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Simple Generalization of the Quantum Mechanical Virial Theorem for Nonrelativistic Systems with Rotational Symmetry

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Author's contribution

The sole author designed, analyzed, interpreted and prepared the manuscript.

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ABSTRACT

In this paper we show that the generalization of the virial theorem can be achieved for nonrelativistic quantum mechanical systems under the conditions of rotational symmetry and the constancy of the trace of moment of inertia tensor. Under these conditions the matrix elements of the commutator of the generator of dilations G and the Hamiltonian H are equal to zero on the subspace of the Hilbert space generated by the simultaneous eigenvectors of the particular maximal set of commuting self-adjoint operators which contains H, J^2, J_z, the trace of the moment of inertia tensor TrI and additional operators. The result obtained is relevant for an important class of N-particle nonrelativistic quantum mechanical systems.

Keywords: Quantum mechanics; virial theorem; rotational symmetry; moment of inertia tensor; dilations.

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1. INTRODUCTION

In general, virial theorem represents a very important information about the dynamical behaviour of many integrable and nonintegrable systems with useful applications. The literature on the quantum mechanical virial theorem for the nonrelativistic systems described by Schrödinger equation, and relativistic systems described by Klein–Gordon, Salpeter or Dirac equation, is large and extensive, an here we mention only a part [1-16]. Quantum mechanical virial theorem in general is a statement [3] that the expectation values of the commutator of the generator of dilations G and the Hamiltonian H are equal to zero,

$$\langle n|[G,H]|n\rangle = 0, \tag{1}$$

when taken with respect to the normalized eigenvectors of H,

$$H|n\rangle = E_n|n\rangle, \qquad \langle n|n\rangle = 1 \tag{2}$$

This argument is only formal since the generator of dilations G, given for *N*-particle system by

$$G = \frac{1}{2}\sum_{i=1}^{N}(\mathbf{r}_i\cdot\mathbf{p}_i + \mathbf{p}_i\cdot\mathbf{r}_i), \tag{3}$$

is an unbounded operator, and therefore, $|n\rangle$ need not be in a domain of operator G [6, Vol. 4, 231].

If the *N*-particle Hamiltonian has the form $H(\mathbf{r},\mathbf{p}) = T(\mathbf{p}) + V(\mathbf{r})$, then using (1), and the relations derived in reference [3], it follows that

$$\langle n|\sum_{i=1}^{N}\mathbf{p}_i\cdot\frac{\partial T(\mathbf{p})}{\partial \mathbf{p}_i}|n\rangle = \langle n|\sum_{i=1}^{N}\mathbf{r}_i\cdot\frac{\partial V(\mathbf{r})}{\partial \mathbf{r}_i}|n\rangle \tag{4}$$

Here, $T(\mathbf{p})$ and $V(\mathbf{r})$ are the kinetic and potential energy operators, respectively; $\mathbf{p}$ denotes the set of momentum operators $(\mathbf{p}_1,\ldots,\mathbf{p}_N)$ and $\mathbf{r}$ denotes the set of position operators $(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ of the *N*-particle system. Therefore, quantum mechanical virial theorem is a relation between the expectation values of the directional derivatives of the kinetic and potential energy operators taken with respect to the eigenvectors of H.

In the recent paper [15] we have shown that the generalization of the virial theorem (1) can be proved for translationally and rotationally invariant nonrelativistic and relativistic Hamiltonians, under certain strong additional conditions, on the subspace $D(H, J^2, J_z, \{\Omega^\alpha\})$ of the Hilbert space. $D(H, J^2, J_z, \{\Omega^\alpha\})$ is generated by the set of normalized simultaneous eigenvectors $\{|n\rangle\}$ of the maximal set of commuting self-adjoint operators which contains H, J^2, J_z and additional operators $\{\Omega^\alpha\}$.

Under the conditions required in [15], the matrix elements of the commutator $[G,H]$, taken between all $|n\rangle, |m\rangle \in \{|n\rangle\}$ are equal to zero

$$\langle m|[G,H]|n\rangle = 0, \qquad \forall |n\rangle, |m\rangle \in \{|n\rangle\} \tag{5}$$

Therefore, for an arbitrary state vector $|\psi\rangle = \sum_n c_n|n\rangle$ in the subspace $D(H, J^2, J_z, \{\Omega^\alpha\})$ generated by the basis $\{|n\rangle\}$, the relation

$$\langle\psi|[G,H]|\psi\rangle = 0, \qquad \forall\psi \in D(H, J^2, J_z, \{\Omega^\alpha\}), \tag{6}$$

is obtained. This is a generalization of the quantum mechanical virial theorem, on the subspace $D(H, J^2, J_z, \{\Omega^\alpha\})$ of the Hilbert space.

In this paper, we set out to prove that for rotationally symmetric nonrelativistic quantum mechanical systems, with the constant trace of the moment of inertia tensor, such a generalization is possible under much weaker conditions:

Theorem 1

Suppose that commutator of the *N*-particle nonrelativistic Hamiltonian $H = T(\mathbf{p}) + V(\mathbf{r})$ with the generator of rotations, operator of total angular momentum $\mathbf{J}$, is equal to zero. Let the commutator of the Hamiltonian H with the trace of the moment of inertia tensor $\mathrm{Tr}\mathbf{I}$ also be equal to zero. Additional self-adjoint operators that commute with H may also exist. The additional self-adjoint operators Ω^α which commute with H, J^2, J_z, $\mathrm{Tr}\mathbf{I}$ and also among themselves form the set $\{\Omega^{\alpha}\}$. Normalized simultaneous eigenvectors of the maximal set of commuting operators $\{H, J^2, J_z, \mathrm{Tr}\mathbf{I}, \{\Omega^{\alpha}\}\}$ which belong to the Hilbert space form an orthonormal basis in the subspace $D(H, J^2, J_z, \mathrm{Tr}\mathbf{I}, \{\Omega^{\alpha}\})$. Suppose that the generator of dilations G is defined on $D(H, J^2, J_z, \mathrm{Tr}\mathbf{I}, \{\Omega^{\alpha}\})$. Then the matrix elements of the commutator of the Hamiltonian H with the generator of dilations G are equal to zero on the subspace $D(H, J^2, J_z, \mathrm{Tr}\mathbf{I}, \{\Omega^{\alpha}\})$ of the Hilbert space.

2. THE PROOF OF THEOREM 1

Under Theorem 1, the condition of rotational symmetry is satisfied, since it is required that the following commutator is equal to zero

$$[H, \mathbf{J}] = 0, \tag{7}$$

Here, $\mathbf{J} = \sum_{i=1}^{N} \mathbf{J}_i$ is the operator of the total angular momentum for a system of *N* particles. As given by (3), the generator of dilations G is a scalar operator and therefore invariant to rotations. This means that G commutes with the generator of rotations, operator of the total angular momentum $\mathbf{J}$,

$$[G, \mathbf{J}] = 0. \tag{8}$$

In classical mechanics, the components of the moment of inertia tensor $\mathbf{I}$ are given by,

$$I_{\alpha\beta} = \sum_{i=1}^{N} m_i \left(r_i^2 \delta_{\alpha\beta} - r_{i\alpha} r_{i\beta}\right), \tag{9}$$

where m_i is the mass and $r_{i\alpha}$, $r_{i\beta}$, with $\alpha, \beta = 1,2,3$, are the Cartesian components of the position vector $\mathbf{r}_i$ of the i th particle. The trace of the moment of inertia tensor $\mathrm{Tr}\mathbf{I}$ is a scalar defined by

$$\mathrm{Tr}\mathbf{I} = \sum_{\alpha=1}^{3} I_{\alpha\alpha} = 2\sum_{i=1}^{N} m_i r_i^2. \tag{10}$$

Therefore, in quantum mechanics the trace of the moment of inertia tensor $\mathrm{Tr}\mathbf{I}$ is a scalar operator, invariant to rotations. In classical mechanics, $\mathrm{Tr}\mathbf{I}$ is equal to

$$\mathrm{Tr}\mathbf{I} = I_1 + I_2 + I_3, \tag{11}$$

where I_1, I_2 and I_3 are the components of the moment of inertia tensor in the system of principal axes, where it is diagonal.

Furthermore, under the conditions of Theorem 1, the trace of the moment of inertia tensor $\mathrm{Tr}\mathbf{I}$ commutes with the Hamiltonian H,

$$[H, \mathrm{Tr}\mathbf{I}] = 0. \tag{12}$$

This means that, together with the total angular momentum operator $\mathbf{J}$ in (7), operator $\mathrm{Tr}\mathbf{I}$ is also a constant of the Heisenberg equation of motion. Suppose that in addition $\mathbf{J}$ and $\mathrm{Tr}\mathbf{I}$, other self-adjoint operators that commute with H exist. The set $\{\Omega^{\alpha}\}$ is then formed by all self-adjoint operators satisfying the following relations:

$$\begin{aligned}
&[H, \Omega^{\alpha}], && \forall \Omega^{\alpha} \in \{\Omega^{\alpha}\} \\
&[J^2, \Omega^{\alpha}], && \forall \Omega^{\alpha} \in \{\Omega^{\alpha}\} \\
&[J_z, \Omega^{\alpha}], && \forall \Omega^{\alpha} \in \{\Omega^{\alpha}\} \\
&[\mathrm{Tr}\mathbf{I}, \Omega^{\alpha}], && \forall \Omega^{\alpha} \in \{\Omega^{\alpha}\} \\
&[\Omega^{\alpha}, \Omega^{\beta}], && \forall \Omega^{\alpha}, \Omega^{\beta} \in \{\Omega^{\alpha}\}
\end{aligned} \tag{13}$$

Therefore, the set $\{H, J^2, J_z, \mathrm{Tr}\mathbf{I}, \{\Omega^{\alpha}\}\}$ is the maximal set of commuting self-adjoint operators. The subspace $D(H, J^2, J_z, \mathrm{Tr}\mathbf{I}, \{\Omega^{\alpha}\})$ of the Hilbert space is generated by the set of normalized simultaneous eigenvectors $\{|n\rangle\}$,

$$|n\rangle \equiv \left| E_n, j_n, m_n, I_n^{Tr}, \{\Omega_n^{\alpha}\} \right\rangle, \tag{14}$$

of the maximal set of commuting self-adjoint operators $\{H, J^2, J_z, \mathrm{Tr}\mathbf{I}, \{\Omega^{\alpha}\}\}$;

$$\begin{aligned}
&H|n\rangle = E_n|n\rangle, \\
&J^2|n\rangle = j_n(j_n+1)\hbar^2|n\rangle, \\
&J_z|n\rangle = m_n\hbar|n\rangle, \\
&\mathrm{Tr}\mathbf{I}|n\rangle = I_n^{Tr}|n\rangle, \\
&\Omega^{\alpha}|n\rangle = \Omega_n^{\alpha}|n\rangle, \qquad \forall \Omega^{\alpha} \in \{\Omega^{\alpha}\}
\end{aligned} \tag{15}$$

From (8) and (15) it follows that the commutators of the operators J^2 and J_z, with the operator G, if taken between any $|n\rangle, |m\rangle \in \{|n\rangle\}$, are equal to

$$\begin{aligned}&\langle m|[G, J^2]|n\rangle \\ &= \langle m|G|n\rangle[j_n(j_n+1) - j_m(j_m+1)]\hbar^2 = 0,\end{aligned} \tag{16}$$

and

$$\langle m|[G, J_z]|n\rangle = \langle m|G|n\rangle[m_n - m_m]\hbar = 0. \tag{17}$$

From (16) and (17) it follows that the matrix elements of the operator G are equal to zero, if taken between the eigenvectors with different j and between the eigenvectors with different m,

$$\langle m|G|n\rangle = \begin{cases} 0, & \forall |n\rangle, |m\rangle \in \{|n\rangle\}: j_n \neq j_m \\ 0, & \forall |n\rangle, |m\rangle \in \{|n\rangle\}: m_n \neq m_m \end{cases} \tag{18}$$

Using (18), we then obtain that for the following cases the matrix elements of the commutator $[G, H]$ are equal to zero:

$$\begin{aligned}&\langle m|[G, H]|n\rangle = \langle m|G|n\rangle(E_n - E_m) \\ &= \begin{cases} 0, & \forall |n\rangle, |m\rangle \in \{|n\rangle\}: j_n \neq j_m \\ 0, & \forall |n\rangle, |m\rangle \in \{|n\rangle\}: m_n \neq m_m \\ 0, & \forall |n\rangle, |m\rangle \in \{|n\rangle\}: E_n = E_m \end{cases}\end{aligned} \tag{19}$$

Therefore, to complete the proof that $\langle m|[G, H]|n\rangle = 0$ for all eigenvectors $\forall |n\rangle, |m\rangle \in \{|n\rangle\}$, we still have to show that the relation $\langle m|G|n\rangle = 0$ is true for all eigenvectors $|n\rangle, |m\rangle \in \{|n\rangle\}$ for which $j_n = j_m$, $m_n = m_m$ and $E_n \neq E_m$.

The Heisenberg equation of motion for the position operator $\mathbf{r}_i$ of i th particle in the nonrelativistic quantum mechanics gives

$$\dot{\mathbf{r}}_i = \frac{1}{i\hbar}[\mathbf{r}_i, H] = \frac{\mathbf{p}_i}{m_i}. \tag{20}$$

Using (3), (10) and (20), we obtain that

$$\begin{aligned}&[H, \mathrm{Tr}\mathbf{I}] = 2\left[H, \sum_{i=1}^{N} m_i r_i^2\right] \\ &= -2i\hbar \sum_{i=1}^{N} (\mathbf{r}_i \cdot \mathbf{p}_i + \mathbf{p}_i \cdot \mathbf{r}_i) \\ &= -4i\hbar G.\end{aligned} \tag{21}$$

The trace of the moment of inertia tensor $\mathrm{Tr}\mathbf{I}$ commutes with the Hamiltonian H, as given by relation (12). In general, if A and B are both unbounded self-adjoint operators, the commutator $[A, B]$ a priori is only defined as a quadratic form on the intersection of their domains, i.e. on $D(A) \cap D(B)$ [7]. Therefore, relations (12) and (21) really mean that on the subspace $D(H, J^2, J_z, \mathrm{Tr}\mathbf{I}, \{\Omega^\alpha\})$, generated by the set of simultaneous eigenvectors $\{|n\rangle\}$ of the set of commuting operators $\{H, J^2, J_z, \mathrm{Tr}\mathbf{I}, \{\Omega^\alpha\}\}$, where the commutator $[H, \mathrm{Tr}\mathbf{I}]$ is defined, the matrix elements of operator G are all equal to zero

$$\langle m|G|n\rangle = 0, \qquad \forall |n\rangle, |m\rangle \in \{|n\rangle\}. \tag{22}$$

Using (15) and (22) we then obtain that

$$\langle m|[G, H]|n\rangle = 0, \qquad \forall |n\rangle, |m\rangle \in \{|n\rangle\}, \tag{23}$$

which is what we set out to prove.

3. CONCLUSION

In this work we derived the generalized version of the quantum mechanical virial theorem for nonrelativistic *N*-particle systems with rotational symmetry, which are characterized by the constant trace of the moment of inertia tensor. In that sense, the work also represents the application of the generalized hypervirial relation on the example of trace of the moment of inertia tensor. It is known that hypervirial approaches lead to important recurrence relations between the matrix elements [17]. Classically, the trace of the moment of inertia tensor is equal to the sum $I_1 + I_2 + I_3$ of the moments of inertia about the principal axes. The result obtained could be applicable to quantum systems known to have this property. There are many possible applications, for example, in nonrelativistic models for nuclei with the constant moments of inertia, where the nucleons are moving in a self-consistent field [18]. Also in a molecular models, when the electronic contribution to the tensor of inertia, and coupling between the rotational motion of the molecule and its other degrees of freedom (vibrational and electronic) could be neglected.

COMPETING INTERESTS

Author has declared that no competing interests exist.

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