

# Particle density and non-local kinetic energy density functional for two-dimensional harmonically confined Fermi vapors

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**Abstract.** We evaluate analytically some ground state properties of two-dimensional harmonically confined Fermi vapors with isotropy and for an arbitrary number of closed shells. We first derive a differential form of the virial theorem and an expression for the kinetic energy density in terms of the fermion particle density and its low-order derivatives. These results allow an explicit differential equation to be obtained for the particle density. The equation is third-order, linear and homogeneous. We also obtain a relation between the turning points of kinetic energy and particle densities, and an expression of the non-local kinetic energy density functional.

**PACS.** 03.65.Db Functional analytical methods – 05.30.Fk Fermion systems and electron gas

## 1 Introduction

We have previously studied in detail the ground-state properties of harmonically confined non-interacting fermions in one dimension (1D) [1,2], because of current interest in experiments on ultracold gases of the <sup>40</sup>K and <sup>6</sup>Li fermionic isotopes populating hyperfine states inside magnetic traps [3–5]. The *s*-wave collisions between fermions in the same hyperfine state are suppressed by the Pauli principle, while *p*-wave scattering and dipole-dipole magnetic interactions are very weak at very low temperature [6]. A one-component gas of Fermi atoms in a fully spin-polarized state inside a magnetic trap thus is a close laboratory realization of the ideal non-interacting Fermi gas in an external harmonic potential, allowing access to the kinetic energy functional which is invoked in the density functional theory of inhomogeneous fluids [7].

The current experimental setups are usually based on axially symmetric magnetic traps with variable aspect ratio. It is thus possible to range from a quasi-1D “cigar-shaped” trap to a quasi-2D “pancake-shaped” trap [8], and to the spherical case of a fully isotropic trap. The interest in such experiments has motivated us to study by essentially analytical methods the extension of the results of references [1,2] to treat independent fermions with two-dimensional (2D) isotropic harmonic confinement, for an arbitrary number of closed shells. The case of 3D isotropic confinement has been considered in reference [9]. Through-

out we study singly filled levels because of the experimental situation involving spin-polarized fermions.

The outline of the paper is then as follows. In Section 2 below, we derive an explicit form of the kinetic energy density for 2D harmonic confinement for an arbitrary number of closed shells. In Section 3 a differential form of the usual integral virial theorem, but now specific to 2D harmonic confinement, is invoked and this allows the kinetic energy density result of Section 2 to be rewritten as a differential equation for the particle density. Section 4 gives the derivation of a relation between the turning points of the kinetic energy and particle densities. This allows the construction of an explicit form of the kinetic energy density functional solely in terms of the particle density and its low-order derivatives. This provides the third example – after the homogeneous electron gas and the one-particle problem presented by the hydrogen atom – for which the exact functional is derived. Illustrative numerical results are presented in Section 5. The final section constitutes a summary, together with some proposals for further studies.

## 2 Derivation of the relation between average kinetic energy density and particle density

Three forms of the kinetic energy density are used in the paper: (i)  $t(r) = -(\hbar^2/2m) \sum_i \psi_i \nabla^2 \psi_i$ , (ii)  $t_G(r) = (\hbar^2/2m) \sum_i |\nabla \psi_i|^2$  and (iii) an average of  $t(r)$  and  $t_G(r)$

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called  $\bar{t}(r)$ . The quantity  $2\bar{t}(r)$  equals the trace of the tensorial momentum flux density and the difference  $t_G(r) - t(r)$  is simply  $(\hbar^2/4m)\nabla^2\rho(r)$  where  $\rho(r)$  is the particle density. All three kinetic energy densities defined above lead to the correct total kinetic energy  $T = \int d^2r t(r)$  etc. A brief reminder of the solution of the Schrödinger equation for the problem of present interest is given in Appendix A.

Our starting point is the result for the 2D fermion particle density in the presence of the harmonic confinement  $V(r) = m\omega^2 r^2/2$ , as obtained by Brack and van Zyl [10], namely

$$\rho(r) = \frac{1}{\pi a_{\text{ho}}^2} \sum_{\mu=0}^M (M+1-\mu)(-1)^\mu L_\mu(y) \exp(-y/2) \quad (1)$$

after adaptation to the case of single occupancy of the trap levels. Here  $a_{\text{ho}} = (\hbar/m\omega)^{1/2}$ ,  $y = 2(r/a_{\text{ho}})^2$ ,  $(M+1)$  is the number of filled shells and  $L_\mu(y)$  are the Laguerre polynomials. The average kinetic energy density  $\bar{t}(r)$  is given by [10]

$$\bar{t}(r) = \frac{\hbar\omega}{2\pi a_{\text{ho}}^2} \sum_{\mu=0}^M (M+1-\mu)^2 (-1)^\mu L_\mu(y) \exp(-y/2). \quad (2)$$

We now define the following summations over the Laguerre polynomials:

$$Q_i^{(M+1)}(y) = \sum_{\mu=0}^M \mu^i (-1)^\mu L_\mu(y) : \quad i = 0, 1, 2. \quad (3)$$

Then the particle density and the average kinetic energy density are readily expressed in the form

$$\rho(r) = \frac{1}{\pi a_{\text{ho}}^2} \left[ (M+1)Q_0^{(M+1)}(y) - Q_1^{(M+1)}(y) \right] \exp(-y/2) \quad (4)$$

and

$$\bar{t}(r) = \frac{\hbar\omega}{2\pi a_{\text{ho}}^2} \left[ (M+1)^2 Q_0^{(M+1)}(y) - 2(M+1)Q_1^{(M+1)}(y) + Q_2^{(M+1)}(y) \right] \exp(-y/2). \quad (5)$$

The next step is to utilize the differential equation for the Laguerre polynomials, namely

$$\left[ y \frac{d^2}{dy^2} + (1-y) \frac{d}{dy} + \mu \right] L_\mu(y) = 0. \quad (6)$$

This is readily shown to lead to the following relations for the summations  $Q_i^{(M+1)}(y)$ :

$$\left[ y \frac{d^2}{dy^2} + (1-y) \frac{d}{dy} \right] Q_i^{(M+1)}(y) + Q_{i+1}^{(M+1)}(y) = 0 \quad (7)$$

for  $i = 0$  and  $1$ . These allow us to express  $\rho(r)$  and  $\bar{t}(r)$  solely in terms of  $Q_0^{(M+1)}(y)$  and of its first two derivatives, leading after some manipulations to the result

$$\bar{t}(r) = \frac{\hbar\omega}{2} \left[ \frac{a_{\text{ho}}^2}{8} \nabla^2 \rho(r) + \left( M + \frac{3}{2} - \frac{r^2}{2a_{\text{ho}}^2} \right) \rho(r) \right]. \quad (8)$$

Equation (8) is one of the central relations for the present study.

### 3 Differential equation for fermion particle density

Having related the kinetic energy density  $\bar{t}(r)$  to the particle density  $\rho(r)$  and the potential energy  $m\omega^2 r^2/2$  in equation (8), for an arbitrary number of closed shells, we shall next invoke a differential form of the usual integral virial theorem. This we write in the form:

$$\frac{\partial \bar{t}(r)}{\partial r} = -\rho(r) \frac{\partial V(r)}{\partial r}. \quad (9)$$

For the specific case of 2D harmonic confinement with filled shells, the differential virial theorem (9) can be proven starting from equations (1, 2) for any given number of shells. The demonstration is given in Appendix B.

Forming the virial  $\mathbf{r} \cdot \mathbf{F}$  of the force  $\mathbf{F}$ , as  $-r\partial V(r)/\partial r$ , and integrating over  $2\pi r dr$  we find

$$\int_0^\infty 2\pi r^2 \frac{\partial \bar{t}(r)}{\partial r} dr = \langle \mathbf{r} \cdot \mathbf{F} \rangle = \int d^2r \rho(r) r \frac{\partial V(r)}{\partial r}. \quad (10)$$

Integrating the LHS of equation (10) by parts we obtain  $2T$  for the integral value,  $T$  being the total kinetic energy, which confirms that equation (9) contains the integral virial theorem.

Having established equation (9), we can combine it with equation (8) relating  $\bar{t}(r)$  to  $V(r)$  and  $\rho(r)$  to obtain a third-order, linear, homogeneous differential equation for the particle density  $\rho(r)$  for  $(M+1)$  closed shells:

$$\frac{\hbar^2}{8m} \frac{\partial [\nabla^2 \rho(r)]}{\partial r} + \left[ \left( M + \frac{3}{2} \right) \hbar\omega - \frac{m\omega^2 r^2}{2} \right] \frac{\partial \rho(r)}{\partial r} + m\omega^2 r \rho(r) = 0. \quad (11)$$

As one immediate check of equation (11), it is readily verified that

$$\rho(r) = \mathcal{N} \exp(-r^2/a_{\text{ho}}^2), \quad (12)$$

where  $\mathcal{N}$  is a known (irrelevant for present purposes) normalization factor, satisfies equation (11) for  $M = 0$ .

Equation (11) achieves a long-term aim of density functional theory for the present case of 2D harmonic confinement of independent fermions: namely to allow the direct calculation of the particle density from the potential energy ( $m\omega^2 r^2/2$  in this case), without recourse to individual wave functions. It constitutes the two-dimensional generalization of the result of Lawes and March [11] for one-dimensional (1D) harmonic confinement of fermions.

## 4 Kinetic energy functional

The first object of the present section is to obtain a relation between  $t'(r) = \partial t(r)/\partial r$  and  $\rho'(r) = \partial \rho(r)/\partial r$  for this isotropic 2D harmonically confined fermion assembly. The result for 1D harmonic confinement is (see *e.g.* [2])

$$\frac{t'(x)}{\rho'(x)} = \left( N\hbar\omega - \frac{m\omega^2 x^2}{2} \right). \quad (13)$$

We first use the definition of  $\bar{t}(r)$  and the relation  $t_G(r) = \bar{t}(r) + (\hbar^2/4m)\nabla^2\rho(r)$  to obtain

$$t(r) = \bar{t}(r) - \frac{\hbar^2}{8m}\nabla^2\rho(r). \quad (14)$$

After differentiation of equation (14) with respect to  $r$ , the use of the virial theorem (9) and of the differential equation (11) for  $\rho(r)$  allows us to obtain

$$\frac{t'(r)}{\rho'(r)} = \left( \mu - \frac{m\omega^2 r^2}{2} \right), \quad (15)$$

which is the desired generalization of equation (13) to 2D harmonic confinement, where the chemical potential for 2D harmonic confinement is  $\mu = (M + 3/2)\hbar\omega$ . Evidently equation (15) relates directly the turning points of kinetic energy and particle densities for any chosen number of closed shells.

Equation (15) allows us to eliminate the presence of the external potential and to obtain the non-local kinetic energy density functional solely in terms of the particle density and of its low-order derivatives. To this aim, we first write an equation for the quantity  $Q(r) = t'(r)/\rho'(r)$  by differentiation of equation (15) and by using equations (9, 14):

$$\frac{\partial}{\partial r} \left[ \frac{Q(r)}{\rho(r)} \right] = \frac{\hbar^2}{8m} \frac{1}{\rho^2(r)} \frac{\partial}{\partial r} \nabla^2 \rho(r). \quad (16)$$

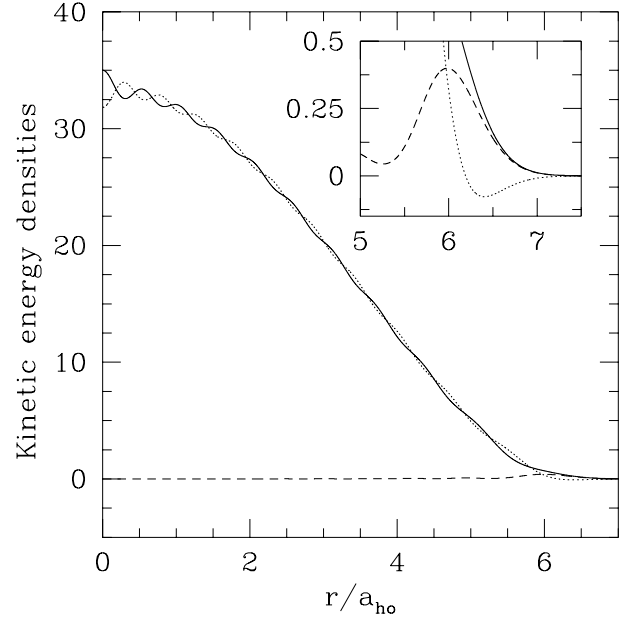
As a second step, we obtain the function  $Q(r)$  by integration:

$$Q(r) = \frac{\mu}{\rho(0)}\rho(r) + \frac{\hbar^2}{8m}\rho(r) \int_0^r ds \frac{1}{\rho^2(s)} \frac{\partial}{\partial s} \nabla^2 \rho(s), \quad (17)$$

the integration constant being fixed by the condition  $Q(0) = \mu$ . A further integration and elimination of the high-order derivatives through integration by parts leads to the final expression

$$t(r) = \frac{t_W(r)}{2} + \left[ C + \frac{\hbar^2}{16m} \int_0^r ds \frac{[\rho'(s)]^2}{\rho^3(s)} \left( \frac{2}{s} + \frac{3\rho'(s)}{\rho(s)} \right) \right] \rho^2(r) \quad (18)$$

where  $t_W(r) = (\hbar^2/8m)[\rho'(r)]^2/\rho(r)$  is the von Weizsäcker ‘‘surface’’ contribution to the kinetic energy density [12] and the constant  $C$  is given by  $C = \mu/(2\rho(0)) - (\hbar^2/16m) \times (\nabla^2\rho(r))_{r=0}/\rho^2(0)$ . In the second term on the RHS of



**Fig. 1.** Kinetic energy densities (in units  $\hbar\omega/a_{\text{ho}}^2$ ) as given by the different definitions in Sections 2 and 4 for a 2D Fermi gas in isotropic harmonic confinement with 20 filled shells, as functions of the radial coordinate  $r/a_{\text{ho}}$ . Solid line:  $t_G(r)$ , dotted line:  $t(r)$ , dashed line:  $t_W(r)$ . The inset shows an enlargement of the turning point region, in the same units.

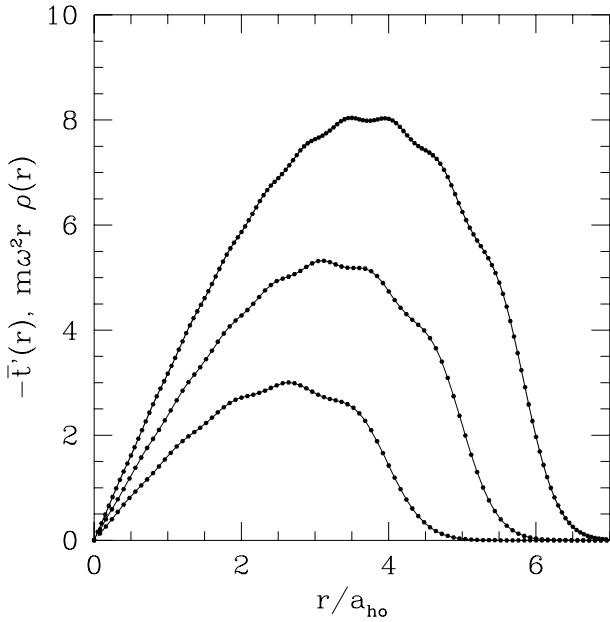
equation (18) we recognize the 2D Thomas-Fermi kinetic energy density functional, as given by  $t_{\text{TF}} = \pi\hbar^2\rho^2(r)/m$ . By comparing this simple expression with equation (18), we understand that the role of the non-local functional is highly non-trivial, leading to the formation of oscillations along the density profile. This provides a generalization of the result obtained by March *et al.* [13] to the 2D harmonic confinement. By integration of equation (18) over the system one obtains an explicit expression for the kinetic energy functional.

## 5 Illustrative numerical results

Equations (1, 2) can be employed to numerically evaluate all the ground state properties defined in Section 2. Typical values for the units of frequency and length in the experiments on atomic Fermi gases are  $\omega = 2\pi \times 200 \text{ s}^{-1}$  and  $a_{\text{ho}} = \sqrt{\hbar/m\omega} \simeq 3 \mu\text{m}$ , respectively.

In Figure 1 we plot the exact kinetic energy densities  $t(r)$  and  $t_G(r)$  for 20 filled shells ( $M = 19$ ). Different physical phenomena are described by  $t(r)$  and  $t_G(r)$ : while  $t(r)$  is relevant in the context of Density-Functional Theory,  $t(r) + t_G(r)$  gives the trace of the momentum flux density entering the equations of generalized hydrodynamics.

Figure 1 clearly displays the shell structure arising from single-level occupancy and the spill-out beyond the Thomas-Fermi radius arising from quantum mechanical



**Fig. 2.** Illustration of the differential virial theorem: negative of  $\partial\bar{t}(r)/\partial r$  (solid line) and  $m\omega^2 r\rho(r)$  (dots) in units  $\hbar\omega/a_{\text{ho}}^3$  as functions of the radial coordinate  $r/a_{\text{ho}}$ , for a 2D Fermi gas in isotropic harmonic confinement with 20, 15 and 10 filled shells (from top to bottom).

tunnelling. There is seen to be a tiny negative region of  $t(r)$ , whereas  $t_G(r)$  is by definition everywhere positive. A negative behaviour in the tails of  $t(r)$  was also observed in the 1D geometry [1]. In the same figure we also show the von Weizsäcker kinetic energy density  $t_W(r)$ . It is seen that  $t_W(r)$  is practically zero until the classically forbidden region is reached, while well outside the classically allowed region it eventually merges with  $t_G(r)$ : *i.e.*  $t_G(r) \rightarrow t_W(r)$  for  $r$  greater than the Fermi radius. This property is shown in the inset of Figure 1. Again, this generalizes a result which was previously known to be valid only in the 1D geometry [2].

In Figure 2 the differential virial theorem (9) is illustrated in the case of harmonic confinement by comparing the negative of  $\partial\bar{t}/\partial r$  with the quantity  $m\omega^2 r\rho(r)$  for various numbers of filled shells. The shell structure is again very evident.

## 6 Summary and proposed future directions

We have derived a set of analytic relations for the ground state properties of a 2D Fermi gas under harmonic confinement, with the proviso that the Fermi particles always fill  $(M + 1)$  closed shells. Our work was aimed mainly at transforming the description of the system from one given in terms of wave functions to one which takes as the main variable the particle density. This procedure, typical of Density Functional Theory (DFT), is here possible in an explicit way due to the simplicity of the system.

Five basic equations have been obtained, namely equations (8, 9, 11, 15, 18). Equation (8) is a differential relation which gives the average kinetic energy density in terms of the particle density, and equation (9) is a differential version of the usual virial theorem. These relations allow the derivation of equation (11), a third-order differential equation for the particle density profile as determined by the external confining potential and by the number of filled shells, and equation (15), a relation between the turning points of the kinetic energy density and the particle density. The latter is finally used to obtain the kinetic energy density functional (18) in terms of the particle density, which is a main task in DFT.

What seems to us therefore to remain outstanding in 2D is to solve the differential equation (11), hopefully analytically and without summation over shells. The motivation for expecting this is the “folklore” that the properties of a fermion fluid are determined by its highest occupied level [11]. Of course, the challenge of the three-dimensional oscillator problem remains as a high priority for further study.

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## Appendix A: Two-dimensional Fermi gas in harmonic confinement: wave functions and Dirac density matrix

The Schrödinger equation in 2D reads

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{1}{2}m\omega^2 r^2\psi = \varepsilon\psi. \quad (19)$$

Using  $a_{\text{ho}} \equiv (\hbar/m\omega)^{1/2}$  and  $\hbar\omega$  as units of length and energy, the eigenfunctions of equation (19) are expressed through the Laguerre polynomials  $L_n^m(r^2)$  as

$$\psi_{n,m}(r, \phi) = \left(\frac{n!}{\pi(n+m)!}\right)^{1/2} r^m L_n^m(r^2) e^{-r^2} e^{im\phi}, \quad (20)$$

in correspondence to the energy eigenvalues

$$\varepsilon_{n,m} = 2n + m + 1. \quad (21)$$

The various shells are filled by taking all integer values of  $n$  and  $m$  which satisfy  $2n + m = N$ ,  $N$  being the shell index.

The “off-diagonal density”, that is the Dirac density matrix can be immediately written from equation (20) as

$$n(\mathbf{r}, \mathbf{r}') = \frac{1}{\pi} e^{-(r^2+r'^2)/2} \sum_{N=0}^M \sum_{h=0}^N \frac{(N-h)!}{h!} (rr')^{2h-N} \times L_{N-h}^{2h-N}(r^2) L_{N-h}^{2h-N}(r'^2) e^{i[(2h-N)(\phi-\phi')]} \quad (22)$$

From this matrix, the density profile  $\rho(r)$  for  $(M+1)$  filled shells is obtained by taking  $\mathbf{r}' = \mathbf{r}$ , the result being the same as the one obtained by Brack and van Zyl [10]. Similarly, the kinetic energy density can be directly constructed in either the form of  $t(r)$  or  $t_G(r)$  by appropriate differentiation on the Dirac matrix (22), and afterwards allowing  $\mathbf{r}'$  to tend to  $\mathbf{r}$ .

## Appendix B: Proof of the differential virial theorem for a 2D harmonically confined Fermi gas

We demonstrate here equation (9) for the specific case  $V(r) = m\omega^2 r^2/2$ , which is the one relevant for the present work. The units  $a_{ho}$  and  $\hbar\omega$  for length and energy are used throughout.

As a first step, we derive from equations (1, 2) recursion relations for the particle density  $\rho_{M+1}(r)$  and the average kinetic energy density  $\bar{t}_{M+1}(r)$  of a system with  $(M+1)$  filled shells in terms of those of a system with  $M$  filled shells. These relations are

$$\rho_{M+1}(r) = \rho_M(r) + Q_0^{(M+1)}(y) \exp(-y/2)/\pi \quad (23)$$

and

$$\bar{t}_{M+1}(r) = \bar{t}_M(r) + \rho_M(r) + Q_0^{(M+1)}(y) \exp(-y/2)/(2\pi). \quad (24)$$

These involve the function  $Q_0^{(M+1)}(y)$  defined in equation (3).

We then proceed by induction. The differential virial theorem is readily proven for the case  $M=1$  of a singly occupied shell by direct substitution of the expressions  $\rho_1(r) = \exp(-r^2)/\pi$  and  $\bar{t}_1(r) = \exp(-r^2)/2\pi$  into equation (9). Assuming that the theorem holds for  $M$  filled shells, we are left to prove that

$$\frac{\partial}{\partial r} \left[ \rho_{M+1}(r) - \frac{e^{-y/2}}{2\pi} Q_0^{(M+1)}(y) \right] = -r \frac{e^{-y/2}}{\pi} Q_0^{(M+1)}(y). \quad (25)$$

Physically this means that the theorem holds separately for each filled shell.

By the use of equation (4) for the density profile, equation (25) can be rewritten solely in terms of the functions

$Q_i^{(M+1)}(y)$  with  $i=0, 1$ :

$$\left( M + \frac{1}{2} \right) \frac{\partial Q_0^{(M+1)}(y)}{\partial y} - 2MQ_0^{(M+1)}(y) = \frac{\partial Q_1^{(M+1)}(y)}{\partial y} - 2Q_1^{(M+1)}(y). \quad (26)$$

We can now employ the definition of the Laguerre polynomials

$$L_\mu(y) = \sum_{k=0}^{\mu} \binom{\mu}{\mu-k} \frac{(-y)^k}{k!} \quad (27)$$

and of the functions  $Q_i^{(M+1)}(y)$  to transform equation (26) into a double sum:

$$\sum_{\mu=1}^M (-1)^\mu \sum_{k=0}^{\mu-1} (2M+1-2\mu) \binom{\mu}{\mu-k-1} \frac{(-y)^k}{k!} + \sum_{\mu=0}^M (-1)^\mu \sum_{k=0}^{\mu} (M-\mu) \binom{\mu}{\mu-k} \frac{(-y)^k}{k!} = 0. \quad (28)$$

Exchanging the order of the sums allows us to collect all terms of the same order in  $k$ : each coefficient must then vanish independently because of the principle of identity between polynomials. Thus, we have finally to prove the simplified expression

$$\sum_{\mu=k}^{M-1} (-1)^\mu [(2M-1-2\mu)(\mu+1) - (M-\mu)(k+1)] \times \frac{\mu!}{(\mu-k)!} = 0. \quad (29)$$

The above finite sum must be shown to yield zero for any integer value  $M$  and  $k \leq (M-1)$ . This statement is proven by applying twice again the reasoning by induction on the index  $M$ : the validity of equation (29) for  $M=1$  is easily checked, and assuming that it holds for a fixed  $M$  leads to prove that

$$\sum_{\mu=k}^{M-1} (-1)^\mu (2\mu-k+1) \frac{\mu!}{(\mu-k)!} = (-1)^{M+1} \frac{M!}{(M-k-1)!}. \quad (30)$$

Applying again induction to the LHS of equation (30) leads to the proof of its validity, which implies the validity of the differential virial theorem.

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