

Spin virial theorem in the time-dependent density-functional theory

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The spin virial theorem is derived in the time-dependent density-functional theory. It establishes a relationship between the differences of kinetic and potential energies and the currents. It provides a way of checking accuracy of approximations.

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I. INTRODUCTION

Exact relations and theorems play a very important role in the density-functional theory [1,2] as they proved to be useful in improving the accuracy of approximate energy functionals. Recently, the time-dependent density-functional theory [3,4] has become a very active research area and a couple of papers have already addressed the problem of deriving new exact theorems in the time-dependent theory. For example, the time-dependent virial theorem [5–7] and hierarchy of equations [8] have been presented.

In this paper the spin virial theorem is generalized to time-dependent systems. The time-independent version was derived several years ago [9]. In the following section the theorem is derived in the Kohn-Sham system. Section III presents the theorem in the real system. The form of the theorem valid in the presence of time-dependent magnetic field is discussed in Sec. IV.

II. DERIVATION IN THE KOHN-SHAM SYSTEM

The time derivative of an operator \hat{A} is given by

$$\frac{d}{dt}\langle\hat{A}\rangle=\left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle+i\langle[\hat{H},\hat{A}]\rangle. \quad (1)$$

Let \hat{H} be the Kohn-Sham one-electron Hamiltonian \hat{h}_{KS} , $\hat{A} = \frac{1}{2}(\mathbf{r}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{r})$ and the average is done with the Kohn-Sham spin orbital $u_{k\sigma}$,

$$\frac{1}{2}\frac{d}{dt}\langle(\mathbf{r}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{r})\rangle_{k\sigma} = 2T_{k\sigma}^s - \langle\mathbf{r}\cdot\nabla v_{s\sigma}\rangle_{k\sigma}, \quad (2)$$

where

$$T_{k\sigma}^s = -\frac{1}{2}\int u_{k\sigma}^*\nabla^2 u_{k\sigma} \quad (3)$$

is the noninteracting kinetic energy for the spin orbital $u_{k\sigma}$. $v_{s\sigma}$ is the Kohn-Sham potential for spin σ . Taking into account the definition of the current density corresponding to the spin orbital $u_{k\sigma}$ (in atomic units),

$$\mathbf{j}_{k\sigma} = \frac{1}{2i}(u_{k\sigma}^*\nabla u_{k\sigma} - u_{k\sigma}\nabla u_{k\sigma}^*), \quad (4)$$

we can immediately notice that

$$\frac{1}{2}\frac{d}{dt}\langle(\mathbf{r}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{r})\rangle_{k\sigma} = \frac{d}{dt}\langle\mathbf{r}\cdot\mathbf{j}_s\rangle_{k\sigma}. \quad (5)$$

From Eqs. (2) and (5) we are led to the virial theorem corresponding to the spin orbital $u_{k\sigma}$:

$$\frac{d}{dt}\langle\mathbf{r}\cdot\mathbf{j}_s\rangle_{k\sigma} = 2T_{k\sigma}^s - \langle\mathbf{r}\cdot\nabla v_{s\sigma}\rangle_{k\sigma}. \quad (6)$$

A summation for the orbitals with the same spin results in

$$\frac{d}{dt}\langle\mathbf{r}\cdot\mathbf{j}_s\rangle_{\sigma} = 2T_{\sigma}^s - \langle\mathbf{r}\cdot\nabla v_{s\sigma}\rangle_{\sigma}. \quad (7)$$

Adding Eq. (7) for spin up and down we obtain the customary virial theorem

$$\frac{d}{dt}\langle\mathbf{r}\cdot\mathbf{j}_s\rangle = 2T^s - \sum_{\sigma}\langle\mathbf{r}\cdot\nabla v_{s\sigma}\rangle_{\sigma}. \quad (8)$$

The difference for spin up and down yields the spin virial theorem

$$\frac{d}{dt}\langle\mathbf{r}\cdot(\mathbf{j}_{s\uparrow} - \mathbf{j}_{s\downarrow})\rangle = 2(T_{\uparrow}^s - T_{\downarrow}^s) - \langle\mathbf{r}\cdot\nabla v_{s\uparrow}\rangle + \langle\mathbf{r}\cdot\nabla v_{s\downarrow}\rangle. \quad (9)$$

For the time-independent case the left-hand side of Eq. (9) is zero and the time-independent form of the spin virial theorem results in Ref. [10].

Another form of the spin virial theorem can be obtained by substituting the Kohn-Sham potential

$$v_{s\sigma} = v_{\sigma} + v_J + v_{xc\sigma} \quad (10)$$

into Eq. (9), where v_{σ} is the time-dependent external potential, $v_{xc\sigma}$ is the exchange-correlation potential, and

$$v_J(\mathbf{r},t) = \int \frac{\varrho(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' \quad (11)$$

is the classical Coulomb potential. Then the spin virial theorem takes the form

$$\frac{d}{dt}\langle\mathbf{r}\cdot\Delta\mathbf{j}_s\rangle = 2\Delta T^s + \Delta V, \quad (12)$$

where

$$\Delta T_s = T_s^\uparrow - T_s^\downarrow \quad (13)$$

and

$$\Delta V = V_\uparrow - V_\downarrow = \Delta w + \Delta y + q_{\uparrow\downarrow} + \Delta x. \quad (14)$$

The first term in the right-hand side of Eq. (14) comes from the virial of the external potential

$$\Delta w = w_\uparrow - w_\downarrow, \quad (15)$$

$$w_\sigma = -\langle \mathbf{r} \cdot \nabla v_\sigma \rangle_\sigma. \quad (16)$$

The second term gives the difference of the electron-electron repulsion energies of electrons with spin up and down:

$$\Delta y = y_{\uparrow\uparrow} - y_{\downarrow\downarrow}, \quad (17)$$

$$y_{\uparrow\uparrow} = \frac{1}{2} \int \frac{\varrho_\uparrow(\mathbf{r}_1)\varrho_\uparrow(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2, \quad (18)$$

$$y_{\downarrow\downarrow} = \frac{1}{2} \int \frac{\varrho_\downarrow(\mathbf{r}_1)\varrho_\downarrow(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|} d\mathbf{r}_1 d\mathbf{r}_2. \quad (19)$$

$q_{\uparrow\downarrow}$ stands for a repulsion term filtered with the factor $(r_1^2 - r_2^2)/|\mathbf{r}_1 - \mathbf{r}_2|^2$:

$$q_{\uparrow\downarrow} = \int \frac{\varrho_\uparrow(\mathbf{r}_1)\varrho_\downarrow(\mathbf{r}_2)}{|\mathbf{r}_1 - \mathbf{r}_2|^3} (r_1^2 - r_2^2) d\mathbf{r}_1 d\mathbf{r}_2. \quad (20)$$

The difference between the exchange-correlation virials gives the last term in Eq. (14):

$$\Delta x = x_\uparrow - x_\downarrow, \quad (21)$$

$$x_\sigma = - \int \varrho_\sigma \mathbf{r} \cdot \nabla v_{xc\sigma} d\mathbf{r}. \quad (22)$$

In an atom or molecule the external potential v_σ can be separated as

$$v_\sigma(\mathbf{r}, t) = v_{ne}(\mathbf{r}) + \tilde{v}_\sigma(\mathbf{r}, t), \quad (23)$$

where $v_{ne}(\mathbf{r})$ is the static electron-nucleon potential

$$v_{ne}(\mathbf{r}) = - \sum_p \frac{Z_p}{|\mathbf{r} - \mathbf{R}_p|} \quad (24)$$

and the second term \tilde{v}_σ is the time-dependent part. In this case we obtain for the virial of the external potential

$$w_\sigma = \int \varrho_\sigma \left(v_{ne} - \sum_p \mathbf{R}_p \cdot \nabla_p \frac{Z_p}{|\mathbf{r} - \mathbf{R}_p|} \right) d\mathbf{r} + \langle \mathbf{r} \cdot \nabla \tilde{v}_\sigma \rangle_\sigma. \quad (25)$$

Another form of the spin virial theorem can be derived by writing the time-dependent total energy as

$$E(t) = \sum_\sigma E_\sigma(t), \quad (26)$$

where

$$E_\sigma(t) = T_\sigma^s(t) + J_\sigma(t) + \int \varrho_\sigma v_\sigma d\mathbf{r} + E_{xc\sigma}(t), \quad (27)$$

$$J_\sigma(t) = \frac{1}{2} \int \varrho_\sigma v_J d\mathbf{r} \quad (28)$$

is the classical Coulomb energy and $E_{xc\sigma}$ is the exchange-correlation energy for electrons with spin σ . In complete analogy with the time-independent density functional theory the exchange-correlation energy functional is defined by Eq. (27). Writing the total energy as

$$E_\sigma(t) = T_\sigma(t) + \int \varrho_\sigma v_\sigma d\mathbf{r} + E_{es}^\sigma(t), \quad (29)$$

where T_σ and E_{es}^σ are the interacting kinetic energy and the Coulomb energy of electrons with spin σ , respectively, the exchange-correlation energy can be expressed with the time-dependent first- and second-order density matrices $\gamma_\sigma, \gamma_\sigma^s, \Gamma_{\sigma\sigma}$ as

$$E_{xc\sigma}(t) = T_\sigma(t) - T_\sigma^s(t) + E_{es}^\sigma(t) - J_\sigma(t), \quad (30)$$

$$T_\sigma(t) = - \frac{1}{2} \int \nabla_1^2 \gamma_\sigma(\mathbf{r}_1, \mathbf{r}'_1; t) |_{\mathbf{r}'_1 = \mathbf{r}_1} d\mathbf{r}_1, \quad (31)$$

$$T_\sigma^s(t) = - \frac{1}{2} \int \nabla_1^2 \gamma_\sigma^s(\mathbf{r}_1, \mathbf{r}'_1; t) |_{\mathbf{r}'_1 = \mathbf{r}_1} d\mathbf{r}_1, \quad (32)$$

and

$$E_{es}^\sigma(t) = \int \frac{\Gamma_{\sigma\sigma}(\mathbf{r}_1, \mathbf{r}_2; t) + \Gamma_{\sigma\sigma'}(\mathbf{r}_1, \mathbf{r}_2; t)}{r_{12}} d\mathbf{r}_1 d\mathbf{r}_2. \quad (33)$$

This is, of course, a very formal expression for the time-dependent exchange-correlation energy. In the density-functional theory the exchange-correlation energy is given as a functional of the density or the orbitals.

Using the total energy difference

$$\Delta E = E_\uparrow - E_\downarrow, \quad (34)$$

the spin virial theorem can be given by

$$\Delta E + \Delta T_s = \Delta E_{xc} - q_{\uparrow\downarrow} - \Delta x + \int (\varrho_\uparrow v_\uparrow - \varrho_\downarrow v_\downarrow) d\mathbf{r} - \Delta w + \frac{d}{dt} \langle \mathbf{r} \cdot \Delta \mathbf{j}_s \rangle. \quad (35)$$

This form of the theorem connects the total and kinetic energy differences. While the previous form of the spin virial theorem [Eq. (9)] gives a method to check the accuracy of the potentials, expression (35) provides a way to judge the energy functionals. In an atom or molecule it can also be written as

$$\begin{aligned} \Delta E + \Delta T_s = & \Delta E_{xc} - q_{\uparrow\downarrow} - \Delta x + \int (\varrho_{\uparrow}\tilde{v}_{\uparrow} - \varrho_{\downarrow}\tilde{v}_{\downarrow})d\mathbf{r} \\ & + \int Q \sum_p \mathbf{R}_p \cdot \nabla_p \frac{Z_p}{|\mathbf{r} - \mathbf{R}_p|} d\mathbf{r} - \int (\varrho_{\uparrow}\mathbf{r} \cdot \nabla \tilde{v}_{\uparrow} \\ & - \varrho_{\downarrow}\mathbf{r} \cdot \nabla \tilde{v}_{\downarrow})d\mathbf{r} + \frac{d}{dt} \langle \mathbf{r} \cdot \Delta \mathbf{j}_s \rangle, \end{aligned} \quad (36)$$

where

$$Q(\mathbf{r}) = \varrho_{\uparrow}(\mathbf{r}) - \varrho_{\downarrow}(\mathbf{r}) \quad (37)$$

is the (spin) magnetization density.

III. DERIVATION IN THE REAL SYSTEM

Let us now turn to the real, interacting system and calculate again the time derivative of the operator \hat{A} with the Hamiltonian of the real system

$$\hat{H} = \hat{T} + \hat{V}_{ee} + \hat{V}, \quad (38)$$

where \hat{T} , \hat{V}_{ee} , and \hat{V} are the kinetic, the electron-electron repulsion, and the external potential operators, respectively. After some algebra we obtain

$$\frac{1}{2} \frac{d}{dt} \langle (\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}) \rangle_{\sigma} = 2T_{\sigma} + \tilde{V}_{ee}^{\sigma} - \langle \mathbf{r} \cdot \nabla v_{\sigma} \rangle_{\sigma}, \quad (39)$$

where

$$\tilde{V}_{ee}^{\uparrow} = - \left\langle \sum_{j=1}^{N_{\uparrow}} \sum_{l=1}^N \frac{\mathbf{r}_j \cdot (\mathbf{r}_j - \mathbf{r}_l)}{r_{jl}^3} \right\rangle \quad (40)$$

and a similar equation stands for electrons with spin down. Eq. (39) can also be written as

$$\frac{d}{dt} \langle \mathbf{r} \cdot \mathbf{j} \rangle_{\sigma} = 2T_{\sigma} + V_{ee}^{\sigma} - \langle \mathbf{r} \cdot \nabla v_{\sigma} \rangle_{\sigma}. \quad (41)$$

The difference for spin up and down yields the spin virial theorem

$$\frac{d}{dt} \langle \mathbf{r} \cdot \Delta \mathbf{j} \rangle = 2\Delta T + \Delta U, \quad (42)$$

where the first term in the right-hand side of Eq. (42) is the kinetic energy difference of electrons with spin up and down

$$\Delta T = T_{\uparrow} - T_{\downarrow}. \quad (43)$$

The second term can be written as

$$\Delta U = \Delta W + \Delta Y + \Delta w, \quad (44)$$

where $W_{\sigma\sigma}$ denotes the Coulomb interaction energy between electrons with spin σ :

$$\Delta W = W_{\uparrow\uparrow} - W_{\downarrow\downarrow}, \quad (45)$$

$$W_{\sigma\sigma} = \frac{1}{2} \left\langle \sum_{j=1}^{N_{\sigma}} \sum_{l=1}^{N_{\sigma}} \frac{1}{r_{jl}} \right\rangle, \quad (46)$$

$$\Delta Y = Y_{\uparrow\downarrow} - Y_{\downarrow\uparrow} \quad (47)$$

gives the difference of electronic repulsion between electrons with different spin

$$Y_{\uparrow\downarrow} = \frac{1}{2} \left\langle \sum_{j=1}^{N_{\uparrow}} \sum_{l=1}^{N_{\downarrow}} \frac{\mathbf{r}_j^2 - \mathbf{r}_l^2}{r_{jl}^3} \right\rangle, \quad (48)$$

$$Y_{\downarrow\uparrow} = \frac{1}{2} \left\langle \sum_{j=1}^{N_{\downarrow}} \sum_{l=1}^{N_{\uparrow}} \frac{\mathbf{r}_j^2 - \mathbf{r}_l^2}{r_{jl}^3} \right\rangle. \quad (49)$$

Δw is the energy difference arriving from the external potential [Eq. (16)].

In an atom or molecule, relation (23) can also be used and ΔU can be written as

$$\Delta U = \Delta W + \Delta Y + \Delta \tilde{w} - \int Q \sum_p \mathbf{R}_p \cdot \nabla_p \frac{Z_p}{|\mathbf{r} - \mathbf{R}_p|} d\mathbf{r}, \quad (50)$$

$$\tilde{w}_{\sigma} = \langle \mathbf{r}_{\sigma} \cdot \nabla \tilde{v}_{\sigma} \rangle_{\sigma}. \quad (51)$$

The spin virial theorem of Eq. (42) is the time-dependent generalization of the theorem derived by Ishiara [10]. For stationary case we get back the spin virial theorem of Ishiara.

IV. THE TIME-DEPENDENT SPIN VIRIAL THEOREM IN THE PRESENCE OF MAGNETIC FIELD

In the presence of a magnetic field of z direction $b(\mathbf{r}, t)$ the Kohn-Sham potentials have the form

$$v_{s\sigma}(\mathbf{r}, t) = v_{\sigma}(\mathbf{r}, t) + v_J(\mathbf{r}, t) + v_{xc\sigma}(\mathbf{r}, t) + v_{b\sigma}(\mathbf{r}, t), \quad (52)$$

where

$$v_{b\uparrow} = \beta b(\mathbf{r}, t), \quad (53)$$

$$v_{b\downarrow} = -\beta b(\mathbf{r}, t), \quad (54)$$

and β is the Bohr magneton. Substituting Eq. (52) into Eq. (9) we arrive at the spin virial theorem

$$\frac{d}{dt} \langle \mathbf{r} \cdot \Delta \mathbf{j}_s \rangle = 2\Delta T^s + \Delta V + B, \quad (55)$$

where the additional term B ,

$$B = \beta \int Q(\mathbf{r}, t) \mathbf{r} \cdot \nabla b(\mathbf{r}, t) d\mathbf{r}, \quad (56)$$

is the virial of the magnetic field $b(\mathbf{r}, t)$. In case of constant field B disappears.

In the total energy expression (26), E_{σ} now has the form

$$E_{\sigma}(t) = T_{\sigma}^s(t) + J_{\sigma}(t) + \int \varrho_{\sigma} v_{\sigma} d\mathbf{r} + E_{xc\sigma} + E_{b\sigma}, \quad (57)$$

where the new terms are

$$E_{b\uparrow} = \beta \int \varrho_{\uparrow}(\mathbf{r}, t) b(\mathbf{r}, t) d\mathbf{r} \quad (58)$$

and

$$E_{b\downarrow} = \beta \int \varrho_{\downarrow}(\mathbf{r}, t) b(\mathbf{r}, t) d\mathbf{r}. \quad (59)$$

The new form of the spin virial theorem is

$$\begin{aligned} \Delta E + \Delta T_s = \Delta E_{xc} - q_{\uparrow\downarrow} - \Delta x + \int (\varrho_{\uparrow} v_{\uparrow} - \varrho_{\downarrow} v_{\downarrow}) d\mathbf{r} - \Delta w \\ + \frac{d}{dt} \langle \mathbf{r} \cdot \Delta \mathbf{j} \rangle - \Delta E_b + B, \end{aligned} \quad (60)$$

where

$$\Delta E_b = E_{b\uparrow} - E_{b\downarrow} = \beta \int \varrho(\mathbf{r}, t) b(\mathbf{r}, t) d\mathbf{r}. \quad (61)$$

V. DISCUSSION

Equation (8) has been derived in Ref. [5] in the form

$$\frac{1}{2} \frac{d}{dt} \langle (\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}) \rangle = 2T^s - \langle \mathbf{r} \cdot \nabla v_s \rangle. \quad (62)$$

Equation (8) can be written in this case as

$$\frac{1}{2} \frac{d}{dt} \langle (\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}) \rangle = 2T^s - \sum_{\sigma} \langle \mathbf{r} \cdot \nabla v_{s\sigma} \rangle_{\sigma}. \quad (63)$$

The corresponding relation in the real system can be obtained by adding Eq. (39) for spin up and down,

$$\frac{1}{2} \frac{d}{dt} \langle (\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}) \rangle = 2T + \tilde{V}_{ee} - \sum_{\sigma} \langle \mathbf{r} \cdot \nabla v_{\sigma} \rangle_{\sigma}, \quad (64)$$

It was shown in Ref. [5] that the left-hand side of Eqs. (63) and (64) is equal. It follows from the fact that

$$\frac{d}{dt} \langle r^2 \rangle = \langle (\mathbf{r} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{r}) \rangle \quad (65)$$

and $\langle r^2 \rangle$ is the same for the Kohn-Sham and the real systems because the density is same in both the systems. Equating the right-hand side of Eqs. (63) and (64) leads to the usual form of the virial theorem. Another consequence of Eq. (65) is the relation

$$\frac{d}{dt} \langle \mathbf{r} \cdot \mathbf{j}_s \rangle = \frac{d}{dt} \langle \mathbf{r} \cdot \mathbf{j} \rangle. \quad (66)$$

It is an unsolved question whether the Kohn-Sham and the true currents are equal. In a recent paper [11] it is emphasized that they are not necessarily equal. Defining the exchange-correlation part of the current by

$$\mathbf{j} = \mathbf{j}_s + \mathbf{j}_{xc}, \quad (67)$$

it follows from the continuity equation that

$$\nabla \cdot \mathbf{j}_{xc} = \nabla \cdot \mathbf{j} - \nabla \cdot \mathbf{j}_s = 0. \quad (68)$$

For a finite system in which the densities and the currents vanish at infinity, the continuity equation leads to

$$\int \mathbf{j}_{xc} = 0, \quad (69)$$

that is, the Kohn-Sham and the true systems have the same momentum. For specific systems further relations are derived in Ref. [11]. It was conjectured [12] that $\mathbf{j} = \mathbf{j}_s$ and $\mathbf{j}_{xc} = 0$ hold in general. Equation (66) would be in accordance with it, but the question still remains open.

The spin virial theorem derived here for time-dependent systems is significant from conceptual and practical points of view. As it gives a relation between the difference of spin up and down kinetic and potential energy terms, it can be used to check the accuracy of approximations. It can be rather important as there is a growing interest in studying spin dynamics within the time-dependent density-functional theory [13]. As this theorem is independent from the ‘‘usual’’ virial theorem it provides a way of judging accuracy. The spin virial theorem is a theorem of quantum mechanics. Contrary to the virial theorem it has no classical counterpart.

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