.38)

Therefore, for singular potential the virial theorem differs from that of regular ones by the extra term

$$b = \frac{P^2}{m} a_{st} a_{add} \tag{3.39}$$

This term vanishes when we take only standard or only additional solutions.

Comment: A Separate consideration needs the case P = 0. As is indicated in [15], we have in this case

$$u_{\to 0} \approx a_{st} r^{\frac{1}{2}} + a_{add} r^{\frac{1}{2}} \ln r$$
 (3.40)

Clearly u(0) = 0.Now instead of (3.36) it follows

$$\left\langle 2qr^{q-1}A + r^{q}A' \right\rangle - \left[2l(l+1)(1-q) + \frac{1}{2}q(q-1)(q-2) \right] \left\langle r^{q-3} \right\rangle = 0$$
 (3.41)

And virial theorem for the Schrodinger theory takes the form

$$E = \left\langle V + \frac{1}{2}rV' \right\rangle \tag{3.42}$$

which is analogous to the regular potential case, but difference appears in averaging by the function (3.40).

For pure singular potential

$$V = -\frac{V_0}{r^2}; (V_0 > 0)$$
(3.43)

it follows from (3.37) that

$$E = \frac{P^2}{m} a_{st} a_{add} \tag{3.44}$$

This is a single level, which appears in quantum mechanical consideration, when we retain the additional solution as necessary ingredient for providing self-adjointness of Hamiltonian via self-adjoint extension (SAE) [15].

This level disappears immediately as we neglect pure standard or pure additional solutions. It is evident that the equality (3.37) is a rather general relation leading to many physical consequences. Consider, for example, Klein-Gordon equation for two particles with equal masses *m*:

$$u'' + \left[\frac{V^2}{4} - \frac{MV}{2} + \frac{M^2}{4} - m^2\right]u - \frac{l(l+1)}{r^2}u = 0;$$
(3.45)

M is the mass of the composite state. Comparison to (2.1) and (3.1) gives

$$A = \frac{V^2}{4} - \frac{MV}{2} + \frac{M^2}{4} - m^2$$

Using this in (3.36), we obtain

$$\left\langle \frac{V^2}{2} - MV + \frac{rV'}{2} (V - M) + \frac{M^2}{2} - 2m^2 \right\rangle = 4P^2 a_{st} a_{add}$$
 (3.46)

Let us now consider the following problem: Can two massive particles produce massless bound state in the case of the Coulomb potential (attraction or repulsion)? Existence of bound states for both cases is a consequence of the relativistic structure of Klein-Gordon equation, where for M = 0 there remains only V^2 in (3.45). This problem was considered in [17].

Taking M = 0 in (3.46), we derive

$$\left\langle \frac{V^2}{2} + \frac{rV'}{2}V - 2m^2 \right\rangle = 4P^2 a_{st} a_{add}$$
 (3.47)

For the Coulomb potential one has

$$-m^2 = 2P^2 a_{st} a_{add} \tag{3.48}$$

and we see that there is a positive answer to this problem only if $a_{st} \neq 0$ and $a_{add} \neq 0$ (if $a_{st}a_{add} < 0$). This result may be verified also by direct solution of the Klein-Gordon equation. Indeed, substituting M = 0 in (3.45), one finds

$$u'' + \left[\frac{V^2}{4} - m^2\right]u - \frac{l(l+1)}{r^2}u = 0;$$
(3.49)

If we take here $V = \mp \frac{\alpha}{r}$ this equation becomes

$$u'' + \left[-m^2 - \frac{P^2 - 1/4}{r^2} \right] u = 0$$
(3.50)

where P is given by (3.33). Note that this equation coincides to the Schrodinger equation with the accuracy of notations. Therefore we can use the results of our paper [15] and write down the general solution derived there

$$u(r) = \sqrt{mr} \{ AI_P(mr) + BI_{-P}(mr) \}$$
(3.51)

where I_{P} and I_{-P} are the modified Bessel functions. We have the following behaviour at infinity

$$u(r) \approx \frac{1}{\sqrt{2\pi}} \{A + B\} e^{mr}$$
(3.52)

Requiring that u(r) vanishes at infinity as it is the case for bound state solution we have to take

$$B = -A \tag{3.53}$$

Remembering the well-known relation

$$K_{P}(z) = \frac{\pi}{2\sin P\pi} \left[I_{-P}(z) - I_{P}(z) \right]$$
(3.54)

our wave function takes the form

$$u = -A\frac{2}{\pi}\sqrt{mr}\sin P\pi \cdot K_{P}(mr)$$
(3.55)

which is exponentially damping at infinity and in the interval $0 \le P < 1/2$ satisfies the fundamental requirement (3.6). It is evident, that our solution is derived by the requirements

$$A \neq 0; \quad B \neq 0 \tag{3.56}$$

which means, that M = 0 state can be derived only by SAE procedure. We see that explicit solution of Klein-Gordon equation confirms the conclusion, derived by Virial theorem.

One important remark is in order: W. Krolikowski [17] derived the same solution for l = 0 state only. It is true, because $K_p(z)$ is the only Bessel function, which behaves in a needed fashion at infinity (vanishes!). It appears that a massless bound state for Coulomb potential may be constructed from 2 massive particle in nonzero orbital momentum states as well, $l \neq 0$ [15].But SAE procedure is necessary.

Owing to the fact, that repulsive case also forms a massless bound state, we conclude, that the following <u>alternatives</u> take place:

Those values of SAE parameter $\tau = \frac{a_{add}}{a_{st}}$, for which this strange fact occurs, must be

deflected in order to suppress such unphysical results.

(i) We must recognize, that the SAE procedure produces an <u>effective attraction</u>, which may be seen from the equation (3.50), where the factor $(P^2 - 1/4)$ is negative in the area (3.34) and gives a quantum anticentrifugal potential, which is attractive [15].

(ii) It is not excepted that such unphysical fact is a pathology of the Klein-Gordon equation. For example if we reverse the problem and ask ourselves whether two massless particles can compose a massive bound state in Coulomb field, we can easily see that (3.46) gives a positive answer in the case of Coulomb repulsion, but not for attraction.

b) Cases $q = 1 \pm 2P$ and $q \neq 0, 1, -2l$ may be discussed in full analogy. One derives some recurrence like relations between average values of various powers of r.

IV. Conclusions

In this article we consider problems, related to the singular potentials in the light of hypervirial theorem. Main results can be summarized as follows:

1. We have derived a hypervirial theorem for the general second order differential equation.

2. For regular potentials we generalized known results concerning the Schrodinger equation

(virial theorem, wave function and its derivatives at origin, recurrence relations between average values of different powers of r)

3.We obtain virial theorem for singular potential, by means of which some physical results are derived (existence of one level for pure r^{-2} potential, possibility of having massless bound state for repulsive and attractive Coulomb potential in the two-body Klein – Gordon equation).

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