GENERALIZED VIRIAL THEOREM AND ITS APPLICATION TO THE SALPETER EQUATION

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We derive a generalization of the virial theorem in terms of the canonically conjugate pair of variables. Then, we apply it to the Salpeter equation and to the reductions of the Salpeter equation. It is shown that the linear mass form and the quadratic mass form of the reductions of the Salpeter equation will be the same in the nonrelativistic limit but different in the ultrarelativistic limit. Therefore, different reductions are appropriate for different bound systems.

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1. Introduction

The well-known virial theorem provides us with a very useful tool in studying nonrelativistic quantum-mechanical systems, which relates the kinetic energy of a system to the expectation value of the directional derivative of potential and can allow us to calculate the kinetic energy in complex situations. Many versions of the virial theorem with different forms for both the nonrelativistic and the relativistic systems have come forth [1–15]. In this paper, one generalized virial theorem which comprises some versions of the virial theorem as special cases is presented and then applied to the Salpeter equation and its reductions.

The Bethe–Salpeter equation [16] is the appropriate tool to deal with bound-state problems within the framework of relativistic quantum field theory. However, the Salpeter equation [17], one of the three-dimensional reductions of the Bethe–Salpeter equation, is frequently used in practice due to various practical reasons. Different from the linear mass term in the Salpeter equation, there exists the quadratic mass operator form of the reduction of the Bethe–Salpeter equation [18–20]. The reductions of the

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Salpeter equation also have both linear and quadratic mass form. The former is the familiar spinless Salpeter equation [21], and the latter is the quadratic mass operator equation. In this paper, we apply the generalized virial theorem not only to the Salpeter equation but also to the two kinds of reductions of the Salpeter equation, and show that these two kinds of reductions are the same in the nonrelativistic limit but different in the ultrarelativistic limit.

This paper is organized as follows. In Sec. 2, we derive a general form of the virial theorem, which comprises some versions of the virial theorem as special cases. Then, we apply the obtained generalized virial theorem to the Salpeter equation and the reductions of the Salpeter equation in Sec. 3. The conclusion is in Sec. 4.

2. Generalized virial theorem

Consider a nonrelativistic or relativistic wave equation of the form

$$F(q, p, E)|\psi(q)\rangle = 0, \qquad (1)$$

where q and p are the generalized coordinates and the canonically conjugate momenta, respectively. They satisfy the commutation relation (in natural units $\hbar = c = 1$)

$$[q,p] = qp - pq = i.$$
⁽²⁾

E is the energy of the system, and $|\psi(q)\rangle$ is the normalized eigenfunction. In many cases, the Hamiltonian *H* is shown explicitly in the function *F*, whereas sometimes *H* has no explicit form, for example, in the Klein–Gordon equation case. Generally speaking, $|\psi(q)\rangle$ can be the normalized eigenfunction of any operator *G* with the eigenvalue *g*. Let us assume there is a scale transformation of the variables by some arbitrary scale factor λ ,

$$q = \lambda q', \qquad p = \frac{p'}{\lambda}.$$
 (3)

Equation (3) is also a simple canonical transformation of the canonically conjugate pair of variables which preserves the Dirac bracket

$$\left[q',p'\right] = i\,.\tag{4}$$

Equation (4) assures that the transformed system is also a quantum system related to the system described by Eq. (1). Substituting Eq. (3) into Eq. (1), then differentiating it with respect to λ , and noticing that $\partial E/\partial \lambda = 0$

because E is independent of q and p, which is true whether the considered theory is dilatation invariant or not, we obtain

$$\left\langle \frac{\partial q}{\partial \lambda} \frac{\partial F}{\partial q} + \frac{\partial p}{\partial \lambda} \frac{\partial F}{\partial p} \right\rangle + \left\langle \psi \middle| F \middle| \frac{\partial \psi}{\partial \lambda} \right\rangle + \left\langle \frac{\partial \psi}{\partial \lambda} \middle| F \middle| \psi \right\rangle = 0, \tag{5}$$

where $\langle \cdots \rangle$ denotes the expectation value which is understood to be taken with respect to the normalized eigenstates. Using Eqs. (1), (3) and (5), we have the generalized virial theorem

$$\left\langle q\frac{\partial F}{\partial q}\right\rangle = \left\langle p\frac{\partial F}{\partial p}\right\rangle - \left\langle \psi \middle| F \middle| q\frac{\partial \psi}{\partial q}\right\rangle.$$
(6)

Let us assume that the operator function F is defined over a domain D(F). ψ necessarily belongs to D(F). If $q(\partial \psi/\partial q)$ also belongs to D(F), that is, if the operator function F has the property [1–3] that

$$\left\langle \psi \middle| F \middle| q \frac{\partial \psi}{\partial q} \right\rangle = \left\langle F \psi \middle| q \frac{\partial \psi}{\partial q} \right\rangle = 0, \qquad (7)$$

we can immediately obtain from Eq. (6)

$$\left\langle q\frac{\partial F}{\partial q}\right\rangle = \left\langle p\frac{\partial F}{\partial p}\right\rangle.$$
(8)

Equation (6) is the general form of the generalized virial theorem, while Eq. (8) is the special form. The second term on the right-hand side in Eq. (6) is an additional contribution to Eq. (8) due to $q(\partial \psi/\partial q) \notin D(F)$.

The generalized virial theorems (6) and (8) are expected to be more general than many versions of the virial theorem. The generalized virial theorem can be applicable not only to the nonrelativistic case [4] but also to the relativistic case [1, 5–11], and not only to F with explicit form of the Hamiltonian H as variable [1, 4–9] but also to F with implicit form of H[10, 11]. To our knowledge, there is not any study on it in the literature, although it is inspired from and related to ideas in papers by Lichtenberg [1] and by Papp [10].

If q is chosen as the radial coordinate r, Eq. (8) becomes

$$\left\langle r\frac{\partial F}{\partial r}\right\rangle = \left\langle p_r\frac{\partial F}{\partial p_r}\right\rangle \,,\tag{9}$$

where $p_r = -i \left(\partial / \partial r + 1 / r \right)$. As expressed in coordinates \boldsymbol{x} and momenta \boldsymbol{p} , Eq. (8) becomes

$$\left\langle \boldsymbol{x} \cdot \frac{\partial F}{\partial \boldsymbol{x}} \right\rangle = \left\langle \boldsymbol{p} \cdot \frac{\partial F}{\partial \boldsymbol{p}} \right\rangle,$$
 (10)

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which is obtained in Ref. [12] by means of the generalized Feynman–Hellmann theorem [1]. Using Eqs. (6), (7) and (8), it is found that Eq. (10) also holds in one or two directions

$$\left\langle x_{i}\frac{\partial F}{\partial x_{i}}\right\rangle = \left\langle p_{i}\frac{\partial F}{\partial p_{i}}\right\rangle,$$
$$\left\langle x_{i}\frac{\partial F}{\partial x_{i}} + x_{j}\frac{\partial F}{\partial x_{j}}\right\rangle = \left\langle p_{i}\frac{\partial F}{\partial p_{i}} + p_{j}\frac{\partial F}{\partial p_{j}}\right\rangle,$$
$$x_{i}, x_{j} = x, y, z, \qquad p_{i}, p_{j} = p_{x}, p_{y}, p_{z}.$$
(11)

Equations (9) and (11) are not obvious or cannot be obtained by applying the approach adopted in Ref. [12], while they are the direct results of Eq. (8) in this paper although Eq. (10) can be derived both in Ref. [12] and in this paper.

In the nonrelativistic case, F will be of the form of

$$F = H - \epsilon = \frac{\mathbf{p}^2}{2\mu} + V - \epsilon \,, \tag{12}$$

where ϵ is the binding energy and μ is the reduced mass. Employing Eq. (10) reproduces the well-known virial theorem

$$\langle T \rangle = \left\langle \frac{\boldsymbol{p}^2}{2\mu} \right\rangle = \frac{1}{2} \langle \boldsymbol{x} \cdot \boldsymbol{\nabla} V \rangle \,.$$
 (13)

Then, from Eqs. (12) and (13), it is found that

$$\epsilon = \langle T \rangle + \langle V \rangle = \frac{1}{2} \langle \boldsymbol{x} \cdot \boldsymbol{\nabla} V \rangle + \langle V \rangle .$$
(14)

The particular forms of the virial theorem for the spinless Salpeter equation, the Dirac equation and the Klein–Gordon equation can be obtained by employing Eq. (10), which are consistent with Refs. [1, 6-12].

3. Application of the generalized virial theorem

Now, we apply the generalized virial theorem to the Salpeter equation. For simplicity, we consider the Salpeter equation [17, 22] for the bound states composed of two scalar constituents assumed to interact through a massless scalar field which has an especially simple form. In the center-of-momentum frame of the bound state, the Salpeter equation reads [17, 22, 23]

$$\left[M^2 - (\omega_1 + \omega_2)^2\right] \Psi(\boldsymbol{p}) = \frac{\omega_1 + \omega_2}{2\omega_1\omega_2} \eta(\boldsymbol{p}), \qquad (15)$$

where M is the bound-state mass, $\omega_i = \sqrt{\mathbf{p}^2 + m_i^2}$,

$$\eta(\boldsymbol{p}) = \int \frac{d^3 \boldsymbol{p}'}{(2\pi)^3} V(\boldsymbol{p}, \boldsymbol{p}') \Psi(\boldsymbol{p}') \,. \tag{16}$$

Taking a Fourier transformation, the Salpeter equation (15) can be written as

$$\left[M^2 - (\omega_1 + \omega_2)^2 - \mathcal{V}\right]\psi(\boldsymbol{x}) = 0, \qquad (17)$$

where $\psi(\boldsymbol{x})$ is the Fourier transform of $\Psi(\boldsymbol{p})$, ω_i is the nonlocal operator $\sqrt{-\boldsymbol{\nabla}^2 + m_i^2}$ obtained as the formal Fourier transform of ω_i , and $\mathcal{V}(\boldsymbol{x})$ is the Fourier transform of $(\omega_1 + \omega_2)/(2\omega_1\omega_2)V(\boldsymbol{p}, \boldsymbol{p}')$, which is taken as an effective potential [23, 24]. In this case, function F takes the form

$$F = (\omega_1 + \omega_2)^2 + \mathcal{V} - M^2 \,. \tag{18}$$

Applying Eq. (10) to (18), we obtain

$$\langle \boldsymbol{x} \cdot \boldsymbol{\nabla} \mathcal{V} \rangle = \left\langle \frac{(\omega_1 + \omega_2)^2}{\omega_1 \omega_2} 2\left(-\boldsymbol{\nabla}^2\right) \right\rangle .$$
 (19)

This is the virial theorem for the Salpeter equation for the bound state with two scalar constituents. In the nonrelativistic case, Eq. (19) reduces to

$$\langle \boldsymbol{x} \cdot \boldsymbol{\nabla} \mathcal{V} \rangle = \left\langle \frac{(m_1 + m_2)^2}{m_1 m_2} 2\left(-\boldsymbol{\nabla}^2\right) \right\rangle.$$
 (20)

In the nonrelativistic limit, the factor $(\omega_1 + \omega_2)/(2\omega_1\omega_2)$ in \mathcal{V} reduces to $(m_1 + m_2)/(2m_1m_2)$. The denominator $2m_1m_2$ is part of the coupling constant $\lambda = g_1g_2/(4m_1m_2)$. $m_1m_2/(m_1+m_2)$ in Eq. (20) is the reduced mass. Therefore, Eq. (20) is, in fact, the nonrelativistic virial theorem.

It is straightforward to obtain the mass of the bound state from Eq. (18)

$$M^{2} = \left\langle (\omega_{1} + \omega_{2})^{2} \right\rangle + \left\langle \mathcal{V} \right\rangle.$$
(21)

In the nonrelativistic limit, Eq. (21) reduces to

$$M^{2} = (m_{1} + m_{2})^{2} + \frac{(m_{1} + m_{2})^{2}}{m_{1}m_{2}} \langle \boldsymbol{p}^{2} \rangle + \langle \mathcal{V} \rangle.$$
(22)

Letting $M = m_1 + m_2 + \epsilon$, where ϵ is the binding energy, neglecting the higher order term ϵ^2 , we obtain from Eq. (22)

$$\epsilon = \frac{1}{2} \left\langle \boldsymbol{x} \cdot \boldsymbol{\nabla} \mathcal{V}' \right\rangle + \left\langle \mathcal{V}' \right\rangle, \tag{23}$$

where $\mathcal{V}' = \mathcal{V}/[2(m_1 + m_2)]$. From the definitions of \mathcal{V} and \mathcal{V}' , one can find easily that Eq. (23) gives the binding energy of the nonrelativistic binding system, see Eq. (14).

In the following part, we use the generalized virial theorem to discuss the semirelativistic reduction of the Salpeter equation and take the fermion– antifermion system as an example. In the center-of-momentum frame of the bound state, the Salpeter equation for a fermion–antifermion system reads [17, 22, 23]

$$\Psi(\boldsymbol{p}) = \frac{\Lambda_1^+(\boldsymbol{p})\gamma^0\eta(\boldsymbol{p})\gamma^0\Lambda_2^-(-\boldsymbol{p})}{M-\omega_1-\omega_2} - \frac{\Lambda_1^-(\boldsymbol{p})\gamma^0\eta(\boldsymbol{p})\gamma^0\Lambda_2^+(-\boldsymbol{p})}{M+\omega_1+\omega_2}, \qquad (24)$$

where

$$\eta(\mathbf{p}) = \int \frac{d^3 \mathbf{p}'}{(2\pi)^3} V(\mathbf{p}, \mathbf{p}') \psi(\mathbf{p}') \,. \tag{25}$$

The generalized virial theorem can be applied easily to the Salpeter equation for the fermion–antifermion system if Eq. (24) is rewritten in another form, see Eqs. (10)–(93) in Ref. [22], and we will not give it in this paper.

Assuming that

$$M - \omega_1 - \omega_2 \ll M + \omega_1 + \omega_2 \tag{26}$$

holds [21], which may be justified for semirelativistic and weakly-bound heavy constituents, we argue that by neglecting the small term and then neglecting all the spin degrees of freedom of constituents, one can obtain two (semi-)relativistic equations. One is the spinless Salpeter equation [21] which is familiar to us

$$(M - \omega_1 - \omega_2 - V_1) \psi(\mathbf{x}) = 0, \qquad (27)$$

where V_1 arises as the Fourier transform of $V(\boldsymbol{p}, \boldsymbol{p}')$. Another form of the reduction of the Salpeter equation (24) reads

$$[M^{2} - (\omega_{1} + \omega_{2})^{2} - V_{2}] \psi(\boldsymbol{x}) = 0, \qquad (28)$$

where $V_2 = 2(m_1 + m_2)V_1$ in the nonrelativistic limit. Equation (28) is a quadratic mass operator equation just like Eq. (17), which was also obtained in Ref. [19] from the first principle.

In the case of Eq. (27), function F reads

$$F = \omega_1 + \omega_2 + V_1 - M \,. \tag{29}$$

Applying Eq. (10) to (29), we obtain

$$\langle \boldsymbol{x} \cdot \boldsymbol{\nabla} V_1 \rangle = \left\langle \frac{\omega_1 + \omega_2}{\omega_1 \omega_2} \left(-\boldsymbol{\nabla}^2 \right) \right\rangle,$$
 (30)

which is derived in Ref. [9] by means of the dilatation operator method. In the nonrelativistic case, the virial theorem (30) reduces to the familiar form

$$\langle \boldsymbol{x} \cdot \boldsymbol{\nabla} V_1 \rangle = \left\langle \frac{m_1 + m_2}{m_1 m_2} \left(-\boldsymbol{\nabla}^2 \right) \right\rangle.$$
 (31)

It is straightforward to obtain from Eq. (29) the mass of the bound state

$$M = \langle \omega_1 + \omega_2 \rangle + \langle V_1 \rangle \,. \tag{32}$$

In the nonrelativistic case, Eq. (32) becomes

$$M = m_1 + m_2 + \frac{1}{2} \left\langle \boldsymbol{x} \cdot \boldsymbol{\nabla} V_1 \right\rangle + \left\langle V_1 \right\rangle.$$
(33)

Letting $M = m_1 + m_2 + \epsilon$, where ϵ is the binding energy, we have

$$\epsilon = \frac{1}{2} \left\langle \boldsymbol{x} \cdot \boldsymbol{\nabla} V_1 \right\rangle + \left\langle V_1 \right\rangle. \tag{34}$$

Similarly, we have for Eq. (28)

$$\langle \boldsymbol{x} \cdot \boldsymbol{\nabla} V_2 \rangle = \left\langle \frac{(\omega_1 + \omega_2)^2}{\omega_1 \omega_2} 2\left(-\boldsymbol{\nabla}^2\right) \right\rangle,$$
 (35)

$$M^{2} = \left\langle (\omega_{1} + \omega_{2})^{2} \right\rangle + \left\langle V_{2} \right\rangle.$$
(36)

In the nonrelativistic limit, Eqs. (35) and (36) reduce to

$$\langle \boldsymbol{x} \cdot \boldsymbol{\nabla} V_2 \rangle = \left\langle \frac{(m_1 + m_2)^2}{m_1 m_2} 2\left(-\boldsymbol{\nabla}^2\right) \right\rangle,$$
 (37)

$$\epsilon = \frac{1}{2} \left\langle \boldsymbol{x} \cdot \boldsymbol{\nabla} V_2' \right\rangle + \left\langle V_2' \right\rangle \,, \tag{38}$$

where $V'_2 = V_2 / [2(m_1 + m_2)]$.

Equations (31), (34), (37), (38) and the definitions of V_1 and V_2 suggest that Eqs. (27) and (28) are equivalent in the nonrelativistic limit. From the derivations of Eq. (27), it is clear and evident that Eq. (27) is a semirelativistic equation, although in Refs. [9, 21], Eq. (27) is applied not only to the nonrelativistic case but also to the relativistic case, even to the ultrarelativistic case. To discriminate between these two equations, we discuss them in the ultrarelativistic limit. In the ultrarelativistic case $|\mathbf{p}| \gg m_1, m_2$, using Eq. (30), Eq. (32) reduces to

$$M = \langle \boldsymbol{x} \cdot \boldsymbol{\nabla} V_1 \rangle + \langle V_1 \rangle, \qquad (39)$$

and using Eq. (35), Eq. (36) reduces to

$$M^{2} = \frac{1}{2} \left\langle \boldsymbol{x} \cdot \boldsymbol{\nabla} V_{2} \right\rangle + \left\langle V_{2} \right\rangle.$$
(40)

When the potential is of the form of r^n , the difference between Eqs. (40) and (39) will be clear and evident. Even after the factors in V_1 and V_2 are considered, Eqs. (27) and (28) are still different. This suggests that although they are equivalent in the nonrelativistic limit, Eqs. (27) and (28) will be different in the ultrarelativistic limit and expected to be also different in the relativistic case.

In Refs. [19, 20], the numerical results are given for the linear mass operator and the quadratic mass operator. The results show that for the heavy-heavy quarkonium, the difference between the linear mass operator and the quadratic mass operator will be very small and can be neglected because the heavy-heavy quarkonium can be regarded as one nonrelativistic system, while for the heavy-light and light-light quarkonia, the difference will be significant due to the relativistic motion of the light quark. Our results are consistent with the numerical results in Refs. [19, 20]. Therefore, Eq. (28) will be better than Eq. (27) when the heavy-light and light-light quarkonia are considered.

Moreover, it can be seen easily from Eqs. (30) and (35) that the ratio of the expectation value of the kinetic energy to the expectation value of potential varies with the ratio of the masses of the components. When two constituents are equally massive, the ratio reaches its minimum. In contrast to the relativistic case, the ratio will be constant and independent of the masses of components in the nonrelativistic limit, n/2 for power-law potential r^n .

4. Conclusion

In this paper, we have derived the generalized virial theorem which will be more general than many previous versions of the virial theorem. Then, we apply the generalized virial theorem to the Salpeter equation for the bound state composed of two scalar constituents and to the reductions of the Salpeter equation for the fermion–antifermion system. The results show that the linear mass form and the quadratic mass form of the reductions of the Salpeter equation will be the same in the nonrelativistic limit, but different in the ultrarelativistic limit. Therefore, one should be cautious of applying the different versions of the reductions of the Salpeter equation in practice. This work was supported by the Natural Science Foundation of Shanxi Province of China under Grant No. 2013011008.

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