Quantum mechanical virial theorem in systems with translational and rotational symmetry

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Abstract

Generalized virial theorem for quantum mechanical nonrelativistic and relativistic systems with translational and rotational symmetry is derived in the form of the commutator between the generator of dilations G and the Hamiltonian H. If the conditions of translational and rotational symmetry together with the additional conditions of the theorem are satisfied, the matrix elements of the commutator $[G, H]$ are equal to zero on the subspace of the Hilbert space. Normalized simultaneous eigenvectors of the particular set of commuting operators which contains H, $\mathbf{J}^2$, J_z and additional operators form an orthonormal basis in this subspace. It is expected that the theorem is relevant for a large number of quantum mechanical N-particle systems with translational and rotational symmetry.

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I. INTRODUCTION

As is the case with many interesting quantum mechanical systems, bound states seem beyond standard perturbation theory and are difficult to grasp, even more so because very few systems are known to be solved exactly. Considering the limitations, virial theorem remains a very useful tool in studying bound states and quantum mechanical systems in general. Historically, derivation of the quantum mechanical virial theorem has been led by analogy with the classical counterpart. Quantum mechanical virial theorem in the nonrelativistic form is the relation between expectation values of the kinetic energy and the directional derivative of the potential energy. For a system described by a relativistic Hamiltonian, quantum mechanical virial theorem is the relation between expectation values of directional derivatives of the kinetic and potential energy. An account of virial theorems in quantum mechanics, including relativistic and nonrelativistic Hamiltonians and wave equations (Schrödinger, Salpeter, Dirac, Klein-Gordon) is found in [1].

Relations between virial theorem in classical mechanics and virial theorem in quantum mechanics are noted here in Section II. Explanation is given on the basis of Ehrenfest's theorem and the correspondence principle. Derivations in Sec. II follow similar derivations of virial theorem in standard classical and quantum mechanics textbooks [2, 3]. Quantum mechanical virial theorem is derived from the time derivative of the expectation value of operator G, i.e. from the expectation value of the commutator between G and H. It is a simple fact in quantum mechanics that the expectation value of the commutator $[G, H]$ vanishes for eigenvectors of the Hamiltonian H and the quantum mechanical virial theorem follows. It is known that this argument is only formal since the generator of dilations G is an unbounded operator and an eigenvector of H need not be in a domain of operator G [4, Vol. 4, 231]. Review of the various assumptions under which abstract versions of the quantum mechanical virial theorem have been proved is found in [5]. Other ways of deriving the quantum mechanical virial theorem include an approach using dilations. This is the focus of Section IV. There is also an approach using variational calculation [6]. For relativistic particles described by the Dirac or the Klein-Gordon equation and bound in scalar and/or vector type potentials an example of variational approach is given in [7].

Section III represents a step further under assumption of certain symmetry properties of the Hamiltonian. In the proof of the theorem in Sec. III no reference is made if the particular system on which the theorem applies is described by a nonrelativistic or relativistic Hamiltonian. It is required, among other conditions of the theorem in Sec. III, that the Hamiltonian is invariant to translations and rotations, i.e. that the system described by the Hamiltonian has translational and rotational symmetry. If in addition to translations and rotations, the Hamiltonian is invariant to other symmetry operations, there is an additional condition. This additional condition of the theorem in Sec. III is important if, in addition to H, $\mathbf{J}^2$ and J_z, there is a set of self-adjoint operators $\{\Omega^\alpha\}$ which are members of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$. It is then required that all operators Ω^α in the set $\{\Omega^\alpha\}$ commute with the generator of dilations G. If this requirement is satisfied along with translational and rotational symmetry and other conditions of the theorem in Sec. III, the matrix elements of the commutator $[G, H]$ are equal to zero on the subspace $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$ of the Hilbert space. Normalized simultaneous eigenvectors of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$ which belong to the Hilbert space form an orthonormal basis in the subspace $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$.

The conditions of the theorem in Sec. III are not satisfied if a member of the set $\{\Omega^\alpha\}$ exists which does not commute with the operator G. Therefore, possible applications of the theorem in Sec. III should be considered with this limitation in mind. Another limitation is that an eigenvector of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$ need not be in a domain of operator G. These and other limitations are discussed in more detail in Sec. III. The proof of the theorem in Sec. III includes the use of analytic functions and distributions. Part of the proof extends to Appendix. It is expected that the theorem in Sec. III relates to a large number of nonrelativistic and relativistic quantum mechanical N-particle systems with translational and rotational symmetry.

II. VIRIAL THEOREM IN CLASSICAL AND QUANTUM MECHANICS

In classical mechanics virial theorem is closely related to systems with bounded coordinates and momenta. If the forces are all derivable from the potential which is a homogeneous function of the coordinates, it relates the time average of the kinetic and potential energy of the system. In classical mechanics virial theorem is derived from the quantity

$$G = \sum_i \mathbf{r}_i \cdot \mathbf{p}_i, \tag{1}$$

i.e. the sum over all the particles of the system, of the scalar product of the momentum and position vector. The total time derivative of this quantity is

$$\frac{dG}{dt} = \sum_i \dot{\mathbf{r}}_i \cdot \mathbf{p}_i + \sum_i \mathbf{r}_i \cdot \mathbf{F}_i, \tag{2}$$

where the momentum time derivatives $\dot{\mathbf{p}}_i$ are equal to the forces $\mathbf{F}_i$. The nonrelativistic relation between the time derivative of the position vector and the momentum is $\dot{\mathbf{r}}_i = \frac{\mathbf{p}_i}{m_i}$ and

$$T(\mathbf{p}) \equiv \sum_i \frac{\mathbf{p}_i^2}{2m_i} = \frac{1}{2}\sum_i \dot{\mathbf{r}}_i \cdot \mathbf{p}_i, \tag{3}$$

is the total kinetic energy of the nonrelativistic system of particles. Taking the time average of (2)

$$\frac{1}{\tau}\int_0^\tau \frac{dG}{dt}dt \equiv \overline{\frac{d}{dt}\left(\sum_i \mathbf{r}_i \cdot \mathbf{p}_i\right)} = 2\overline{T(\mathbf{p})} + \overline{\sum_i \mathbf{r}_i \cdot \mathbf{F}_i}, \tag{4}$$

leads to a relation

$$\frac{1}{\tau}\left[G(\tau) - G(0)\right] = 2\overline{T(\mathbf{p})} + \overline{\sum_i \mathbf{r}_i \cdot \mathbf{F}_i}. \tag{5}$$

As explained below, in classical mechanics virial theorem is known as a relation

$$\overline{T(\mathbf{p})} = -\frac{1}{2}\overline{\sum_i \mathbf{r}_i \cdot \mathbf{F}_i}. \tag{6}$$

If the motion is periodic with the time interval τ as the period, the left-hand side of equation (5) vanishes. A similar result is obtained even if the motion is not periodic but is confined in a bounded domain in the phase space so that G is bounded. By choosing the time interval τ in the time average sufficiently long, the left-hand side of Eq. (5) can be made as small as desired [2, 82-85].

If the forces $\mathbf{F}_i$ are derivable from a potential, a consequence of relation (6) is the relation between the time average of the kinetic energy and the time average of the directional derivative of potential energy of the system of particles,

$$\overline{T(\mathbf{p})} = \frac{1}{2}\overline{\sum_{i=1}^{N} \mathbf{r}_i \cdot \nabla_i V(\mathbf{r})}. \tag{7}$$

In relation (7) written for a system of N particles, $\mathbf{r}$ denotes the set of N position vectors $(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ and $\mathbf{p}$ denotes the set of N momentum vectors $(\mathbf{p}_1, \ldots, \mathbf{p}_1)$. If the potential is a homogeneous function of degree λ [1], with $3N$ Cartesian coordinates $(x_1, y_1, z_1, \ldots, x_N, y_N, z_N)$ as variables, then

$$\sum_{i=1}^{N} \mathbf{r}_i \cdot \nabla_i V(\mathbf{r}) = \lambda V(\mathbf{r}). \tag{8}$$

[1] A function f such that for all points $(x_1, \ldots, x_n)$ in its domain of definition and all real $s > 0$, the equation $f(sx_1, \ldots, sx_n) = s^\lambda f(x_1, \ldots, x_n)$ holds, where λ is a real number; here it is assumed that for every point $(x_1, \ldots, x_n)$ in the domain of f, the point $(sx_1, \ldots, sx_n)$ also belongs to this domain for any $s > 0$. If the domain of definition E of f is an open set and f is continuously differentiable on E, then the function is homogeneous of degree λ if and only if for all $(x_1, \ldots, x_n)$ in its domain of definition it satisfies the Euler formula $\sum_{i=1}^n x_i \frac{\partial f}{\partial x_i} = \lambda f$, [8].

Equations (7) and (8) lead to relation between the time average of the kinetic and potential energy of the system of N particles

$$\overline{T(\mathbf{p})} = \frac{\lambda}{2}\overline{V(\mathbf{r})}. \tag{9}$$

In quantum mechanics Ehrenfest's theorem [9] proves that the equations of motion for the expectation values of quantum mechanical operators[2] are analogous to the equations of motion for the corresponding classical quantities. Ehrenfest's theorem provides an example of the correspondence between classical and quantum mechanics [3, 28-30]. This is true also for the equations of motion for quantum mechanical operators in the Heisenberg picture,

$$\dot{\mathbf{p}}_i = \frac{1}{i\hbar}[\mathbf{p}_i, H] = -\nabla_i V(\mathbf{r}) \ ,$$

$$\dot{\mathbf{r}}_i = \frac{1}{i\hbar}[\mathbf{r}_i, H]. \tag{10}$$

For simplicity, it is assumed that the Hamiltonian H in Eqs. (10) has the form

$$H = T(\mathbf{p}) + V(\mathbf{r}), \tag{11}$$

where $T(\mathbf{p})$ is the kinetic energy operator and $V(\mathbf{r})$ is the potential energy operator. For Hamiltonian H of a system of N particles, $\mathbf{r}$ denotes the set of N position operators $(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ and $\mathbf{p}$ denotes the set of N momentum operators $(\mathbf{p}_1, \ldots, \mathbf{p}_1)$.

By this analogy, classical quantities in the virial theorem (7) for the classical nonrelativistic system can be replaced by the expectation values of corresponding quantum mechanical operators, if the following relation

$$\frac{1}{\tau}\int_0^\tau \frac{d}{dt}\langle\psi|G|\psi\rangle dt = \frac{1}{\tau}\int_0^\tau \frac{1}{i\hbar}\langle\psi|[G,H]|\psi\rangle dt = 0, \tag{12}$$

is true for the quantum mechanical state vector denoted by $|\psi\rangle$ representing the physical state of the system. If the state vector $|\psi\rangle$ is an eigenvector of the Hamiltonian H and the expectation value of the commutator $[G, H]$ is equal to zero, then (12) is obviously true. If the virial theorem (7) for the corresponding classical system holds, relation (12) is expected to be true in the classical or correspondence-principle limit. In the classical limit expectation value of the operator G corresponds to a classical quantity in Eq. (1). The operator $\sum_{i=1}^N \mathbf{r}_i \cdot \mathbf{p}_i$ is not hermitian and is

[2] All quantum mechanical operators in this work are denoted in the same way classical quantites at the beginning of Sec. II were denoted, since the rest of the work is focused on the quantum mechanical virial theorem.

replaced by

$$G = \frac{1}{2}\sum_{i=1}^{N}\left(\mathbf{r}_i\cdot\mathbf{p}_i+\mathbf{p}_i\cdot\mathbf{r}_i\right). \tag{13}$$

Operator G given by Eq. (13) is different from $\sum_{i=1}^{N}\mathbf{r}_i\cdot\mathbf{p}_i$ by a constant term proportional to $\hbar$ which vanishes in the classical limit.[3] This constant term commutes with the Hamiltonian and is irrelevant in the time evolution of operator G.

The main difference between the classical and quantum mechanical virial theorem is that the former is given in terms of the time averages of classical quantities and the latter in terms of the expectation values of quantum mechanical operators. In analogy to derivation in classical mechanics, the derivation of virial theorem for the quantum mechanical system starts with the quantum mechanical analogue of Eq. (2), with the operator G given by Eq. (13),

$$\begin{aligned}\frac{d}{dt}\langle\psi|G|\psi\rangle &= \frac{1}{i\hbar}\langle\psi|[G,H]|\psi\rangle \\ &= 2\langle\psi|T(\mathbf{p})|\psi\rangle - \langle\psi|\sum_{i=1}^{N}\mathbf{r}_i\cdot\nabla_i V(\mathbf{r})|\psi\rangle.\end{aligned} \tag{14}$$

In the last line of Eq. (14) it is assumed that the Hamiltonian H has the form given by Eq. (11) and that the kinetic energy operator $T(\mathbf{p})$ is the quantum mechanical analogue of the nonrelativistic kinetic energy in Eq. (3). If the relation (14) is equal to zero, virial theorem for the quantum mechanical system follows. In this way, for the nonrelativistic quantum mechanical system with the Hamiltonian (11), the relation

$$\langle\psi|T(\mathbf{p})|\psi\rangle = \frac{1}{2}\langle\psi|\sum_{i=1}^{N}\mathbf{r}_i\cdot\nabla_i V(\mathbf{r})|\psi\rangle, \tag{15}$$

is established. If the potential $V(\mathbf{r})$ is a homogeneous function of degree λ, from relation (15) one obtains the relation between the expectation values of the kinetic and potential energy of the system,

$$\langle\psi|T(\mathbf{p})|\psi\rangle = \frac{\lambda}{2}\langle\psi|V(\mathbf{r})|\psi\rangle\ . \tag{16}$$

Similar derivations of quantum mechanical virial theorem are standard in the textbooks of nonrelativistic quantum mechanics, for example in [3, 180].

[3] A quote important for this work is [3, 176]: "it is important to realize that there is no unique way of making the transition from classical to quantum mechanics. Terms can always be added to the quantum equations of motion that vanish in the classical or correspondence-principle limit. On the other hand, if the classical behavior of a system is known, certain restrictions are placed on its quantum equations."

For the relativistic quantum mechanical system with the Hamiltonian in the form (11), virial theorem is established in the similar way, but the expectation value of the operator $2T(\mathbf{p})$ in the last line of Eq. (14) and subsequently, should be replaced with the expectation value of an operator which involves the relativistic kinetic energy. In Section IV this operator is derived and is equal to directional derivative of the kinetic energy operator. To keep the presentation as simple as possible, electromagnetic four-vector potential $A^\mu = (\phi, \mathbf{A})$ and scalar-type potentials are not discussed here, but details regarding the virial theorem can be found in [7].

In nonrelativistic quantum mechanics and in relativistic quantum mechanics, where the Hamiltonian for the system described by the particular wave equation can be given, virial theorem follows for eigenvectors of the Hamiltonian as a consequence of hermiticity of the Hamiltonian, $H^\dagger = H$. Quantum mechanical virial theorem [1] is in this way equivalent to a statement that the expectation values of the commutator $[G, H]$ are equal to zero

$$\langle\psi|[G, H]|\psi\rangle = 0, \tag{17}$$

taken with respect to the normalized eigenvectors of the Hamiltonian H,

$$H|\psi\rangle = E|\psi\rangle, \qquad \langle\psi|\psi\rangle = 1. \tag{18}$$

This argument is formal since G is an unbounded operator and $|\psi\rangle$ need not be in a domain of operator G, [4, Vol. 4, 231].

III. SYSTEMS WITH TRANSLATIONAL AND ROTATIONAL SYMMETRY

A. Symmetry conditions

In Section II quantum mechanical virial theorem was given in the form that is common in the literature for the nonrelativistic and relativistic cases. This form of quantum mechanical virial theorem directly depends on the state vectors; the proof is formal and is given only for eigenvectors of the Hamiltonian. It is shown here in Section III, that under the conditions of translational and rotational symmetry of the Hamiltonian and the additional conditions, the theorem can be derived in the form of the commutator between the generator of dilations G and the Hamiltonian H and the matrix elements of this commutator are equal to zero on the subspace of the Hilbert space. In this section, the proof of quantum mechanical virial theorem is given without reference to the detailed form of the Hamiltonian. It works for the nonrelativistic and relativistic Hamiltonians, if along with other conditions, the conditions of translational and rotational symmetry are satisfied, i.e. the following commutators are equal to zero

$$[H, \mathbf{P}] = 0, \qquad [H, \mathbf{J}] = 0. \tag{19}$$

Other conditions additional to (19) exist, and will be discussed. The generator of translations, operator of the total momentum $\mathbf{P} = \sum_{i=1}^{N} \mathbf{p}_i$ and the generator of rotations, operator of the total angular momentum $\mathbf{J} = \sum_{i=1}^{N} \mathbf{J}_i$, do not commute. Possible set of commuting operators can contain operators H, $\mathbf{J}^2$ and J_z, or it can contain operators H and $\mathbf{P}$, but can not contain operators H, $\mathbf{J}^2$, J_z and $\mathbf{P}$.

Next, the properties of operators G, H and $\mathbf{J}$ are discussed. As given by Eq. (13), G is a scalar operator and therefore is invariant to rotations. This means that G commutes with the generator of rotations, operator of the total angular momentum $\mathbf{J} = \sum_{i=1}^{N} \mathbf{J}_i$. The commutators of the operator G with the operators $\mathbf{J}$ and $\mathbf{P}$ are equal to

$$[G, \mathbf{J}] = 0, \qquad [G, \mathbf{P}] = i\hbar\mathbf{P}. \tag{20}$$

The discussion in this section is limited to quantum mechanical N-particle systems that have the following symmetry properties:

The Hamiltonian H of the system considered here is invariant to translations, rotations and can be invariant to additional symmetry operations. The commutators of the Hamiltonian H with the generators of translations and rotations, operators $\mathbf{P}$ and $\mathbf{J}$, are equal to zero. If, in addition to $\mathbf{P}$ and $\mathbf{J}$, other self-adjoint operators which commute with H exist, then the additional condition is required from these operators. Those of them which commute with $\mathbf{J}^2$, J_z and among themselves, and hence are members of the set of commuting operators containing H, $\mathbf{J}^2$ and J_z, should commute with the operator G.

Suppose that in addition to $\mathbf{P}$ and $\mathbf{J}$, other self-adjoint operators which commute with H exist. Suppose that they satisfy the aforementioned additional condition. The set $\{\Omega^\alpha\}$ is formed by all self-adjoint operators Ω^α satisfying the following relations:

$$\begin{aligned}
[H, \Omega^\alpha] &= 0, && \forall\Omega^\alpha \in \{\Omega^\alpha\}, \\
[\mathbf{J}^2, \Omega^\alpha] &= 0, && \forall\Omega^\alpha \in \{\Omega^\alpha\}, \\
[J_z, \Omega^\alpha] &= 0, && \forall\Omega^\alpha \in \{\Omega^\alpha\}, \\
[\Omega^\alpha, \Omega^{\alpha'}] &= 0, && \forall\Omega^\alpha, \forall\Omega^{\alpha'} \in \{\Omega^\alpha\},
\end{aligned} \tag{21}$$

and since the additional condition is fulfilled,

$$[G, \Omega^\alpha] = 0, \qquad \forall \Omega^\alpha \in \{\Omega^\alpha\}. \tag{22}$$

For example, if the Hamiltonian H, invariant to translations and rotations, is also parity invariant, an obvious candidate for the set $\{\Omega^\alpha\}$ is the parity operator π, since it commutes with the operators $\mathbf{J}$ and G. It will be shown here that under the conditions of the theorem given at the end of this section, the matrix elements of the commutator $[G, H]$ are equal to zero on the subspace of the Hilbert space. This subspace is generated by the simultaneous eigenvectors of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$ which belong to the Hilbert space.

B. Subspace $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$

Simultaneous eigenvectors of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$ which belong to the Hilbert space are denoted

$$|n\rangle \equiv |E_n, j_n, m_n, \{\Omega_n^\alpha\}\rangle. \tag{23}$$

In this simple notation $|n\rangle$ denotes the simultaneous eigenvector of operators H, $\mathbf{J}^2$, J_z and $\{\Omega^\alpha\}$, with the eigenvalues

$$H|n\rangle = E_n|n\rangle,$$

$$\mathbf{J}^2|n\rangle = j_n(j_n+1)\hbar^2|n\rangle,$$

$$J_z|n\rangle = m_n\hbar|n\rangle,$$

$$\Omega^\alpha|n\rangle = \Omega_n^\alpha|n\rangle, \qquad \forall \Omega^\alpha \in \{\Omega^\alpha\}. \tag{24}$$

If all members Ω^α of the set of operators $\{\Omega^\alpha\}$ are known, the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$ is maximal. All members of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$ are self-adjoint operators. Any simultaneous eigenvector of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$, denoted by (23), is uniquely determined by the eigenvalues (24). A basis in the subspace of the Hilbert space formed from the normalized simultaneous eigenvectors (23) is orthonormal

$$\langle n|m\rangle = \delta_{n,m}. \tag{25}$$

This basis is denoted by $\{|n\rangle\}$. Subspace of the Hilbert space generated by the basis $\{|n\rangle\}$ is denoted $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$.

The commutators of the operators $\mathbf{J}^2,\ J_z$ and $\{\Omega^\alpha\}$ with the operator G, if taken between any simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$, are equal to:

$$\langle n|[G, \mathbf{J}^2]|m\rangle = \langle n|G|m\rangle[j_m(j_m+1) - j_n(j_n+1)]\hbar^2 = 0,$$

$$\langle n|[G, J_z]|m\rangle = \langle n|G|m\rangle(m_m - m_n)\hbar = 0,$$

$$\langle n|[G, \Omega^\alpha]|m\rangle = \langle n|G|m\rangle(\Omega_m^\alpha - \Omega_n^\alpha) = 0, \qquad \forall\Omega^\alpha \in \{\Omega^\alpha\}. \tag{26}$$

From the commutators (20) and (22), it follows that the matrix elements in (26) are equal to zero. Furthermore, from the matrix elements in (26), it follows that the matrix elements of the operator G are equal to zero if taken between the eigenvectors with different j, between the eigenvectors with different m and between the eigenvectors with different Ω^α. This follows independently in all aforementioned cases,

$$\langle n|G|m\rangle = \begin{cases} 0\,, & \forall|n\rangle, \forall|m\rangle \in \{|n\rangle\} :\ j_n \neq j_m \\ 0\,, & \forall|n\rangle, \forall|m\rangle \in \{|n\rangle\} :\ m_n \neq m_m \\ 0\,, & \forall|n\rangle, \forall|m\rangle \in \{|n\rangle\} :\ \Omega_n^\alpha \neq \Omega_m^\alpha \end{cases}. \tag{27}$$

From the relation (27), it follows that in aforementioned cases matrix elements of the commutator $[G, H]$ are equal to zero, i.e.

$$\langle n|[G, H]|m\rangle = \langle n|G|m\rangle\,(E_m - E_n) = \begin{cases} 0\,, & \forall|n\rangle, \forall|m\rangle \in \{|n\rangle\} :\ j_n \neq j_m \\ 0\,, & \forall|n\rangle, \forall|m\rangle \in \{|n\rangle\} :\ m_n \neq m_m \\ 0\,, & \forall|n\rangle, \forall|m\rangle \in \{|n\rangle\} :\ \Omega_n^\alpha \neq \Omega_m^\alpha \\ 0\,, & \forall|n\rangle, \forall|m\rangle \in \{|n\rangle\} :\ E_n = E_m \end{cases}. \tag{28}$$

It is clear, from relation (28), that to complete the proof of the relation $\langle n|[G, H]|m\rangle = 0$ for all eigenvectors $|n\rangle$ and $|m\rangle$, it still remains to show that the relation $\langle n|G|m\rangle = 0$ is true for all cases (for all eigenvectors) not already contained in relation (27) for which $E_n \neq E_m$. Therefore to complete the proof, it remains to show that the relation $\langle n|G|m\rangle = 0$ is true for the eigenvectors $|n\rangle$ and $|m\rangle$ for which $j_n = j_m,\ m_n = m_m,\ \Omega_n^\alpha = \Omega_m^\alpha$ and $E_n \neq E_m$. Relation $\langle n|[G, H]|m\rangle = 0$ is established in this way by direct calculation, for all simultaneous eigenvectors of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$ which belong to the Hilbert space, denoted by (23), i.e. on the subspace $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$ of the Hilbert space. *Sufficient condition under* *which relations (26), (27) and (28) are defined without ambiguity, is that operator G is defined on the subspace $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$.*[4] *Therefore, assumption that $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\}) \subset D(G)$, where $D(G)$ represents the domain of operator G, should be tested initially.*

C. Analytic functions $f(\mathbf{p})$

The commutator of the operator G with an analytic function $f(\mathbf{p})$ is equal to

$$[G, f(\mathbf{p})] = i\hbar \mathbf{p} \cdot \frac{\partial f(\mathbf{p})}{\partial \mathbf{p}}. \tag{29}$$

In relation (29), the set of N momentum operators $(\mathbf{p}_1, \ldots, \mathbf{p}_N)$ is denoted by $\mathbf{p}$ and $\mathbf{p} \cdot \frac{\partial}{\partial \mathbf{p}}$ is a notation for the directional derivative $\sum_{i=1}^{N} \mathbf{p}_i \cdot \frac{\partial}{\partial \mathbf{p}_i}$. For analytic functions $f(\mathbf{p})$ relation (29) is derived in Sec. IV using the canonical commutation relations. For analytic functions[5] $f(\mathbf{P}) = f\left(\sum_{i=1}^{N} \mathbf{p}_i\right)$, the commutator with the operator G is equal to

$$[G, f(\mathbf{P})] = i\hbar \mathbf{P} \cdot \frac{\partial f(\mathbf{P})}{\partial \mathbf{P}}. \tag{30}$$

Relation (30) is obtained from relation (29) using the definition of the total momentum operator $\mathbf{P} = \sum_{i=1}^{N} \mathbf{p}_i$.

It easy to show that the second commutator in (20) can be obtained from the relation (30), if it is applied on the components P_i of vector operator $\mathbf{P}$, where $i = 1, 2, 3$, in place of the function $f(\mathbf{P})$. If the relation (30) is applied on the set of operators formed by the components P_i of r vector operators $\mathbf{P}$,

$$\underbrace{P_i P_j \cdots P_n}_{\text{r operators}}, \qquad \underbrace{i, j, \ldots, n}_{\text{r indices}} = 1, 2, 3 \ , \tag{31}$$

it is straightforward to obtain

$$[G, P_i P_j \cdots P_n] = i\hbar r P_i P_j \cdots P_n, \qquad i, j, \ldots, n = 1, 2, 3 \ . \tag{32}$$

Relation (32) applies for all r where $r = 1, 2, \ldots$. The operators (31) can be considered components of the 3^r-component tensor operator. The second commutator in (20) represents a special case of (32) for $r = 1$.

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[4] 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 $D(A) \cap D(B)$ [5].

[5] A function f is called holomorphic (analytic) at a point $\alpha \in \mathbb{C}^n$ if it is holomorphic in some neighbourhood of this point. According to the Cauchy-Riemann criterion, a function of several variables which is holomorphic at a point α is holomorphic with respect to each variable (if the values of the other variables are fixed). The converse proposition is also true: if, in a neighbourhood of some point, a function f is holomorphic with respect to each variable separately, then it is holomorphic at this point (Hartogs' fundamental theorem) [8].

The next step in the proof involves translational invariance of the Hamiltonian. The commutator (19) of the Hamiltonian H with the generator of translations, operator of total momentum $\mathbf{P}$, is equal to zero. Using this commutation relation, one easily obtains that the commutators of H with the operators (31) are equal to zero,

$$[H, P_i P_j \cdots P_n] = 0, \qquad i, j, \ldots, n = 1, 2, 3 \ , \tag{33}$$

for all $r = 1, 2, \ldots$. For the matrix elements of the commutators (33) taken between simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$, the following relation is obtained:

$$\langle n|[H, P_i P_j \cdots P_n]|m\rangle = \langle n|P_i P_j \cdots P_n|m\rangle(E_n - E_m) = 0, \tag{34}$$

for all $r = 1, 2, \ldots$ and $i, j, \ldots, n = 1, 2, 3$. Relation (34) gives

$$\langle n|P_i P_j \cdots P_n|m\rangle = 0, \qquad \forall|n\rangle, \forall|m\rangle \in \{|n\rangle\} : \ E_n \neq E_m, \tag{35}$$

for all $r = 1, 2, \ldots$ and $i, j, \ldots, n = 1, 2, 3$. *Sufficient condition under which relations (34) and (35) are defined without ambiguity, is that operators $P_i P_j \cdots P_n$ in (31) are defined on the subspace $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$, for all $r = 1, 2, \ldots$ and $i, j, \ldots, n = 1, 2, 3$.*

D. Projection operator into $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$

Any simultaneous eigenvector $|n\rangle$ of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$ is an eigenvector of the Hamiltonian H. Since the commutators (33) of the operators $P_i P_j \cdots P_n$ in (31) with the Hamiltonian H are equal to zero, it follows that $P_i P_j \cdots P_n|n\rangle$ is an eigenvector of H, or a zero vector. In either case

$$H P_i P_j \cdots P_n|n\rangle = E_n P_i P_j \cdots P_n|n\rangle. \tag{36}$$

Relation (36) follows in this way for all operators $P_i P_j \cdots P_n$ in (31). The commutators of the operator G with the operators $\mathbf{J}^2$, J_z and $\{\Omega^\alpha\}$ are equal to zero. It follows, for any simultaneous eigenvector $|n\rangle$ of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$, that $G|n\rangle$ is a simultaneous eigenvector of operators $\mathbf{J}^2$, J_z and $\{\Omega^\alpha\}$, or a zero vector. In either case

$$\mathbf{J}^2 G|n\rangle = j_n(j_n + 1)\hbar^2 G|n\rangle,$$

$$J_z G|n\rangle = m_n \hbar G|n\rangle,$$

$$\Omega^\alpha G|n\rangle = \Omega_n^\alpha G|n\rangle, \qquad \forall \Omega^\alpha \in \{\Omega^\alpha\}. \tag{37}$$

Projection operator $\mathcal{P}_{\mathcal{D}(H)}$ maps every state vector onto its orthogonal projection in the subspace $\mathcal{D}(H)$, generated by the eigenvectors of the Hamiltonian H. Projection operator $\mathcal{P}_{\mathcal{D}(H)}$ is a bounded hermitian operator and it is idempotent, $\mathcal{P}^2_{\mathcal{D}(H)} = \mathcal{P}_{\mathcal{D}(H)}$. This is true for projection operators into any subspace of Hilbert space [10, 348]. Projection operator into the subspace $\mathcal{D}(\mathbf{J}^2, J_z, \{\Omega^\alpha\})$, generated by the simultaneous eigenvectors of operators $\mathbf{J}^2$, J_z and $\{\Omega^\alpha\}$, is denoted by $\mathcal{P}_{\mathcal{D}(J^2,J_z,\{\Omega^\alpha\})}$. Since the operators H, $\mathbf{J}^2$, J_z and $\{\Omega^\alpha\}$ form the set of commuting operators, it is straightforward to show that the projection operators $\mathcal{P}_{\mathcal{D}(J^2,J_z,\{\Omega^\alpha\})}$ and $\mathcal{P}_{\mathcal{D}(H)}$ commute and

$$\mathcal{P}_{\mathcal{D}(H)}\mathcal{P}_{\mathcal{D}(J^2,J_z,\{\Omega^\alpha\})} = \mathcal{P}_{\mathcal{D}(J^2,J_z,\{\Omega^\alpha\})}\mathcal{P}_{\mathcal{D}(H)} = \mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}. \tag{38}$$

Introduced here in relation (38), $\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}$ is a projection operator into the subspace $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$ generated by the simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$. Relation (38) is a special case of the property of projection operators associated to self-adjoint commuting operators. It follows from the definition of commutativity for self-adjoint operators and the properties of their associated projection-valued measures, [4, Vol. 1]. It is easily seen from relation (38), that $\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}$ is hermitian and idempotent. With the help of relations (36), (37) and (38), the following relations are obtained,

$$\langle n|GP_iP_j\cdots P_n|m\rangle = \langle n|G\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}P_iP_j\cdots P_n|m\rangle, \tag{39}$$

and

$$\langle n|P_iP_j\cdots P_nG|m\rangle = \langle n|P_iP_j\cdots P_n\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}G|m\rangle, \tag{40}$$

for all operators $P_iP_j\cdots P_n$ in (31) and for all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$.

From relation (32) it follows that on the subspace $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$ the expectation value of the operator $P_iP_j\cdots P_n$ is equal (up to a constant factor) to the expectation value of the commutator $[G, P_iP_j\cdots P_n]$. This inference is correct under conditions introduced in the analysis in previous subsections. It is useful when calculating matrix elements of the operators $P_iP_j\cdots P_n$ in (31). For the expectation value taken with respect to any simultaneous eigenvector (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$, relation (32) gives

$$\langle n|[G, P_iP_j\cdots P_n]|n\rangle = i\hbar r\langle n|P_iP_j\cdots P_n|n\rangle. \tag{41}$$

With the help of relations (39) and (40), it is easy to show that the left side of relation (41) is equal to

$$\langle n|G\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}P_iP_j\cdots P_n|n\rangle - \langle n|P_iP_j\cdots P_n\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}G|n\rangle. \tag{42}$$

Then, using relations (27), (35) and (42) one obtains

$$\langle n|G|n\rangle\left\{\langle n|P_iP_j\cdots P_n|n\rangle - \langle n|P_iP_j\cdots P_n|n\rangle\right\} = i\hbar r\langle n|P_iP_j\cdots P_n|n\rangle. \tag{43}$$

The factor in the brackets on the left side of relation (43) is equal to zero. It follows from relation (43) that the expectation values of operators $P_iP_j\cdots P_n$ in (31), taken with respect to all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$ are equal to zero

$$\langle n|P_iP_j\cdots P_n|n\rangle = 0, \qquad \forall|n\rangle\in\{|n\rangle\}\subset\mathcal{D}(H,\mathbf{J}^2,J_z,\{\Omega^\alpha\}). \tag{44}$$

Relation (44) is true for all operators $P_iP_j\cdots P_n$ in (31). By applying similar procedures when calculating the matrix elements of commutators (32) between all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$, and using relations (27), (35) and (44) one obtains

$$\langle n|P_iP_j\cdots P_n|m\rangle = 0, \qquad \forall|n\rangle,\forall|m\rangle\in\{|n\rangle\}\subset\mathcal{D}(H,\mathbf{J}^2,J_z,\{\Omega^\alpha\}). \tag{45}$$

Relation (45) follows for all operators $P_iP_j\cdots P_n$ in (31).

E. Multiple power series

Analytic function $f(\mathbf{P})$ is represented by a multiple power series. In abbreviated notation it is written as

$$f(\mathbf{P}) = \sum_{k=0}^{\infty}\frac{1}{k!}\frac{\partial^k f}{\partial\mathbf{P}^k}(0)\mathbf{P}^k, \tag{46}$$

with the terms in the series (46) given by

$$\frac{1}{k!}\frac{\partial^k f}{\partial\mathbf{P}^k}(0)\mathbf{P}^k \equiv \sum_{k_1,k_2,k_3\geq 0}^{k_1+k_2+k_3=k}\frac{1}{k_1!k_2!k_3!}\frac{\partial^{k_1+k_2+k_3}f}{\partial P_1^{k_1}\partial P_2^{k_2}\partial P_3^{k_3}}(0)P_1^{k_1}P_2^{k_2}P_3^{k_3}. \tag{47}$$

It is clear from (47) that all terms in the multiple power series (46) are equal (up to constant factors) to operators $P_1^{k_1}P_2^{k_2}P_3^{k_3}$, which are of the form (31):

$$P_1^{k_1}P_2^{k_2}P_3^{k_3} = \underbrace{P_1\cdots P_1}_{\mathrm{k_1}}\underbrace{P_2\cdots P_2}_{\mathrm{k_2}}\underbrace{P_3\cdots P_3}_{\mathrm{k_3}}. \tag{48}$$

Relation (45) is useful for evaluating matrix elements of the function (46) between the simultaneous eigenvectors (23) of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$. As it clearly follows from relations (45), (47) and (48), the matrix elements of the function $f(\mathbf{P})$ represented by (46) between all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$ are equal to

$$\langle n|f(\mathbf{P})|m\rangle = f(0)\langle n|m\rangle = f(0)\delta_{n,m}. \tag{49}$$

If the coefficient $f(0)$ in the multiple power series (46) is equal to zero, it follows that all matrix elements in (49) are equal to zero. Under conditions in this analysis, relation (49) is true for all functions $f(\mathbf{P})$ represented by multiple power series (46).

F. Translational invariance in $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$

The translation operator for a spatial displacement of the system by a displacement vector $\mathbf{d}$ is given by

$$U(\mathbf{d}) = \exp\left(\frac{-i\mathbf{d}\cdot\mathbf{P}}{\hbar}\right), \tag{50}$$

Total momentum operator $\mathbf{P} = \sum_{i=1}^{N} \mathbf{p}$ divided by $\hbar$ is the generator of translations for the system. Translation operator $U(\mathbf{d})$ given in (50) is represented by a multiple power series of the form (46). From relation (49) applied on the translation operator $U(\mathbf{d})$, one obtains

$$\langle n|U(\mathbf{d})|m\rangle = \langle n|m\rangle = \delta_{n,m}, \tag{51}$$

for all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$. Translation operator $U(\mathbf{d})$ is a unitary operator, $U(\mathbf{d})^\dagger U(\mathbf{d}) = U(\mathbf{d})U(\mathbf{d})^\dagger = I$. From the unitarity of $U(\mathbf{d})$ it follows that

$$\langle n|U(\mathbf{d})^\dagger U(\mathbf{d})|n\rangle = \langle n|U(\mathbf{d})U(\mathbf{d})^\dagger|n\rangle = \langle n|n\rangle = 1. \tag{52}$$

Relations (51) and (52) are equivalent to invariance of all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$ to translations,

$$U(\mathbf{d})|n\rangle = |n\rangle. \tag{53}$$

Eigenfunctions ψ_n correspond to simultaneous eigenvectors (23) of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$. The basis of simultaneous eigenvectors $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$ of the set of N position operators $(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is introduced in Appendix. In the usual notation of wave mechanics eigenfunctions ψ_n are recognized as

$$\langle \mathbf{r}_1, \ldots, \mathbf{r}_N | n \rangle = \psi_n(\mathbf{r}_1, \ldots, \mathbf{r}_N). \tag{54}$$

Equivalently, relation (53) implies that the eigenfunctions (54) are invariant to space displacements and depend on the relative position vectors of N particles,

$$\psi_n(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \psi_n(\{\mathbf{r}_i - \mathbf{r}_j\}). \tag{55}$$

In Eq. (55), $\{\mathbf{r}_i - \mathbf{r}_j\}$ is the set of relative position vectors $\mathbf{r}_i - \mathbf{r}_j$, where $i, j = 1, \ldots, N$ and $i \neq j$.

G. Gaussian function $\phi_a(\mathbf{P}, \mathbf{K})$

Gaussian function $\phi_a(x)$ of the independent variable x is given by

$$\phi_a(x) = \frac{1}{2a\sqrt{\pi}} \exp\left(-\frac{x^2}{4a^2}\right). \tag{56}$$

It has the following properties: it is normalized to unity

$$\int_{-\infty}^{\infty} \phi_a(x)dx = 1, \qquad\qquad a \in \mathbb{R} \setminus \{0\}, \tag{57}$$

and more importantly

$$\lim_{a\to 0} \int_{-\infty}^{\infty} \phi_a(x)g(x)dx = g(0). \tag{58}$$

Relation (58) can be rigorously proved for any "reasonably behaving" function $g(x)$; for instance, differentiability at $x = 0$ is sufficient [11, 231]. With the distributional[6] definition of $\delta(x)$, it is safe to write the relation (58) in the form

$$\lim_{a\to 0} \int_{-\infty}^{\infty} \phi_a(x)g(x)dx = \int_{-\infty}^{\infty} \delta(x)g(x)dx = g(0). \tag{59}$$

Generalization of (56) to three dimensions is given by

$$\phi_a(\mathbf{x}) = \frac{1}{(2a\sqrt{\pi})^3} \exp\left(-\frac{\mathbf{x}^2}{4a^2}\right), \tag{60}$$

[6] In the theory of distributions, the sequence of functions $f_n(x) = (n/\sqrt{\pi}) \exp\left(-n^2x^2\right)$ corresponds to the distribution $\phi(x)$ with the property $\lim_{n\to\infty} \int_{-\infty}^{\infty} f_n(x)g(x)dx = \int_{-\infty}^{\infty} \phi(x)g(x)dx = g(0)$ for all test functions $g(x)$. Variety of different sequences of functions $\{f_n(x)\}$ have this property for all test functions $g(x)$, and one such sequence is given by $f_n(x) = (n/\sqrt{\pi}) \exp\left(-n^2x^2\right)$. Such equivalent sequences correspond to the same distribution $\phi(x)$, better known as delta distribution or delta function $\delta(x)$, although no ordinary function with the corresponding property exists. The concept of a distribution can be extended to two and more dimensions. For example, in two dimensions delta distribution can be defined by the sequence of functions $f_n(x, y) = \left(n^2/\pi\right) \exp\left\{-n^2(x^2 + y^2)\right\}$ [11].

where $\mathbf{x}$ is the vector in three-dimensional Euclidean space $\mathbb{R}^3$. The function $\phi_a(\mathbf{x})$ in (60) corresponds to delta distribution $\delta^3(\mathbf{x})$.

Important function represented by a multiple power series of the form (46) is the Gaussian function

$$\phi_a(\mathbf{P},\mathbf{K}) = \frac{1}{\left(2a\sqrt{\pi}\right)^3} \exp\left[-\frac{(\mathbf{P}-\mathbf{K})^2}{4a^2}\right], \tag{61}$$

where $\mathbf{P}$ is the total momentum operator and $\mathbf{K}$ is the vector in Euclidean space $\mathbb{R}^3$. From the relation (49) for the functions represented by a multiple power series (46), it follows that the matrix elements of the Gaussian function $\phi_a(\mathbf{P},\mathbf{K})$, taken between all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$ are equal to

$$\langle n|\phi_a(\mathbf{P},\mathbf{K})|m\rangle = \phi_a(0,\mathbf{K})\langle n|m\rangle = \left(2a\sqrt{\pi}\right)^{-3} e^{-\frac{\mathbf{K}^2}{4a^2}}\delta_{n,m}. \tag{62}$$

H. Operator $\phi_a(\mathbf{P},\mathbf{K})$ and $a \to 0$ limit

Provided that the limit $a \to 0$ of the matrix element of the function $\phi_a(\mathbf{P},\mathbf{K})$ taken between the vectors $|\Psi\rangle$ and $|\Phi\rangle$ in the Hilbert space is finite, this limit is denoted as

$$\lim_{a\to 0}\langle\Phi|\phi_a(\mathbf{P},\mathbf{K})|\Psi\rangle = \langle\Phi|\delta^3(\mathbf{P},\mathbf{K})|\Psi\rangle. \tag{63}$$

The limit (63) is evaluated in relations (A.5), (A.6) and (A.7) in Appendix. It is shown in Appendix, that the matrix representation $\langle\mathbf{p}|\delta^3(\mathbf{P},\mathbf{K})|\mathbf{p}'\rangle$ in the basis $|\mathbf{p}_1,\ldots,\mathbf{p}_N\rangle$ in relation (A.8), is related to the matrix representation in the basis $|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle$ by a unitary transformation. In this way the matrix $\langle\mathbf{r}|\delta^3(\mathbf{P},\mathbf{K})|\mathbf{r}'\rangle$ in relation (A.17) is obtained. With the inverse transformation the matrix $\langle\mathbf{p}|\delta^3(\mathbf{P},\mathbf{K})|\mathbf{p}'\rangle$ is again obtained. This is important as the matrix representations (A.8) and (A.17) are useful in evaluating the limit (63). However, it should be stressed for clarity that neither vectors $|\mathbf{p}_1,\ldots,\mathbf{p}_N\rangle$ nor vectors $|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle$ introduced in Appendix, are normalizable and do not themselves actually belong to Hilbert space. Therefore, in the technical sense, they do not form a basis in the Hilbert space.

For the vectors $|\Psi\rangle$ and $|\Phi\rangle$ in the Hilbert space, the limit (63) is evaluated here using the relation (A.17). In the limit (63) one obtains

$$\langle\Phi|\delta^3(\mathbf{P},\mathbf{K})|\Psi\rangle = (2\pi\hbar)^{-3}\,\mathcal{I}_k(\mathbf{K}), \tag{64}$$

where $\mathcal{I}_k(\mathbf{K})$ is the integral

$$\mathcal{I}_k(\mathbf{K}) = \int e^{\frac{i}{\hbar}\mathbf{K}\cdot\left(\mathbf{r}_k-\mathbf{r}'_k\right)}\Phi^*(\mathbf{r}_1,\ldots,\mathbf{r}_N)\Psi(\mathbf{r}_1+\mathbf{r}'_k-\mathbf{r}_k,\ldots,\mathbf{r}_N+\mathbf{r}'_k-\mathbf{r}_k)d^3r'_k\prod_{i=1}^{N}d^3r_i. \tag{65}$$

Functions $\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ and $\Phi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ correspond to vectors $|\Psi\rangle$ and $|\Phi\rangle$ in the Hilbert space. The vector $\mathbf{r}'_k$ in relation (65) is any position vector from the set $(\mathbf{r}'_1,\ldots,\mathbf{r}'_N)$. If the functions $\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ and $\Phi(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ belong to the vector space $D(\mathbb{R}^{3N})$ of infinitely differentiable functions on $\mathbb{R}^{3N}$ with compact support, the integral (65) is convergent and the limit (63) is finite. All functions in $D(\mathbb{R}^{3N})$ belong to the Hilbert space $L^2(\mathbb{R}^{3N})$ of square integrable complex-valued functions and $D(\mathbb{R}^{3N})$ is a dense subspace of $L^2(\mathbb{R}^{3N})$.

The limit (63) is defined for all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$. The eigenfunctions ψ_n and ψ_m correspond to eigenvectors $|n\rangle$ and $|m\rangle$, as given by the relation (54). Using the property of translational invariance (55) of eigenfunctions ψ_n, one obtains the following equality from relations (63), (64) and (65),

$$\langle n|\delta^3(\mathbf{P},\mathbf{K})|m\rangle = \delta^3(\mathbf{K}) \int e^{\frac{i}{\hbar}\mathbf{K}\cdot\mathbf{r}_k} \psi_n^*(\{\mathbf{r}_j-\mathbf{r}_l\})\psi_m(\{\mathbf{r}_j-\mathbf{r}_l\}) \prod_{i=1}^{N} d^3r_i. \tag{66}$$

Relation (66) can be written in the form

$$\langle n|\delta^3(\mathbf{P},\mathbf{K})|m\rangle = \delta^3(\mathbf{K})\mathcal{F}_{(n,m),k}(\mathbf{K}). \tag{67}$$

The function $\mathcal{F}_{(n,m),k}(\mathbf{K})$ in relation (67) is equal to the Fourier transform

$$\mathcal{F}_{(n,m),k}(\mathbf{K}) = \int e^{\frac{i}{\hbar}\mathbf{K}\cdot\mathbf{r}_k} \psi_n^*(\{\mathbf{r}_j-\mathbf{r}_l\})\psi_m(\{\mathbf{r}_j-\mathbf{r}_l\}) \prod_{i=1}^{N} d^3r_i. \tag{68}$$

The Fourier transform (68) is defined since all eigenfunctions $\psi_n(\{\mathbf{r}_j-\mathbf{r}_l\})$ belong to the Hilbert space $L^2(\mathbb{R}^{3N})$ of square integrable complex-valued functions. Therefore, functions $e^{\frac{i}{\hbar}\mathbf{K}\cdot\mathbf{r}_k}\psi_n(\{\mathbf{r}_j-\mathbf{r}_l\})$ also belong to the Hilbert space $L^2(\mathbb{R}^{3N})$ and the integral (68) is convergent. The following properties of $\mathcal{F}_{(n,m),k}(\mathbf{K})$ are observed,

$$\mathcal{F}_{(n,m),k}(0) = \langle n|m\rangle = \delta_{n,m}, \tag{69}$$

and

$$\mathcal{F}_{(n,m),k}(0) = \mathcal{F}_{(n,m),l}(0), \tag{70}$$

for all $k,l=1,\ldots,N$. The indices (n,m) correspond to all simultaneous eigenvectors $|n\rangle$ and $|m\rangle$ of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$.

Relations (67), (68), (69) and (70) are consistent with the limit $a\to 0$ of relation (62). From relations (62) and (63) it is clear that the matrix elements $\langle n|\delta^3(\mathbf{P},\mathbf{K}=0)|m\rangle$ between simultaneous eigenvectors (23) of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$ are unbounded.

Relations (64), (65) and (66) indicate that operator $\delta^3(\mathbf{P}, \mathbf{K} = 0)$ is not defined on the subspace $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$ of the Hilbert space. This is verified with the help of relations (54), (55) and (A.17),

$$\|\delta^3(\mathbf{P}, \mathbf{K})|n\rangle\|^2 = \delta^3(\mathbf{K})\delta^3(\mathbf{K}), \tag{71}$$

for all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$. The norm of a vector $|\Psi\rangle$ in the Hilbert space, denoted by $\||\Psi\rangle\|$, is defined to be the nonnegative real number $\||\Psi\rangle\| = \sqrt{\langle\Psi|\Psi\rangle} \geq 0$. In the representation (A.17) it is straightforward to show that the vector subspace $D_{\partial_x}(\mathbb{R}^{3N})$ of the Hilbert space $L^2(\mathbb{R}^{3N})$,

$$D_{\partial_x}(\mathbb{R}^{3N}) = \left\{ \varphi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \,\middle|\, \varphi = \sum_{i=1}^{N} \frac{\partial \chi}{\partial x_i}, \quad \chi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \in D(\mathbb{R}^{3N}) \right\}, \tag{72}$$

is a vector subspace of the null space of operator $\delta^3(\mathbf{P}, \mathbf{K} = 0)$ and also that $D_{\partial_x}(\mathbb{R}^{3N}) \subset D(\mathbb{R}^{3N})$. The same is true for $D_{\partial_y}(\mathbb{R}^{3N})$ and $D_{\partial_z}(\mathbb{R}^{3N})$.

I. Properties of operator G on $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$

The commutator of the operator G with the function $\phi_a(\mathbf{P}, \mathbf{K})$ follows from relation (30):

$$[G, \phi_a(\mathbf{P}, \mathbf{K})] = i\hbar \mathbf{P} \cdot \frac{\partial \phi_a(\mathbf{P}, \mathbf{K})}{\partial \mathbf{P}}. \tag{73}$$

With the help of relations (49) and (61), one obtains that the matrix elements of the commutator (73) taken between all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$ are equal to zero,

$$\langle n|[G, \phi_a(\mathbf{P}, \mathbf{K})]|m\rangle = 0. \tag{74}$$

Function $\phi_a(\mathbf{P}, \mathbf{K})$ is represented by a multiple power series of the form (46). With the help of commutators (33), one obtains that the commutator of the Hamiltonian H with the function $\phi_a(\mathbf{P}, \mathbf{K})$ is equal to zero,

$$[H, \phi_a(\mathbf{P}, \mathbf{K})] = 0. \tag{75}$$

Any simultaneous eigenvector $|n\rangle$ of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$ is an eigenvector of H. Since the commutator (75) of the operators H and $\phi_a(\mathbf{P}, \mathbf{K})$ is equal to zero, it follows that $\phi_a(\mathbf{P}, \mathbf{K})|n\rangle$ is an eigenvector of H,

$$H\phi_a(\mathbf{P}, \mathbf{K})|n\rangle = E_n \phi_a(\mathbf{P}, \mathbf{K})|n\rangle. \tag{76}$$

With the help of relations (37), (38) and (76), one obtains the following relations

$$\langle n|G\phi_a(\mathbf{P},\mathbf{K})|m\rangle = \langle n|G\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}\phi_a(\mathbf{P},\mathbf{K})|m\rangle, \tag{77}$$

and

$$\langle n|\phi_a(\mathbf{P},\mathbf{K})G|m\rangle = \langle n|\phi_a(\mathbf{P},\mathbf{K})\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}G|m\rangle, \tag{78}$$

for all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$. With the help of (77) and (78), relation (74) becomes

$$\langle n|G\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}\phi_a(\mathbf{P},\mathbf{K})|m\rangle - \langle n|\phi_a(\mathbf{P},\mathbf{K})\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}G|m\rangle = 0. \tag{79}$$

Then, from relation (79), with the help of relation (62) one obtains

$$\langle n|G|m\rangle \left(2a\sqrt{\pi}\right)^{-3} e^{-\frac{\mathbf{K}^2}{4a^2}} - \left(2a\sqrt{\pi}\right)^{-3} e^{-\frac{\mathbf{K}^2}{4a^2}} \langle n|G|m\rangle = 0. \tag{80}$$

The notation introduced in Appendix, in particular in relations (A.5), (A.6) and (A.7), suggests that it is possible to write

$$\lim_{a\to 0}\langle\Phi|\mathbf{P}\cdot\frac{\partial\phi_a(\mathbf{P},\mathbf{K})}{\partial\mathbf{P}}|\Psi\rangle = \langle\Phi|\mathbf{P}\cdot\frac{\partial\delta^3(\mathbf{P},\mathbf{K})}{\partial\mathbf{P}}|\Psi\rangle, \tag{81}$$

where $|\Psi\rangle$ and $|\Phi\rangle$ are vectors in the Hilbert space. In this way the following relation is obtained,

$$\langle\Phi|\mathbf{P}\cdot\frac{\partial\delta^3(\mathbf{P},\mathbf{K})}{\partial\mathbf{P}}|\Psi\rangle = \int\langle\Phi|\mathbf{p}\rangle\mathbf{P}\cdot\frac{\partial\delta^3(\mathbf{P}-\mathbf{K})}{\partial\mathbf{P}}\langle\mathbf{p}|\Psi\rangle\prod_{i=1}^{N}d^3p_i. \tag{82}$$

In relation (82) $|\mathbf{p}\rangle$ is a notation for $|\mathbf{p}_1,\dots,\mathbf{p}_N\rangle$. The functions next to the derivative of the delta distribution $\delta^3(\mathbf{P}-\mathbf{K})$ in the integral (82) may have some properties of test functions. If the functions $\langle\mathbf{p}|\Psi\rangle$ and $\langle\mathbf{p}|\Phi\rangle$ do not belong to the space $D(\mathbb{R}^{3N})$ of infinitely differentiable functions on $\mathbb{R}^{3N}$ with compact support (the space of test functions), they still belong to the Hilbert space of square integrable functions $L^2(\mathbb{R}^{3N})$. Depending on differentiability of the functions $\langle\mathbf{p}|\Psi\rangle$ and $\langle\mathbf{p}|\Phi\rangle$, the rules of δ-calculus for derivatives of delta distribution and partial integration may still be applicable.

It is straightforward to prove, that for all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$, the corresponding limit (81) is finite. In a direct way, using the relation (49) for the matrix elements of functions represented by (46) between simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$, and the relation (61), one obtains

$$\lim_{a\to 0}\langle n|\mathbf{P}\cdot\frac{\partial\phi_a(\mathbf{P},\mathbf{K})}{\partial\mathbf{P}}|m\rangle = \lim_{a\to 0}(0) = 0. \tag{83}$$

Therefore, for eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$, the limit (81) is finite and is equal to zero. The limiting procedure is formally equivalent to calculating the matrix elements of the commutator

$$[G, \delta^3(\mathbf{P}, \mathbf{K})] = i\hbar \mathbf{P} \cdot \frac{\partial \delta^3(\mathbf{P}, \mathbf{K})}{\partial \mathbf{P}}, \tag{84}$$

between simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$. It is straightforward to show, with the help of the matrix representation (A.8), that matrix elements of the commutator (84) are defined on the space $D(\mathbb{R}^{3N})$ of infinitely differentiable functions on $\mathbb{R}^{3N}$ with compact support. This is obtained in the representation in the basis $|\mathbf{p}_1, \ldots, \mathbf{p}_N\rangle$. The vector subspace $D(\mathbb{R}^{3N})$ is a dense subspace of the Hilbert space $L^2(\mathbb{R}^{3N})$ of square integrable functions on $\mathbb{R}^{3N}$. With the help of the Plancherel theorem for the Fourier transform on $L^2(\mathbb{R}^{3N})$ ([4, Theorem IX.6]), similar conclusion is inferred also for a dense subspace of the Hilbert space $L^2(\mathbb{R}^{3N})$ obtained by Fourier transforms in the representation in basis $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$.

From the relations (77) and (78) it follows that the limit $a \to 0$ of the matrix element of the commutator $[G, \phi_a(\mathbf{P}, \mathbf{K})]$ in (74) is the same if the projection operator $\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}$ is inserted between the operators G and $\phi_a(\mathbf{P}, \mathbf{K})$. From the relation (79), with the help of relation (63), one then obtains

$$\langle n|G\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}\delta^3(\mathbf{P}, \mathbf{K})|m\rangle - \langle n|\delta^3(\mathbf{P}, \mathbf{K})\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}G|m\rangle = 0. \tag{85}$$

Matrix elements of the commutator (84) between all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$ are defined and are equal to zero. Since they are equivalent to relation (85) each term in the relation (85) is finite. From relations (67), (68), (69) and (70) follows that the matrix elements $\langle n|\delta^3(\mathbf{P}, \mathbf{K})|m\rangle$ between simultaneous eigenvectors (23) of the set of commuting operators $\{H,\ \mathbf{J}^2,\ J_z,\ \{\Omega^\alpha\}\}$ are unbounded if $\mathbf{K} = 0$. As stated in relation (71), operator $\delta^3(\mathbf{P}, \mathbf{K} = 0)$ is not defined on the subspace $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$ of the Hilbert space.

The requirement that the matrix elements in relation (85) are finite for all $|n\rangle$ and $|m\rangle$, and for all $\mathbf{K}$ where $\mathbf{K} \in \mathbb{R}^3$, must be satisfied if the relation (85) is valid. The only vector in $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$ which is orthogonal to all vectors in $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$ is the zero vector. Any linear operator acting upon a zero vector in some vector space maps it into a zero vector. Therefore, the only remaining possibility is that $\delta^3(\mathbf{P}, \mathbf{K})$ acts upon the zero vector in each term in the relation (85). The matrix elements in the relation (85) are finite if and only if

$$\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}G|n\rangle = 0, \tag{86}$$

for all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$.

Projection operator $\mathcal{P}_{\mathcal{D}(H,J^2,J_z,\{\Omega^\alpha\})}$ is a bounded hermitian operator which maps every state vector onto its orthogonal projection in the subspace $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$. From relation (86) follows immediately that the matrix elements of operator G taken between all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$ are equal to zero,

$$\langle n|G|m\rangle = 0, \qquad \forall|n\rangle, \forall|m\rangle \in \{|n\rangle\} \subset \mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\}). \tag{87}$$

By applying the relation (86), or the relation (87), the final result is obtained that the matrix elements of the commutator $[G, H]$, taken between all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$ are equal to zero

$$\langle n|[G, H]|m\rangle = 0, \qquad \forall|n\rangle, \forall|m\rangle \in \{|n\rangle\} \subset \mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\}). \tag{88}$$

At the end of section the result is summarized in the following theorem:

Theorem 1 *Suppose that commutators of the Hamiltonian H with the generators of translations and rotations, operators of total momentum $\mathbf{P}$ and total angular momentum $\mathbf{J}$, are equal to zero. Additional self-adjoint operators that commute with H may also exist. Suppose that the additional self-adjoint operators which commute with H, $\mathbf{J}^2$, J_z and among themselves, and hence are members of the set of commuting operators containing H, $\mathbf{J}^2$ and J_z, commute also with the generator of dilations G. These additional operators Ω^α form the set $\{\Omega^\alpha\}$. Normalized simultaneous eigenvectors of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$ which belong to the Hilbert space form an orthonormal basis in the subspace $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$. Suppose that operator G and all operators $P_iP_j \cdots P_n$, formed by the components P_i of the vector operator $\mathbf{P}$, where $i, j, \ldots, n = 1, 2, 3$, are defined on $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$. Then the matrix elements of the commutator of the Hamiltonian H with the generator of dilations G are equal to zero on the subspace $\mathcal{D}(H, \mathbf{J}^2, J_z, \{\Omega^\alpha\})$ of the Hilbert space.*

IV. DILATIONS

Another approach to quantum mechanical virial theorem is based on scale transformation properties of the Hamiltonian. In this approach the fact that operator G is a generator of dilations is introduced. Dilations are scaling transformations given by operators

$$D \equiv U(s) = \exp\left(\frac{i}{\hbar} sG\right), \qquad s \in \mathbb{R}, \tag{89}$$

which form a continuous one-parameter unitary group, called the dilation group. Generator of the dilation group, operator G, is given for a system of N particles in Eq. (13). The commutator (29) of operator G with an analytic function $f(\mathbf{p})$, $\mathbf{p}$ denoting the set of N momentum operators $(\mathbf{p}_1, \ldots, \mathbf{p}_N)$, was used in the proof of the theorem in Section III. It is derived here using canonical commutation relations.

The canonical commutation relations between the operators corresponding to $3N$ Cartesian coordinates $\{x_k\} \equiv (x_1, y_1, z_1, \ldots, x_N, y_N, z_N)$ and their $3N$ conjugate momenta $\{p_k\} \equiv (p_{1x}, p_{1y}, p_{1z}, \ldots, p_{Nx}, p_{Ny}, p_{Nz})$ are summarized here:

$$[x_k, x_l] = 0, \qquad [p_k, p_l] = 0, \qquad [x_k, p_l] = i\hbar\delta_{kl}, \tag{90}$$

With the help of canonical commutation relations (90), the following relations are obtained for analytic functions $f(\mathbf{r})$ and $f(\mathbf{p})$,

$$[\mathbf{p}, f(\mathbf{r})] = -i\hbar\frac{\partial f(\mathbf{r})}{\partial \mathbf{r}}, \tag{91}$$

and

$$[\mathbf{r}, f(\mathbf{p})] = i\hbar\frac{\partial f(\mathbf{p})}{\partial \mathbf{p}}. \tag{92}$$

In relations (91) and (92) $\mathbf{r}$ denotes the set of N position operators $(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ and $\mathbf{p}$ denotes the set of N momentum operators $(\mathbf{p}_1, \ldots, \mathbf{p}_N)$. Notation for $\frac{\partial}{\partial \mathbf{r}_i}$ and $\frac{\partial}{\partial \mathbf{p}_i}$ are $\frac{\partial}{\partial \mathbf{r}}$ and $\frac{\partial}{\partial \mathbf{p}}$ respectively. With the help of commutators (91) and (92), one easily obtains that the commutators of the generator of dilations, operator G, with analytic functions $f(\mathbf{r})$ and $f(\mathbf{p})$ are equal to

$$[G, f(\mathbf{r})] = -i\hbar\mathbf{r} \cdot \frac{\partial f(\mathbf{r})}{\partial \mathbf{r}}, \tag{93}$$

$$[G, f(\mathbf{p})] = i\hbar\mathbf{p} \cdot \frac{\partial f(\mathbf{p})}{\partial \mathbf{p}}. \tag{94}$$

In relations (93) and (94), $\mathbf{r}\cdot\frac{\partial}{\partial \mathbf{r}}$ and $\mathbf{p}\cdot\frac{\partial}{\partial \mathbf{p}}$ denote directional derivatives $\sum_{i=1}^{N} \mathbf{r}_i\cdot\frac{\partial}{\partial \mathbf{r}_i}$ and $\sum_{i=1}^{N} \mathbf{p}_i\cdot\frac{\partial}{\partial \mathbf{p}_i}$ respectively.

It is straightforward to show, with the help of commutators (93) and (94), that the dilation operators in (89) are transformations which are scalings of position operators $\mathbf{r}$ and inverse scalings of momentum operators $\mathbf{p}$,

$$D\mathbf{r}D^{-1} = \lambda\mathbf{r},$$

$$D\mathbf{p}D^{-1} = \frac{1}{\lambda}\mathbf{p}. \tag{95}$$

The scale parameter λ is equal to $\lambda = \mathrm{e}^s$. If the dilation operator D acts on analytic functions $f(\mathbf{r})$ and $f(\mathbf{p})$, the result is given by

$$Df(\mathbf{r})D^{-1} = \exp\left(s\mathbf{r}\cdot\frac{\partial}{\partial\mathbf{r}}\right)f(\mathbf{r}) = f(\lambda\mathbf{r}),$$

$$Df(\mathbf{p})D^{-1} = \exp\left(-s\mathbf{p}\cdot\frac{\partial}{\partial\mathbf{p}}\right)f(\mathbf{p}) = f(\frac{1}{\lambda}\mathbf{p}). \tag{96}$$

Relations (96) are useful when considering scale transformation properties of the Hamiltonian.

For simplicity of presentation, dilations are considered here only for Hamiltonians that have the form

$$H(\mathbf{p},\mathbf{r}) = T(\mathbf{p}) + V(\mathbf{r}) + K, \tag{97}$$

where $T(\mathbf{p})$ is the kinetic energy operator, $V(\mathbf{r})$ is the potential energy operator and K is the constant term which is neither $\mathbf{r}$ nor $\mathbf{p}$ dependent. As before, $\mathbf{r}$ denotes the set of N position operators $(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ and $\mathbf{p}$ denotes the set of N momentum operators $(\mathbf{p}_1,\ldots,\mathbf{p}_N)$. Detailed discussion of virial theorem and dilations for Hamiltonians of the form (97) is found in [1]. The commutator of the Hamiltonian (97) with the generator of dilations, operator G, is obtained with the help of commutators (93) and (94),

$$[G,H(\mathbf{p},\mathbf{r})] = i\hbar\left(\mathbf{p}\cdot\frac{\partial T(\mathbf{p})}{\partial\mathbf{p}} - \mathbf{r}\cdot\frac{\partial V(\mathbf{r})}{\partial\mathbf{r}}\right). \tag{98}$$

The dilated Hamiltonian is obtained with the help of relations (96) applied on the Hamiltonian (97),

$$DH(\mathbf{p},\mathbf{r})D^{-1} = T(\frac{1}{\lambda}\mathbf{p}) + V(\lambda\mathbf{r}) + K = H(\frac{1}{\lambda}\mathbf{p},\lambda\mathbf{r}). \tag{99}$$

The theorem in Section III is applicable to a particular class of quantum mechanical systems invariant to translations and rotations. If the theorem applies to a specific system, it follows that the expectation values of the commutator $[G,H]$ are equal to zero for all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\,\mathbf{J}^2,\,J_z,\,\{\Omega^\alpha\}\}$. If in addition, the Hamiltonian H has the form (97), from relation (98) it follows:

$$\langle n|\mathbf{p}\cdot\frac{\partial T(\mathbf{p})}{\partial\mathbf{p}}|n\rangle = \langle n|\mathbf{r}\cdot\frac{\partial V(\mathbf{r})}{\partial\mathbf{r}}|n\rangle, \qquad \forall|n\rangle\in\{|n\rangle\}\subset\mathcal{D}(H,\mathbf{J}^2,J_z,\{\Omega^\alpha\}). \tag{100}$$

It is implicitly assumed in relation (100) that the matrix elements of operators $\mathbf{p}\cdot\frac{\partial T(\mathbf{p})}{\partial\mathbf{p}}$ and $\mathbf{r}\cdot\frac{\partial V(\mathbf{r})}{\partial\mathbf{r}}$ are defined on $\mathcal{D}(H,\mathbf{J}^2,J_z,\{\Omega^\alpha\})$. Notation $\mathbf{r}\cdot\frac{\partial}{\partial\mathbf{r}}$ and $\mathbf{p}\cdot\frac{\partial}{\partial\mathbf{p}}$ stands for directional derivatives $\sum_{i=1}^N\mathbf{r}_i\cdot\frac{\partial}{\partial\mathbf{r}_i}$ and $\sum_{i=1}^N\mathbf{p}_i\cdot\frac{\partial}{\partial\mathbf{p}_i}$ respectively.

Relation (100) is recognized as the quantum mechanical virial theorem derived in Section II in analogy with the classical derivation. But for specific systems on which the theorem in Section III applies, and with the Hamiltonian of the form (97), the theorem is a much stronger statement than just Equation (100). From relation (88) for all simultaneous eigenvectors (23) of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$, and from relation (98), it then follows

$$\langle n|\mathbf{p}\cdot\frac{\partial T(\mathbf{p})}{\partial\mathbf{p}}|m\rangle = \langle n|\mathbf{r}\cdot\frac{\partial V(\mathbf{r})}{\partial\mathbf{r}}|m\rangle, \qquad \forall|n\rangle,\forall|m\rangle \in \{|n\rangle\} \subset \mathcal{D}(H,\mathbf{J}^2,J_z,\{\Omega^\alpha\}). \tag{101}$$

Relation (101) is a generalization of relation (100), on the subspace $\mathcal{D}(H,\mathbf{J}^2,J_z,\{\Omega^\alpha\})$ of the Hilbert space.

V. SUMMARY AND PERSPECTIVES

This work is a generalization based on previously known facts on virial theorems in the nonrelativistic and relativistic quantum mechanics. It is demonstrated that this is attainable if certain requirements on symmetry properties of the Hamiltonian are made. The requirements are the conditions of the theorem in Section III. It is shown that if the conditions of translational and rotational symmetry of the Hamiltonian together with the additional conditions of the theorem in Sec. III are satisfied, the matrix elements of the commutator $[G,H]$ are equal to zero on the subspace $\mathcal{D}(H,\mathbf{J}^2,J_z,\{\Omega^\alpha\})$ of the Hilbert space. Normalized simultaneous eigenvectors of the set of commuting operators $\{H,\, \mathbf{J}^2,\, J_z,\, \{\Omega^\alpha\}\}$ which belong to the Hilbert space form an orthonormal basis in the subspace $\mathcal{D}(H,\mathbf{J}^2,J_z,\{\Omega^\alpha\})$.

The well known fact that operator G is a generator of dilations, i.e. scaling transformations of the position operators and inverse scalings of the momentum operators, is introduced in Section IV. This approach is a basis for modern derivations of quantum mechanical virial theorems. In Section IV a relation between directional derivatives of the kinetic and potential energy is derived for systems on which the theorem in Section III applies, and with the Hamiltonian in the form (97). For simplicity of presentation, more detailed forms of the Hamiltonian are not discussed here. Considering the complexity of N-body problems, it is author's expectation that further work on finding systems with the required properties will give more detailed answers.

Quantum mechanical virial theorem has proved important in many different areas. For example, the description of hadrons consisting of light quarks by two seemingly different approaches, in terms of the nonrelativistic Schrödinger formalism and by a semirelativistic Hamiltonian incorporating relativistic kinematics produces comparably good results. The relativistic generalization of the quantum mechanical virial theorem is derived and used to clarify the connection between the nonrelativistic and (semi)relativistic treatment of bound states in [12]. It is concluded in [1] and [7] 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.

Other possibilities lead to reformulation of the virial theorem for quantum systems that are appropriate for a quantum field theoretic treatment. Based on the field theoretical canonical generator for the infinitesimal scale transformation of the second quantized Schrödinger field [13], a rigorous reformulation of the virial theorem for an interacting quantum many-body system with arbitrary spin is presented in [14]. This formulation provides a general procedure applicable in the discussion on the equation of state in the framework of the nonperturbative canonical theory. A gauge invariant canonical generator for the scale transformation of the quantized Schrödinger field is proposed on the basis of the gauge invariance of the virial theorem in [15]. In relativistic field theories scale transformations and virial theorem are more appropriately considered when the space coordinates and time are treated on the same ground. A relation between the trace anomaly of the energy-momentum tensor and the energy of a quantum bound state is obtained in [16]. This anomaly is connected to the scale symmetry breakdown of quantum field theory.

Appendix: Matrix representation of $\delta^3(\mathbf{P},\mathbf{K})$

The limit $a \to 0$ of matrix element (63) of the function $\phi_a(\mathbf{P},\mathbf{K})$ introduced in Eq. (61), is considered here using two different bases. One of them is formed by the simultaneous eigenvectors $|\mathbf{p}_1,\ldots,\mathbf{p}_N\rangle$ of the set of N momentum operators $(\mathbf{p}_1,\ldots,\mathbf{p}_N)$. The eigenvectors $|\mathbf{p}_1,\ldots,\mathbf{p}_N\rangle$ satisfy $3N$ eigenvalue relations

$$p_{il}|\mathbf{p}'_1,\ldots,\mathbf{p}'_N\rangle = p'_{il}|\mathbf{p}'_1,\ldots,\mathbf{p}'_N\rangle, \tag{A.1}$$

where p_{il}, with $l = 1,2,3$, are components of the momentum operator $\mathbf{p}_i$ for the i-th particle. The basis vectors $|\mathbf{p}_1,\ldots,\mathbf{p}_N\rangle$ are also eigenvectors of the total momentum operator $\mathbf{P} = \sum_{i=1}^N \mathbf{p}_i$, satisfying eigenvalue relations

$$P_l|\mathbf{p}'_1,\ldots,\mathbf{p}'_N\rangle = P'_l|\mathbf{p}'_1,\ldots,\mathbf{p}'_N\rangle, \tag{A.2}$$

where P_l, with $l = 1,2,3$, are components of the total momentum operator $\mathbf{P}$.

The eigenvectors $|\mathbf{p}_1,\ldots,\mathbf{p}_N\rangle$ are orthonormal in the sense defined by δ-function normalization of $|\mathbf{p}_1, \ldots, \mathbf{p}_N\rangle$,

$$\langle \mathbf{p}_1, \ldots, \mathbf{p}_N | \mathbf{p}'_1, \ldots, \mathbf{p}'_N \rangle = \prod_{i=1}^{N} \delta^3(\mathbf{p}_i - \mathbf{p}'_i). \tag{A.3}$$

Matrix elements of the function $\phi_a(\mathbf{P}, \mathbf{K})$ between the basis vectors $|\mathbf{p}_1, \ldots, \mathbf{p}_N\rangle$ are obtained using the definition of $\phi_a(\mathbf{P}, \mathbf{K})$ in (61),

$$\langle \mathbf{p}_1, \ldots, \mathbf{p}_N | \phi_a(\mathbf{P}, \mathbf{K}) | \mathbf{p}'_1, \ldots, \mathbf{p}'_N \rangle = \phi_a(\mathbf{P}', \mathbf{K}) \prod_{i=1}^{N} \delta^3(\mathbf{p}_i - \mathbf{p}'_i). \tag{A.4}$$

Evaluating the matrix elements of the function $\phi_a(\mathbf{P}, \mathbf{K})$ between the basis vectors $|\mathbf{p}_1, \ldots, \mathbf{p}_N\rangle$, one obtains the function $\phi_a(\mathbf{P}, \mathbf{K})$ of the total momentum eigenvalue $\mathbf{P} = \sum_{i=1}^{N} \mathbf{p}_i$. In relation (A.4) this is indicated by a prime.

Relation (A.4) is used in evaluating the limit $a \to 0$ of the matrix element of the function $\phi_a(\mathbf{P}, \mathbf{K})$ taken between vectors $|\Psi\rangle$ and $|\Phi\rangle$ in the Hilbert space,

$$\lim_{a \to 0} \langle \Phi | \phi_a(\mathbf{P}, \mathbf{K}) | \Psi \rangle = \lim_{a \to 0} \int \langle \Phi | \mathbf{p} \rangle \phi_a(\mathbf{P}, \mathbf{K}) \langle \mathbf{p} | \Psi \rangle \prod_{i=1}^{N} d^3 p_i. \tag{A.5}$$

In relation (A.5) $|\mathbf{p}\rangle$ is a notation for $|\mathbf{p}_1, \ldots, \mathbf{p}_N\rangle$. The function $\phi_a(\mathbf{P}, \mathbf{K})$ on the right side of relation (A.5) corresponds to the delta distribution $\delta^3(\mathbf{P} - \mathbf{K})$. In accordance with the distributional definition of $\delta^3(\mathbf{x})$, introduced in Section III, relation (A.5) is written in the form

$$\lim_{a \to 0} \langle \Phi | \phi_a(\mathbf{P}, \mathbf{K}) | \Psi \rangle = \int \langle \Phi | \mathbf{p} \rangle \delta^3(\mathbf{P} - \mathbf{K}) \langle \mathbf{p} | \Psi \rangle \prod_{i=1}^{N} d^3 p_i. \tag{A.6}$$

The following notation is introduced:

$$\lim_{a \to 0} \langle \Phi | \phi_a(\mathbf{P}, \mathbf{K}) | \Psi \rangle = \langle \Phi | \delta^3(\mathbf{P}, \mathbf{K}) | \Psi \rangle. \tag{A.7}$$

The limit $a \to 0$ of the matrix elements of the function $\phi_a(\mathbf{P}, \mathbf{K})$ between vectors $|\Psi\rangle$ and $|\Phi\rangle$ in the Hilbert space in relation (A.7) is evaluated in relations (A.5) and (A.6). Furthermore, in the basis $|\mathbf{p}_1, \ldots, \mathbf{p}_N\rangle$ the following notation is introduced:

$$\langle \mathbf{p}_1, \ldots, \mathbf{p}_N | \delta^3(\mathbf{P}, \mathbf{K}) | \mathbf{p}'_1, \ldots, \mathbf{p}'_N \rangle = \delta^3(\mathbf{P}' - \mathbf{K}) \prod_{i=1}^{N} \delta^3(\mathbf{p}_i - \mathbf{p}'_i). \tag{A.8}$$

When it is possible, matrix elements (A.8) are used equivalently with (A.4) when evaluating the limit $a \to 0$ of matrix elements in relation (A.7), as given by relations (A.5) and (A.6).

Evaluation of this limit is possible in another basis formed by the simultaneous eigenvectors $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$ of the set of N position operators $(\mathbf{r}_1, \ldots, \mathbf{r}_N)$. The eigenvectors $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$ satisfy $3N$ eigenvalue relations

$$x_{il} | \mathbf{r}'_1, \ldots, \mathbf{r}'_N \rangle = x'_{il} | \mathbf{r}'_1, \ldots, \mathbf{r}'_N \rangle, \tag{A.9}$$

where x_{il}, with $l = 1, 2, 3$, are components of the position operator $\mathbf{r}_i$ for the i-th particle. The eigenvectors $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$ are orthonormal in the sense defined by δ-function normalization of $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$,

$$\langle \mathbf{r}_1, \ldots, \mathbf{r}_N | \mathbf{r}'_1, \ldots, \mathbf{r}'_N \rangle = \prod_{i=1}^{N} \delta^3(\mathbf{r}_i - \mathbf{r}'_i). \tag{A.10}$$

The basis $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$ and the basis $|\mathbf{p}_1, \ldots, \mathbf{p}_N\rangle$ are related by a unitary transformation

$$|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle = \int |\mathbf{p}_1, \ldots, \mathbf{p}_N\rangle \left(\mathbf{U}\right)_{\mathbf{p},\mathbf{r}} \prod_{i=1}^{N} d^3 p_i. \tag{A.11}$$

Elements of the unitary transformation matrix $\mathbf{U}$ are equal to:

$$\left(\mathbf{U}\right)_{\mathbf{p},\mathbf{r}} = \langle \mathbf{p}_1, \ldots, \mathbf{p}_N | \mathbf{r}_1, \ldots, \mathbf{r}_N \rangle. \tag{A.12}$$

Unitarity of the transformation matrix $\mathbf{U}$ ($\mathbf{U}^\dagger \mathbf{U} = \mathbf{1}$ and $\mathbf{U}\mathbf{U}^\dagger = \mathbf{1}$) follows from the completeness of orthonormal bases $|\mathbf{p}_1, \ldots, \mathbf{p}_N\rangle$ and $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$. The numbers of rows and columns of unitary transformation matrices $\mathbf{U}$ and $\mathbf{U}^\dagger$ are nondenumerably infinite. Each element $\left(\mathbf{U}\right)_{\mathbf{p},\mathbf{r}} = \left(\mathbf{U}^\dagger\right)^*_{\mathbf{r},\mathbf{p}}$ of the matrices is a product of N δ-function normalized plane waves,

$$\left(\mathbf{U}\right)_{\mathbf{p},\mathbf{r}} = \langle \mathbf{p}_1, \ldots, \mathbf{p}_N | \mathbf{r}_1, \ldots, \mathbf{r}_N \rangle = \frac{1}{(2\pi\hbar)^{3N/2}} \prod_{i=1}^{N} e^{-\frac{i}{\hbar}\mathbf{p}_i \cdot \mathbf{r}_i}. \tag{A.13}$$

Finally, with the help of relation (A.11), the matrix (A.4) is transformed to the basis $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$ by a unitary transformation

$$\langle \mathbf{r} | \phi_a(\mathbf{P}, \mathbf{K}) | \mathbf{r}' \rangle = \int \left(\mathbf{U}^\dagger\right)_{\mathbf{r},\mathbf{p}} \langle \mathbf{p} | \phi_a(\mathbf{P}, \mathbf{K}) | \mathbf{p}' \rangle \left(\mathbf{U}\right)_{\mathbf{p}',\mathbf{r}'} \prod_{i=1}^{N} d^3 p_i d^3 p'_i. \tag{A.14}$$

In relation (A.14) $|\mathbf{r}\rangle$ is a notation for $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$ and $|\mathbf{p}\rangle$ is a notation for $|\mathbf{p}_1, \ldots, \mathbf{p}_N\rangle$. With the help of relations (A.4), (A.13) and (A.14) one obtains

$$\langle \mathbf{r} | \phi_a(\mathbf{P}, \mathbf{K}) | \mathbf{r}' \rangle = \frac{1}{(2\pi\hbar)^{3N}} \int \phi_a(\mathbf{P}, \mathbf{K}) \prod_{i=1}^{N} e^{\frac{i}{\hbar}\mathbf{p}_i \cdot \left(\mathbf{r}_i - \mathbf{r}'_i\right)} \prod_{j=1}^{N} d^3 p_j. \tag{A.15}$$

The function $\phi_a(\mathbf{P}, \mathbf{K})$ on the right side of relation (A.15) corresponds to the delta distribution $\delta^3(\mathbf{P} - \mathbf{K})$. The limit $a \to 0$ of relation (A.15) is therefore written in the form

$$\lim_{a \to 0} \langle \mathbf{r} | \phi_a(\mathbf{P}, \mathbf{K}) | \mathbf{r}' \rangle = \frac{1}{(2\pi\hbar)^{3N}} \int \delta^3(\mathbf{P} - \mathbf{K}) \prod_{i=1}^{N} e^{\frac{i}{\hbar}\mathbf{p}_i \cdot \left(\mathbf{r}_i - \mathbf{r}'_i\right)} \prod_{j=1}^{N} d^3 p_j. \tag{A.16}$$

With the help of the rules of δ-calculus and the closure property of δ-function normalized plane waves, one obtains from (A.16) the following relation written in notation (A.7),

$$\langle \mathbf{r} | \delta^3(\mathbf{P}, \mathbf{K}) | \mathbf{r}' \rangle = \frac{1}{(2\pi\hbar)^3} e^{\frac{i}{\hbar}\mathbf{K} \cdot \left(\mathbf{r}_k - \mathbf{r}'_k\right)} \prod_{\substack{i=1 \\ i \neq k}}^{N} \delta^3(\mathbf{r}_i + \mathbf{r}'_k - \mathbf{r}_k - \mathbf{r}'_i). \tag{A.17}$$

Index k in relation (A.17) can be any $k = 1, \ldots, N$. Equivalently, relation (A.17) is obtained directly by transforming the matrix (A.8) to the basis $|\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle$ by the same unitary transformation. Transforming the matrix (A.17) to the basis $|\mathbf{p}_1, \ldots, \mathbf{p}_N\rangle$ by inverse transformation, the matrix (A.8) is again obtained.

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