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RELATIVISTIC VIRIAL THEOREMS

Wolfgang LUCHA

Institut für Hochenergiephysik
Österreichische Akademie der Wissenschaften
A-1050 Wien, Austria

Franz F. SCHÖBERL

Institut für Theoretische Physik
Universität Wien
A-1090 Wien, Austria

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Abstract

Everything you always wanted to know about quantum-mechanical virial theorems but did not dare to ask.

1 Introduction

In quantum theory, the virial theorem provides an extremely useful tool for studying quantum-mechanical systems. In its nonrelativistic version, based on the Schrödinger equation, it relates the kinetic energy of a system to the expectation value of the directional derivative of the interaction potential entering in the Hamiltonian which describes the system. Here we intend to give an elementary account of virial theorems in quantum theory. With the above-mentioned exception of the Schrödinger equation, all of them are of relativistic nature. We leave, however, aside virial theorems in (quantum) field theories.

Historically, the original idea of the derivation of the quantum-mechanical virial theorem was by analogy to the proof of its classical counterpart: The expectation value of the scalar product $\vec{x}\vec{p}$ of the coordinates and momenta was required to be time-independent, i.e., its time derivative to vanish. Later on it was recognized that this scalar product is the generator of dilatations.

The outline of this Review is as follows: Section 2 introduces the concept of dilatations which provides the basis for the modern ways of deriving the quantum-mechanical virial theorems. In Section 3 some sort of "master virial theorem" is derived from a trivial feature of the commutator of two operators between (degenerate) eigenstates of one of them [1]. As is shown in Section 4, the same relation can also be deduced from a variational calculation [2], at the price, however, of postulating an additional requirement. Section 5 compares time-derivative and dilatation approach to the virial theorem. Section 6 illustrates the master virial theorem for the most common wave equations, viz., the Schrödinger equation, its relativistically improved version which is found by adopting the correct relation between energy and momentum, as well as the Dirac equation. Section 7 draws some conclusions regarding the energy eigenvalues of these equations. Section 8 demonstrates how to extend all the previously elaborated formalism to non-Hamiltonian theories like, e.g., systems described by the Klein-Gordon equation. Section 9 recalls the formulation in terms of explicit wave functions. Section 10 concludes with a brief summary. The units chosen are such that $\hbar = c = 1$.

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2 Dilatations

In our opinion, the simplest - and at the same time physically most transparent - derivation of the virial theorem [1] takes advantage of the behaviour of a theory under dilatations. From the fundamental commutation relations between the coordinates $\vec{x} \equiv \{x_i\}$ and their canonically conjugate momenta $\vec{p} \equiv \{p_i\}$,

$$[x_i, p_j] = i\delta_{ij} \quad , \quad (1)$$

one finds for arbitrary analytic functions $f(\vec{x})$ and $f(\vec{p})$

$$\begin{aligned} [\vec{p}, f(\vec{x})] &= -i \frac{\partial}{\partial \vec{x}} f(\vec{x}) \quad , \\ [\vec{x}, f(\vec{p})] &= i \frac{\partial}{\partial \vec{p}} f(\vec{p}) \quad . \end{aligned} \quad (2)$$

It is a simple task to verify (2) by applying (1) to the power-series expansions

$$\begin{aligned} f(\vec{x}) &= \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n f}{\partial \vec{x}^n}(0) \vec{x}^n \quad , \\ f(\vec{p}) &= \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\partial^n f}{\partial \vec{p}^n}(0) \vec{p}^n \end{aligned} \quad (3)$$

of the functions $f(\vec{x})$ and $f(\vec{p})$.

Dilatations are scalings of \vec{x} , accompanied by inverse scalings of \vec{p} . They are thus characterized by a scale parameter $\lambda = e^\tau$. The (symmetrized) generator of dilatations reads

$$G = \frac{1}{2}(\vec{x}\vec{p} + \vec{p}\vec{x}) \quad . \quad (4)$$

With the help of (2) it is then easy to see that the operator

$$D = e^{i\tau G} \quad , \quad (5)$$

when applied to the phase-space variables \vec{x} and \vec{p} , generates the transformations

$$\begin{aligned} D\vec{x}D^{-1} &= \lambda\vec{x} \quad , \\ D\vec{p}D^{-1} &= \frac{1}{\lambda}\vec{p} \quad , \end{aligned} \quad (6)$$

and thus acts on the functions $f(\vec{x})$ and $f(\vec{p})$ as

$$\begin{aligned} Df(\vec{x})D^{-1} &= \exp\left(\tau\vec{x}\frac{\partial}{\partial\vec{x}}\right) f(\vec{x}) = f(\lambda\vec{x}) \quad , \\ Df(\vec{p})D^{-1} &= \exp\left(-\tau\vec{p}\frac{\partial}{\partial\vec{p}}\right) f(\vec{p}) = f\left(\frac{1}{\lambda}\vec{p}\right) \quad . \end{aligned} \quad (7)$$

3 Derivation of the Master Virial Theorem

Let us start from a rather general form of the Hamiltonian $H = H(\vec{p}, \vec{x})$ governing the dynamics of the system under consideration:

$$H = T(\vec{p}) + V(\vec{x}) + K \quad , \quad (8)$$

where $T(\vec{p})$ represents the kinetic energy and $V(\vec{x})$ some potential, while K is a constant, i.e., neither \vec{x} - nor \vec{p} -dependent, term. Still more general forms of the Hamiltonian are somewhat cumbersome to treat and are of very restricted practical interest. Consider normalized eigenstates $|\psi\rangle$ of the Hamiltonian H , with energy eigenvalue E :

$$H|\psi\rangle = E|\psi\rangle \quad , \quad \langle\psi|\psi\rangle = 1 \quad . \quad (9)$$

The virial theorem is equivalent to the statement that the expectation values of the commutator between the dilatation generator G and the Hamiltonian H , taken with respect to the above energy eigenstates $|\psi\rangle$, vanish:

$$\langle\psi|[G, H]|\psi\rangle = 0 \quad . \quad (10)$$

This is a trivial observation following from the hermiticity of H , $H^\dagger = H$. The left-hand side of (10) is a difference of two identical terms, both of which are equal to $E\langle\psi|G|\psi\rangle$. With the help of (2) the above commutator is easily evaluated:

$$[G, T(\vec{p})] = i\vec{p}\frac{\partial}{\partial\vec{p}}T(\vec{p}) \quad , \quad (11)$$

$$[G, V(\vec{x})] = -i\vec{x}\frac{\partial}{\partial\vec{x}}V(\vec{x}) \quad .$$

Inserting this into (10) one obtains the general virial theorem

$$\left\langle\psi\left|\vec{p}\frac{\partial}{\partial\vec{p}}T(\vec{p})\right|\psi\right\rangle = \left\langle\psi\left|\vec{x}\frac{\partial}{\partial\vec{x}}V(\vec{x})\right|\psi\right\rangle \quad . \quad (12)$$

The directional derivative in momentum space of the \vec{p} -dependent term $T(\vec{p})$ in the Hamiltonian is equal to the directional derivative in coordinate space of the \vec{x} -dependent term $V(\vec{x})$ in the Hamiltonian.

According to the fundamental commutator (1) the symmetric form (4) of the dilatation generator G and its frequently used asymmetric form $G = \vec{x}\vec{p}$ differ only by a constant: $\vec{x}\vec{p} + \vec{p}\vec{x} = 2\vec{x}\vec{p} - id$, where d is the dimension of configuration space. It therefore does not matter which one of them is employed in the commutators (10) and (11).

The relation (12) is, of course, nothing else but the representation of the dilatation generator $G \sim \vec{x}\vec{p}$ in the vector space of functions on the phase space (\vec{x}, \vec{p}) , in particular for the special linear combination $T(\vec{p}) + V(\vec{x})$. For homogeneous functions, of degree n ,

$$f(\vec{\xi}) \propto \xi^n \quad , \quad (13)$$

the directional derivative measures their degree of homogeneity, n ,

$$\vec{\xi} \frac{\partial}{\partial \vec{\xi}} f(\vec{\xi}) = n f(\vec{\xi}) \quad . \quad (14)$$

In this sense, the virial theorem (12) compares the degrees of homogeneity of the kinetic term $T(\vec{p})$ and the potential $V(\vec{x})$ in the Hamiltonian (8).

Eq. (10) may, of course, also be approached from the dilatation operator D [1]. For the same reasons as above

$$\langle \psi | [D, H] | \psi \rangle = 0 \quad . \quad (15)$$

If (15), then also

$$\langle \psi | (DHD^{-1})D - HD | \psi \rangle = 0 \quad (16)$$

and

$$\lim_{\tau \rightarrow 0} \frac{1}{\tau} \langle \psi | (DHD^{-1} - H)D | \psi \rangle = 0 \quad . \quad (17)$$

The expansion of the dilated Hamiltonian DHD^{-1} in powers of τ reads

$$DHD^{-1} = H + i\tau[G, H] + O(\tau^2) \quad . \quad (18)$$

Inserting this into (17) and performing the limit $\tau \rightarrow 0$, as indicated, yields again (10).

Explicitly, according to (7), one finds for dilated kinetic term and potential

$$\begin{aligned} DT(\vec{p})D^{-1} &= T\left(\frac{1}{\lambda}\vec{p}\right) = T(\vec{p}) - \tau\vec{p}\frac{\partial}{\partial\vec{p}}T(\vec{p}) + O(\tau^2) \quad , \\ DV(\vec{x})D^{-1} &= V(\lambda\vec{x}) = V(\vec{x}) + \tau\vec{x}\frac{\partial}{\partial\vec{x}}V(\vec{x}) + O(\tau^2) \quad , \end{aligned} \quad (19)$$

and thus for the dilated Hamiltonian

$$\begin{aligned} DHD^{-1} &= T\left(\frac{1}{\lambda}\vec{p}\right) + V(\lambda\vec{x}) + K \\ &= H + \tau \left[-\vec{p}\frac{\partial}{\partial\vec{p}}T(\vec{p}) + \vec{x}\frac{\partial}{\partial\vec{x}}V(\vec{x}) \right] + O(\tau^2) \quad . \quad (20) \end{aligned}$$

4 An Alternative Derivation

An alternative derivation of the virial theorem is established by considering the expectation value of the dilated Hamiltonian DHD^{-1} with respect to the energy eigenstates $|\psi\rangle$ as a function $E(\tau)$ of the scale parameter $\tau \equiv \ln \lambda$,

$$E(\tau) = \langle \psi | DHD^{-1} | \psi \rangle \quad , \quad (21)$$

and by requiring, for *all* eigenstates $|\psi\rangle$, the proper energy eigenvalue E corresponding to $|\psi\rangle$ to be a minimum of $E(\tau)$ at $\tau = 0$ [3,4], i.e.,

$$E(0) = E \quad . \quad (22)$$

Stationarity of $E(0)$ means that

$$\frac{\partial E}{\partial \tau}(0) \equiv \left\langle \psi \left| \frac{\partial(DHD^{-1})}{\partial \tau}(0) \right| \psi \right\rangle = 0 \quad , \quad (23)$$

while $E(0)$ to be a minimum is guaranteed if the concavity condition

$$\frac{\partial^2 E}{\partial \tau^2}(0) \equiv \left\langle \psi \left| \frac{\partial^2(DHD^{-1})}{\partial \tau^2}(0) \right| \psi \right\rangle > 0 \quad (24)$$

is satisfied. From

$$DHD^{-1} = T(e^{-\tau} \vec{p}) + V(e^{\tau} \vec{x}) + K \quad (25)$$

one finds

$$\frac{\partial(DHD^{-1})}{\partial \tau}(0) = -\vec{p} \frac{\partial}{\partial \vec{p}} T(\vec{p}) + \vec{x} \frac{\partial}{\partial \vec{x}} V(\vec{x}) \quad (26)$$

and

$$\frac{\partial^2(DHD^{-1})}{\partial \tau^2}(0) = \left(\vec{p} \frac{\partial}{\partial \vec{p}} \right)^2 T(\vec{p}) + \left(\vec{x} \frac{\partial}{\partial \vec{x}} \right)^2 V(\vec{x}) \quad . \quad (27)$$

Eq. (26), when inserted into (23), gives again the general virial theorem (12),

$$\left\langle \psi \left| \vec{p} \frac{\partial}{\partial \vec{p}} T(\vec{p}) \right| \psi \right\rangle = \left\langle \psi \left| \vec{x} \frac{\partial}{\partial \vec{x}} V(\vec{x}) \right| \psi \right\rangle \quad , \quad (28)$$

whereas Eq. (27), inserted into (24), yields the concavity condition

$$\left\langle \psi \left| \left(\vec{p} \frac{\partial}{\partial \vec{p}} \right)^2 T(\vec{p}) + \left(\vec{x} \frac{\partial}{\partial \vec{x}} \right)^2 V(\vec{x}) \right| \psi \right\rangle > 0 \quad . \quad (29)$$

In three spatial dimensions, for kinetic terms $T(p)$ depending only on $p \equiv |\vec{p}|$ or potentials $V(x)$ depending only on $x \equiv |\vec{x}|$, respectively, the above concavity condition may be recast into either of the two following, asymmetric forms by substituting the virial theorem (28) into (29):

$$\left\langle \psi \left| \vec{p}^2 \Delta_p T(p) + x_i x_j \frac{\partial^2}{\partial x_i \partial x_j} V(\vec{x}) \right| \psi \right\rangle > 0 \quad , \quad (30)$$

since

$$\Delta_p T(\vec{p}) = \left(\frac{d^2}{dp^2} + \frac{2}{p} \frac{d}{dp} \right) T(p) \quad \text{for} \quad T(\vec{p}) = T(p) \quad , \quad (31)$$

or

$$\left\langle \psi \left| p_i p_j \frac{\partial^2}{\partial p_i \partial p_j} T(\vec{p}) + \vec{x}^2 \Delta_x V(x) \right| \psi \right\rangle > 0 \quad , \quad (32)$$

since

$$\Delta_x V(\vec{x}) = \left(\frac{d^2}{dx^2} + \frac{2}{x} \frac{d}{dx} \right) V(x) \quad \text{for} \quad V(\vec{x}) = V(x) \quad . \quad (33)$$

However, in contrast to the derivation of the virial theorem presented in Sec. 3, which does not need any specific requirement, the derivation given here is based on the assumption of the so-called minimum-energy principle, as discussed above, and thus not as general as the other one.

5 Analogy to Classical Mechanics

In classical mechanics, the virial theorem is obtained from considering the classical counterpart $\vec{x}\vec{p}$ of the dilatation generator G and requiring the time average of

$$\frac{d}{dt}(\vec{x}\vec{p})$$

to vanish, as is the case for systems with bounded coordinates and momenta. It should be no great surprise that there is a close relationship between this assumption and the previous quantum-mechanical derivations.

In quantum theory, for an operator O without explicit time dependence, the time derivative of an arbitrary expectation value $\langle \psi | O | \psi \rangle$ is given by

$$i \frac{d}{dt} \langle \psi | O | \psi \rangle = \langle \psi | [O, H] | \psi \rangle \quad . \quad (34)$$

Accordingly, specifying to the energy eigenstates $|\psi\rangle$ from (9), the commutator formulation (10) of the virial theorem implies that the time derivative of the expectation value of the dilatation generator G , $\langle\psi|G|\psi\rangle$, vanishes:

$$\frac{d}{dt}\langle\psi|G|\psi\rangle = 0 \quad . \quad (35)$$

Likewise, the derivative of the dilated Hamiltonian DHD^{-1} with respect to $\tau \equiv \ln \lambda$, evaluated at $\tau = 0$, may also be written as

$$\frac{\partial(DHD^{-1})}{\partial\tau}(0) = i[G, H] \quad . \quad (36)$$

Thus the stationarity condition (23) is also equivalent to the vanishing of the time derivative of $\langle\psi|G|\psi\rangle$, Eq. (35).

6 Application of the General Virial Theorem to Specific Wave Equations

With the general virial theorem (12) at our disposal, we are able to give the specific virial theorem for any particular Hamiltonian.

The Hamiltonian for the nonrelativistic Schrödinger equation is given by

$$H = m + \frac{\vec{p}^2}{2m} + V(\vec{x}) \quad , \quad (37)$$

i.e., $T(\vec{p}) = \vec{p}^2/(2m)$, $K = m$ in the notation of Eq. (8). It entails via (12) the well-known relation

$$\left\langle\psi\left|\frac{\vec{p}^2}{2m}\right|\psi\right\rangle = \langle\psi|T(\vec{p})|\psi\rangle = \frac{1}{2}\left\langle\psi\left|\vec{x}\frac{\partial}{\partial\vec{x}}V(\vec{x})\right|\psi\right\rangle \quad , \quad (38)$$

which is of close formal resemblance to its classical analog.

The shortcomings of the Schrödinger equation due to its inherent nonrelativistic nature may be (partly) circumvented by taking into account correct relativistic kinematics. The result of this improvement is sometimes called "spinless Salpeter equation", its Hamiltonian is given by

$$H = \sqrt{\vec{p}^2 + m^2} + V(\vec{x}) \quad , \quad (39)$$

i.e., $T(\vec{p}) = \sqrt{\vec{p}^2 + m^2}$, $K = 0$. We then find from (12) the relativistic virial theorem [1]

$$\left\langle\psi\left|\frac{\vec{p}^2}{\sqrt{\vec{p}^2 + m^2}}\right|\psi\right\rangle = \left\langle\psi\left|\vec{x}\frac{\partial}{\partial\vec{x}}V(\vec{x})\right|\psi\right\rangle \quad . \quad (40)$$

In the nonrelativistic limit $\vec{p}^2 \ll m^2$ it reduces, of course, to (38).

The Hamiltonian for the Dirac equation is given by

$$H = \vec{\alpha} \cdot \vec{p} + \beta m + V(\vec{x}) \quad , \quad (41)$$

i.e., $T(\vec{p}) = \vec{\alpha} \cdot \vec{p}$, $K = \beta m$, where $\vec{\alpha}$ and β satisfy the relations

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij} \quad , \quad \{\alpha_i, \beta\} = 0 \quad , \quad \beta^2 = 1 \quad (42)$$

and may be represented by (4×4) matrices. Here the potential V may receive contributions from a vector potential (Φ, \vec{A}) as well as from a scalar potential U :

$$V(\vec{x}) = \Phi(\vec{x}) + \vec{\alpha} \cdot \vec{A}(\vec{x}) + \beta U(\vec{x}) \quad . \quad (43)$$

The corresponding virial theorem reads [2,3]

$$\langle \psi | \vec{\alpha} \cdot \vec{p} | \psi \rangle = \left\langle \psi \left| \vec{x} \frac{\partial}{\partial \vec{x}} V(\vec{x}) \right| \psi \right\rangle \quad . \quad (44)$$

7 Implications of the Virial Theorems for the Energy

The main field of application of the virial theorems listed in the preceding section are the corresponding energy eigenvalues $E \equiv \langle \psi | H | \psi \rangle$. In particular, if the kinetic term $T(\vec{p})$ is a homogeneous function of \vec{p} , as is the case for Schrödinger and Dirac equation, the virial theorem can be used to replace the expectation value of $T(\vec{p})$ by the expectation value of the directional derivative of the potential $V(\vec{x})$ entering in the Hamiltonian (8). E is then completely expressed in terms of $V(\vec{x})$. For the spinless Salpeter equation, with the help of the decomposition

$$\sqrt{\vec{p}^2 + m^2} = \frac{\vec{p}^2}{\sqrt{\vec{p}^2 + m^2}} + \frac{m^2}{\sqrt{\vec{p}^2 + m^2}} \quad , \quad (45)$$

one finds in this way

$$\begin{aligned} E &= \langle \psi | \sqrt{\vec{p}^2 + m^2} | \psi \rangle + \langle \psi | V(\vec{x}) | \psi \rangle \\ &= \left\langle \psi \left| \vec{x} \frac{\partial}{\partial \vec{x}} V(\vec{x}) \right| \psi \right\rangle + \langle \psi | V(\vec{x}) | \psi \rangle + \left\langle \psi \left| \frac{m^2}{\sqrt{\vec{p}^2 + m^2}} \right| \psi \right\rangle \quad . \quad (46) \end{aligned}$$

Similarly, for the Dirac equation one obtains

$$\begin{aligned} E &= \langle \psi | \vec{\alpha} \cdot \vec{p} | \psi \rangle + \langle \psi | \beta m | \psi \rangle + \langle \psi | V(\vec{x}) | \psi \rangle \\ &= \left\langle \psi \left| \vec{x} \frac{\partial}{\partial \vec{x}} V(\vec{x}) \right| \psi \right\rangle + \langle \psi | \beta m | \psi \rangle + \langle \psi | V(\vec{x}) | \psi \rangle \quad (47) \end{aligned}$$

For a spherically symmetric potential $V(\vec{x}) = V(r)$, i.e., a potential which depends only on the radial coordinate $r = |\vec{x}|$, the directional derivative reduces to

$$\vec{x} \frac{\partial}{\partial \vec{x}} V(\vec{x}) = r \frac{d}{dr} V(r) \quad (48)$$

For a Coulomb potential

$$V_C(r) = \frac{\kappa}{r} \quad (49)$$

this directional derivative reproduces, apart from a sign, the potential,

$$r \frac{d}{dr} V_C(r) = -V_C(r) \quad (50)$$

In this case the potential and its directional derivative add up to zero,

$$\vec{x} \frac{\partial}{\partial \vec{x}} V_C(\vec{x}) + V_C(\vec{x}) = 0 \quad (51)$$

In contrast to that, due to the factor $\frac{1}{2}$ on the right-hand side of Eq. (38), this cancellation is incomplete in the nonrelativistic version. For the relativistic expressions for the energy E of systems with pure Coulomb interaction one obtains in the case of the spinless Salpeter equation [1,5]

$$E = \left\langle \psi \left| \frac{m^2}{\sqrt{\vec{p}^2 + m^2}} \right| \psi \right\rangle \quad (52)$$

and in the case of the Dirac equation [2,3,6]

$$E = m \langle \psi | \beta | \psi \rangle \quad (53)$$

For a potential which vanishes at infinity, $V(\vec{x}) \rightarrow 0$ for $|\vec{x}| \rightarrow \infty$, in order to be regarded as a bound state, the binding energy of the quantum-mechanical system has to be negative. Consequently, from Eqs. (52) and (53), respectively, one concludes that a massless particle described by the spinless Salpeter equation as well as a massless Dirac particle cannot be bound by a pure Coulomb potential [3].

8 Generalization to Wave Equations Without Corresponding Hamiltonian

There are quantum mechanical systems for which the assumption on the existence of a Hamiltonian of the form (8) is too restrictive. First, it might happen that the Hamiltonian H cannot be decomposed into a purely \vec{p} -dependent part $T(\vec{p})$ and a purely \vec{x} -dependent part $V(\vec{x})$,

$$H \neq T(\vec{p}) + V(\vec{x}) + K \quad . \quad (54)$$

This is already the case if, for instance, the orbital angular momentum $\vec{L} = \vec{x} \times \vec{p}$ enters. Secondly, there are even wave equations for which the corresponding Hamiltonian cannot be given at all. Nevertheless the states describing the system (are supposed to) satisfy an eigenvalue equation of the form

$$O|\psi\rangle = 0 \quad , \quad (55)$$

where the (hermitean) operator O may depend in an arbitrary way on \vec{x} and \vec{p} as well as on the energy eigenvalue E ,

$$O = O(\vec{p}, \vec{x}, E) \quad . \quad (56)$$

There is a straightforward generalization of the procedure proposed in Sec. 3. One has to take advantage of the fact that, very similarly as before, the expectation values of the commutator between the dilatation generator G and the operator O , taken with respect to the eigenstates $|\psi\rangle$ defined in (55), vanish:

$$\langle\psi|[G, O]|\psi\rangle = 0 \quad . \quad (57)$$

The virial theorem entailed by (55) then has to be found by explicit application of (2) to the above relation.

An example for the latter of the two above-mentioned possibilities is the Klein-Gordon equation with potential $V(\vec{x})$,

$$(\vec{p}^2 + m^2)|\psi\rangle = [E - V(\vec{x})]^2|\psi\rangle \quad , \quad (58)$$

i.e., $O = \vec{p}^2 + m^2 - [E - V(\vec{x})]^2$. Evaluation of the commutator in (57) with the help of (2) yields the virial theorem [7]

$$\langle\psi|\vec{p}^2|\psi\rangle = \left\langle\psi\left|[E - V(\vec{x})]\vec{x}\frac{\partial}{\partial\vec{x}}V(\vec{x})\right|\psi\right\rangle \quad . \quad (59)$$

9 Wave-Function Approach to the Virial Theorem

Very often, the discussion of the quantum mechanical virial theorem proceeds in terms of wave functions rather than in terms of state vectors in an abstract Hilbert space. The connection between the former formulation and the latter one - advocated for in this review - can be established immediately.

Denoting by d the dimension of configuration space, the coordinate eigenstates $|\vec{x}\rangle$, defined by $\vec{x}|\vec{x}\rangle = \vec{x}|\vec{x}\rangle$, satisfy the normalization condition $\langle\vec{x}|\vec{y}\rangle = \delta^{(d)}(\vec{x} - \vec{y})$ and completeness relation $\int d^d x |\vec{x}\rangle\langle\vec{x}| = 1$. The dilatation (6), $D\vec{x}D^{-1} = \lambda\vec{x}$, generates the dilated coordinate eigenstates

$$|\lambda\vec{x}\rangle = \frac{1}{\lambda^{d/2}} D^{-1} |\vec{x}\rangle, \quad (60)$$

with normalization

$$\langle\lambda\vec{x}|\lambda\vec{y}\rangle = \frac{1}{\lambda^d} \delta^{(d)}(\vec{x} - \vec{y}) \quad (61)$$

and completeness relation $\lambda^d \int d^d x |\lambda\vec{x}\rangle\langle\lambda\vec{x}| = 1$.

For an arbitrary state $|\psi\rangle$, with normalization $\langle\psi|\psi\rangle = 1$, the corresponding wave function $\psi(\vec{x})$ is given by the projection of $|\psi\rangle$ onto $|\vec{x}\rangle$, $\psi(\vec{x}) \equiv \langle\vec{x}|\psi\rangle$, and is, as a consequence of the normalizations of $|\vec{x}\rangle$ and $|\psi\rangle$, automatically normalized to unity, $\int d^d x |\psi(\vec{x})|^2 = 1$. Accordingly, the dilated wave function $\psi(\vec{x}; \lambda)$ reads

$$\psi(\vec{x}; \lambda) \equiv \lambda^{d/2} \psi(\lambda\vec{x}) = \lambda^{d/2} \langle\lambda\vec{x}|\psi\rangle = \langle\vec{x}|D|\psi\rangle, \quad (62)$$

with normalization $\int d^d x |\psi(\vec{x}; \lambda)|^2 = 1$.

The virial theorem is then derived by sandwiching the coordinate-space representation

$$H\left(-i\frac{\partial}{\partial\vec{x}}, \vec{x}\right)$$

of the Hamiltonian $H(\vec{p}, \vec{x})$ (or of the more general wave-equation operator O) between the dilated eigenfunctions (62) and by rescaling the variables like

$$\vec{x} \rightarrow \frac{1}{\lambda} \vec{x} \quad (63)$$

in order to shift the dilatation to the Hamiltonian, which becomes

$$H\left(-i\lambda\frac{\partial}{\partial\vec{x}}, \frac{1}{\lambda}\vec{x}\right).$$

This expression may in turn be recognized as the coordinate-space representation of the (inverse) dilated Hamiltonian $D^{-1}HD$. After this step, the derivation proceeds along similar lines of arguments as before.

10 Summary

We have discussed quantum-mechanical virial theorems, with emphasis on their formulation in terms of state vectors in an abstract Hilbert space rather than in terms of explicit wave functions.

The resulting expressions for the energy eigenvalues of relativistic wave equations permit to draw some important conclusions for the description of hadrons as bound states of quarks by so-called potential models [8]. Any potential like this should show up two features: At short inter-quark distances it should be essentially Coulomb-like, as is implied by one-gluon exchange between the bound quarks. At large distances it should rise, not very different from linearly, to infinity in order to provide for confinement – the empirical fact that quarks do not appear as free particles but are always bound to hadrons. However, as has been observed in Section 7, the contribution of the Coulomb part in the potential drops out from the expression for the bound-state energy. Hence, apart from the difference in the respective eigenstates, the formal expression for the energy of a massless and thus necessarily relativistic particle in a Coulomb-plus-linear potential is identical to the one of a nonrelativistic particle in a purely linear potential [1,8].

For the sake of simplicity we have restricted our discussion to single-particle wave equations. The way of extension to systems with more than one particles is obvious [1]. The vectors \vec{x} and \vec{p} in (4) then have to be understood to summarize the coordinates and momenta of all the particles.

The previous treatment allows, of course, for generalizations in still more directions. For instance, it is clear from Eq. (10) that the states $\langle\psi|$ and $|\psi\rangle$ in the expectation values need not be identical; it is sufficient that they are degenerate in energy, i.e., belong to the same energy eigenvalue E .

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