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# Virial theorems for trapped quantum gases

Félix Werner

Laboratoire Kastler Brossel, École Normale Supérieure,  
Université Pierre et Marie Curie-Paris 6, CNRS,  
24 rue Lhomond, 75231 Paris Cedex 05, France

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We present a general virial theorem for quantum particles with arbitrary zero-range or finite-range interactions in an arbitrary external potential. We deduce virial theorems for several situations relevant to trapped gases: zero-range interactions with and without Efimov effect, narrow resonances, and finite-range interactions of infinite scattering length.

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## I. INTRODUCTION

In the early days of nuclear physics, Wigner, Bethe and Peierls introduced the zero-range model [1]. This zero-range limit is now realized experimentally to an unprecedentedly good approximation with cold atoms. Moreover the scattering length can be tuned using a Feshbach resonance and one can reach the unitary limit where the scattering length tends to infinity ([2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18] and references therein). Typically, numerics are necessary to solve accurately few-body [6, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28] and many-body problems [22, 23, 27, 29, 30] with resonant interactions. But there also exists some analytical results [1, 31, 32, 33, 34, 35, 36, 37, 38, 39, 41, 42, 47], which are useful to better understand some aspects, and to check the consistency of the zero-range model with numerical calculations [22, 23, 24, 27] and experiments [18, 48].

The most simple analytical result is the virial theorem for the unitary gas in a harmonic trap: the energy equals twice the trapping potential energy

$$E = 2E_{\text{trap}} \quad (1)$$

for any  $N$ -body eigenstate of the zero-range model [40, 41, 42].

This was rederived using non-relativistic conformal field theory [43]. It was also shown to hold within the local-density approximation [18, 44].

Experimentally, the total energy is accessible from the released energy [7, 8], and the trapping potential energy from in-situ measurement of the density profile [9, 10, 11, 13]. If the expansion dynamics is known theoretically, then other experimental methods become available: energy can be precisely added to the gas [14, 18] and the potential energy can be deduced from a time-of-flight image [15, 18]. The expansion dynamics is known if hydrodynamics is valid. This was used in particular to check the virial theorem experimentally [18]. In situations where hydrodynamics break down [17], it could be worth making an additional experimental effort to enter the validity regime of exact scaling solutions [34].

In this paper, we present a very general virial theorem, and use it to generalize Eq. (1) to arbitrary scattering

lengths, trap shapes and space dimensions, to efimovian states, to finite-range resonant interactions and to narrow Feshbach resonances.

## II. GENERAL VIRIAL THEOREM

**Theorem:** Consider a general quantum problem of  $N$  particles, with arbitrary statistics and dispersion relations. The position of particle  $i$  is denoted by  $\mathbf{r}_i$ , which is a vector of arbitrary dimension, with continuous or discrete coordinates. Assume that the Hamiltonian is of the form

$$H = H' + U(\mathbf{r}_1, \dots, \mathbf{r}_N) \quad (2)$$

where

- $H'$  and its domain depend on  $p$  parameters  $l_1, \dots, l_p$  which have the dimension of a length, on  $\hbar$ , and on some arbitrary fixed mass  $m$

- $U(\mathbf{r}_1, \dots, \mathbf{r}_N)$  is an arbitrary smooth [54] function.

Then, as shown below:

$$E = \langle \psi | U + \frac{1}{2} \sum_{i=1}^N \mathbf{r}_i \cdot \nabla_{\mathbf{r}_i} U | \psi \rangle - \frac{1}{2} \sum_{i=1}^p l_i \frac{\partial E}{\partial l_i} \quad (3)$$

for any stationary state. The partial derivatives  $\partial E / \partial l_i$  are taken for a fixed function  $U$ .

**Derivation:** Using dimensional analysis, one can rewrite  $U$  as

$$U(\mathbf{r}_1, \dots, \mathbf{r}_N) = \frac{\hbar^2 \lambda^2}{m} f(\lambda \mathbf{r}_1, \dots, \lambda \mathbf{r}_N) \quad (4)$$

where  $\lambda$  has the dimension of the inverse of a length, and  $f$  is dimensionless function. The theorem directly follows from two lemmas:

*Lemma 1:*

$$\lambda \frac{\partial E}{\partial \lambda} = \langle \psi | 2U + \sum_{i=1}^N \mathbf{r}_i \cdot \nabla_{\mathbf{r}_i} U | \psi \rangle. \quad (5)$$

*Lemma 2:*

$$\lambda \frac{\partial E}{\partial \lambda} = 2E + \sum_{i=1}^p l_i \frac{\partial E}{\partial l_i}. \quad (6)$$

Here the partial derivatives with respect to  $\lambda$  are taken for a fixed function  $f$  and for fixed  $l_1, \dots, l_p$ .

Lemma 1 follows from the Hellmann-Feynman theorem [55, 56] and from Eq. (4).

Lemma 2 follows from the fact that, by dimensional analysis, the energy can be rewritten as

$$E(l_1, \dots, l_p, [U]) = \frac{\hbar^2 \lambda^2}{m} F(\lambda l_1, \dots, \lambda l_p, [f]) \quad (7)$$

where  $F$  is a dimensionless functional.

### III. A PARTICULAR CASE: THE TRADITIONAL VIRIAL THEOREM

The traditional virial theorem concerns the case where  $H'$  is just the kinetic energy

$$T = - \sum_{i=1}^N \frac{\hbar^2}{2m_i} \Delta_{\mathbf{r}_i}, \quad (8)$$

$m_i$  being the mass of particle  $i$ . Since this operator and its domain do not depend on any length, the general virial theorem Eq. (3) reduces to the traditional one:

$$\langle \psi | T | \psi \rangle = \frac{1}{2} \langle \psi | \sum_{i=1}^N \mathbf{r}_i \cdot \nabla_{\mathbf{r}_i} U | \psi \rangle \quad (9)$$

and if  $U$  is a homogeneous function of degree  $n$ ,

$$\langle \psi | T | \psi \rangle = \frac{n}{2} \langle \psi | U | \psi \rangle. \quad (10)$$

This theorem is as old as many-particle quantum mechanics [52]. It is used e. g. to calculate and understand the properties of many-electron atoms [53].

### IV. VIRIAL THEOREMS FOR TRAPPED GASES

In this Section we restrict to the case where  $U$  is a sum of trapping potentials:

$$U(\mathbf{r}_1, \dots, \mathbf{r}_N) = \sum_{i=1}^N U_i(\mathbf{r}_i). \quad (11)$$

In this case it is convenient to rewrite the general virial theorem Eq. (3) as:

$$E = 2\tilde{E}_{\text{trap}} - \frac{1}{2} \sum_{i=1}^p l_i \frac{\partial E}{\partial l_i}, \quad (12)$$

where

$$\tilde{E}_{\text{trap}} \equiv \langle \psi | \sum_{i=1}^N [2U_i(\mathbf{r}_i) + \mathbf{r}_i \cdot \nabla U_i(\mathbf{r}_i)] | \psi \rangle / 4. \quad (13)$$

If each  $U_i$  is a harmonic trap,  $\tilde{E}_{\text{trap}}$  reduces to the trapping potential energy:

$$\tilde{E}_{\text{trap}} = \langle \psi | \sum_{i=1}^N U_i(\mathbf{r}_i) | \psi \rangle = E_{\text{trap}}. \quad (14)$$

#### A. Zero-range interactions

We first assume that each pair of particles either interacts *via* a zero-range interaction of scattering length  $a$ , or does not interact. Zero-range interactions are well-known in  $d = 1, 2$  and 3 dimensions. For  $d = 1$ , the zero-range interaction is simply the interaction potential  $-\hbar^2/(\mu a)\delta(x)$ ,  $\mu$  being the reduced particle mass [32, 57, 58]. For  $d = 2$  and  $d = 3$ , the zero-range interaction is most simply expressed as an  $a$ -dependent boundary condition on the many-body wavefunction in the limit of vanishing distance between two particles [59]. For  $d = 3$  this is called Bethe-Peierls boundary condition. This boundary condition defines the domain of the Hamiltonian.

We call *universal state* a stationary state of the zero-range model which depends only on the scattering length. All eigenstates are believed to be universal in dimension  $d = 1$  and  $d = 2$  ([57, 58, 61] and references therein). In  $d = 3$ , in some cases (e. g. for  $N = 3$  bosons of zero total orbital angular momentum), there is the so-called Efimov effect, leading to non-universal states which we call efimovian states (in the absence of trapping potential, these states are the well-known Efimov trimers). Even in cases where the Efimov effect occurs, some of the eigenstates can be universal [33, 39].

##### 1. Universal states

In the Hilbert space generated by universal states, the domain of the Hamiltonian depends only on the scattering length. Thus Eq. (12) gives for any universal state:

$$E = 2\tilde{E}_{\text{trap}} - \frac{1}{2} a \frac{\partial E}{\partial a}, \quad (15)$$

or equivalently

$$E = 2\tilde{E}_{\text{trap}} + \frac{1}{2a} \frac{\partial E}{\partial(1/a)}. \quad (16)$$

This result generalizes the virial theorem Eq. (1) to an arbitrary scattering length, trapping potential and space dimension.

Thus it also applies to quantum gases in low dimensions ([3, 82, 83, 84, 85, 86] and references therein).

For the 3D Fermi gas, it was shown by Shina Tan that the quantity  $\frac{\partial E}{\partial(1/a)}$  is related to the large-momentum tail of the momentum distribution of the gas [37] and to its total energy [36]. It would therefore be interesting to

measure this fundamental quantity [36, 37]. This could not yet be done by measuring the momentum distribution, although measurements of the momentum distribution already exist [16, 17]. An alternative method would be to measure  $E$  and  $\tilde{E}_{\text{trap}}$ , as discussed in the introduction, and to use Eq. (16). This method can work if one is sufficiently far from the Feshbach resonance, since  $E - 2\tilde{E}_{\text{trap}}$  needs to be larger than experimental error bars.

For  $a = \infty$  (which is the unitary limit for  $d = 3$  and the non-interacting limit for  $d = 1$  and 2), Eq. (16) becomes:

$$E = 2\tilde{E}_{\text{trap}}. \quad (17)$$

This last result was obtained by Yvan Castin [62].

Of course it also holds for  $a = 0$  (which is the Tonks-Girardeau limit for  $d = 1$  and the non-interacting limit for  $d = 2$  and 3) in accordance with Eq. (15).

Finally we note that taking the derivative of Eq. (16) with respect to  $1/a$  at  $a = \infty$ , one obtains:

$$\left. \frac{\partial E}{\partial(1/a)} \right|_{a=\infty} = 4 \left. \frac{\partial \tilde{E}_{\text{trap}}}{\partial(1/a)} \right|_{a=\infty}. \quad (18)$$

## 2. Efimovian states

In cases where the Efimov effect occurs, the Bethe-Peierls boundary condition is not sufficient to define a hermitian problem, and one has to add a boundary condition on the wavefunction when all 3 particles approach each other. This boundary condition can be expressed in terms of a 3-body parameter which we call  $R_t$  and has the dimensions of a length [65]. This model is known to be self-adjoint and physically meaningful for  $N = 3$  particles [6, 31, 33, 39, 63, 64]. The case of  $N \geq 4$  is still under debate [25].

Applying the general virial theorem Eq. (12) to this 2-parameter model, we get the virial theorem for an efimovian state:

$$E = 2\tilde{E}_{\text{trap}} + \frac{1}{2} \left[ \frac{1}{a} \frac{\partial E}{\partial(1/a)} - R_t \frac{\partial E}{\partial R_t} \right]. \quad (19)$$

For  $a = \infty$  this reduces to

$$E = 2\tilde{E}_{\text{trap}} - \frac{R_t}{2} \frac{\partial E}{\partial R_t}. \quad (20)$$

This allows to calculate the trapping potential energy in the exactly solvable case of 3 bosons in an isotropic harmonic trap, as shown in Appendix A.

## B. Weakly repulsive interactions

Let us consider the regime of weak repulsive interactions, which is relevant to many experiments. In  $1D$  this

situation is well-described by the zero-range model (with a large scattering length). But in 2 or 3 dimensions, it is not obvious whether this regime can be described by universal eigenstates of the zero-range model, and it is simpler to use a finite-range repulsive potential. Results become model-independent in the limit of small positive scattering length [88]. We may thus choose the simple model of a hard-sphere interaction potential of radius  $a$  (or a hard-disc interaction  $2D$ ). Applying the general virial theorem with a single length scale then gives:

$$E = 2\tilde{E}_{\text{trap}} - \frac{1}{2} a \frac{\partial E}{\partial a}. \quad (21)$$

Within the  $3D$  Gross-Pitaevskii theory,  $a \partial E / \partial a$  is the interaction energy [89], so that Eq. (21) agrees with the virial theorem of [51].

## C. Finite-range interactions of infinite scattering length

In 3 dimensions, a particularly interesting case is an interaction  $V_{ij}$  between particles  $i$  and  $j$  which has an infinite scattering length, a finite range  $l$ , and does not depend on any other length [76]. The virial theorem Eq. (12) then reduces to:

$$E = 2\tilde{E}_{\text{trap}} - \frac{l}{2} \frac{\partial E}{\partial l}. \quad (22)$$

Let us apply this to a universal state. In the zero-range limit  $l \rightarrow 0$  one recovers the virial theorem for the unitary gas Eq. (17), as expected. In numerical calculations, it is useful and sometimes crucial to perform an extrapolation to  $l \rightarrow 0$ , which is typically done as follows: one performs calculations at different values of  $l$ , checks that the variation with  $l$  is linear, and extrapolates using a linear fit [23, 29, 39, 78]. Interestingly, Eq. (22) allows to obtain the first order correction to the energy,  $l \partial E / \partial l$ , by calculating  $E - 2\tilde{E}_{\text{trap}}$  for a *single* value of  $l$ .

## D. Narrow Feshbach resonances

In  $d = 3$  dimensions, there exists an alternative zero-range model with two parameters, the scattering length  $a$  and a finite *effective* range  $r_e$  [28, 45, 47, 66, 67]. This model describes a narrow Feshbach resonance, as realized in [28] and further justified using a 2-channel model for 2 particles [45] and 3 particles [46, 47]. For  $r_e \rightarrow 0$ , this model has a limit cycle which is described by the zero-range model of Section IV A 2 with  $R_t = C r_e$ , where the constant  $C$  was obtained numerically [28] and analytically [47]. The model is expected to be hermitian for a modified scalar product, for 2 particles [67] and 3 particles [28, 47, 68]. Thus the Hellmann-Feynman theorem can be used and the generalized virial theorem Eq. (12)

holds, giving:

$$E = 2\tilde{E}_{\text{trap}} + \frac{1}{2} \left[ \frac{1}{a} \frac{\partial E}{\partial(1/a)} - r_e \frac{\partial E}{\partial r_e} \right]. \quad (23)$$

## V. IN A BOX

Finally we discuss what happens if the system is enclosed in a box of size  $L$ . This may be a cubic box with periodic boundary conditions or hard walls, or any other box shape. Consider a system satisfying the assumptions of the general virial theorem, with  $p$  lengths  $l_1, \dots, l_p$ . Adding a box simply means to add an additional length  $l_{p+1} = L$  on which the domain of the Hamiltonian depends. Thus, the virial theorems Eqs. (15,16,17,19,20,21,22,23) remain valid for a system enclosed in a box, provided one adds the term  $-L/2 \cdot \partial E / \partial L$  on the right-hand-side of these equations [90]. If one considers the ground state in a box of volume  $V$ , then  $-L \cdot \partial E / \partial L = dPV$  where  $d$  is the dimension of space and  $P = -\partial E / \partial V$  is the zero-temperature pressure. The same conclusions hold for the standard virial theorem Eq. (9,10), as is well-known [91, 92].

## NOTE

Closely related but independent works were submitted recently [93, 94, 95]. Some of the results found in this paper and in [93, 94] are identical, and a method similar to mine was used in [95].

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## APPENDIX A: APPLICATION TO EFIMOVIAN STATES AT UNITARITY

In this Section we apply the virial theorem for efimovian states Eq. (20) to the case of three equal mass bosons in an isotropic harmonic trap with zero total angular momentum. Since this problem is exactly solvable [33, 39, 69], the virial theorem will allow us to calculate the trapping potential energy.

We take units in which

$$\hbar = m = \omega = 1 \quad (A1)$$

where  $m$  is the particle mass and  $\omega$  is the trapping frequency. Thus the total trapping potential energy is:

$$E_{\text{trap,tot}} = \frac{1}{2} \sum_{i=1}^3 r_i^2. \quad (A2)$$

In the following we call  $E_{\text{tot}}$  and  $\psi_{\text{tot}}$  the energy and the wavefunction of a stationary state of the 3-body problem, so that the virial theorem Eq. (20) becomes:

$$E_{\text{tot}} = 2E_{\text{tot,trap}} - \frac{R_t}{2} \frac{\partial E_{\text{tot}}}{\partial R_t}. \quad (A3)$$

### 1. Separation of the center-of-mass

It is straightforward to deduce a virial theorem for the relative motion. Since the center-of-mass coordinate  $\mathbf{C} = (\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3)/3$  is separable,

$$E_{\text{tot}} = E + E_{\text{CM}} \quad (A4)$$

$$\Psi_{\text{tot}}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \Psi \cdot \Psi_{\text{CM}}(\mathbf{C}). \quad (A5)$$

Here  $E$  denotes the energy for the relative motion of the 3 particles (this notation is inconsistent with the previous Sections but convenient) and  $\Psi$  depends only on the relative coordinates [71], while  $E_{\text{CM}}$  and  $\Psi_{\text{CM}}$  are the well-known energy and wavefunction of the center-of-mass problem of one particle of mass  $N$  in a trapping potential

$$E_{\text{trap,CM}} = \frac{1}{2} N C^2. \quad (A6)$$

Moreover, we have

$$E_{\text{trap,tot}} = E_{\text{trap}} + E_{\text{trap,CM}} \quad (A7)$$

where

$$E_{\text{trap}} = \frac{1}{2} R^2, \quad (A8)$$

$R$  being the hyperradius

$$R = \sqrt{\frac{1}{3} \sum_{1 \leq i < j \leq 3} r_{ij}^2}, \quad (A9)$$

and  $r_{ij} = \|\mathbf{r}_i - \mathbf{r}_j\|$ .

Of course, the virial theorem holds for the center-of-mass problem:

$$E_{\text{CM}} = 2E_{\text{trap,CM}}. \quad (A10)$$

Subtracting Eq. (A10) from Eq. (A3) gives the virial theorem for the relative motion:

$$E = 2E_{\text{trap}} - \frac{R_t}{2} \frac{\partial E}{\partial R_t}. \quad (A11)$$

## 2. Calculation of the trapping potential energy

The spectrum for the relative motion is given by the implicit equation [33, 39]:

$$\arg \Gamma \left( \frac{1+s-E}{2} \right) = -|s| \ln R_t + \arg \Gamma(1+s) \pmod{\pi}. \quad (\text{A12})$$

Here,  $s \simeq i \cdot 1.00624$  is the only solution such that  $s^2 < 0$  of the transcendental equation [31, 72]:

$$s \cos \left( s \frac{\pi}{2} \right) - \frac{8}{\sqrt{3}} \sin \left( s \frac{\pi}{6} \right) = 0. \quad (\text{A13})$$

This allows to calculate  $\partial E / \partial R_t$ , and the virial theorem Eq. (A11) then gives:

$$E_{\text{trap}} = \frac{1}{2} \left( E + \frac{|s|}{\text{Im} \psi \left( \frac{1+s-E}{2} \right)} \right) \quad (\text{A14})$$

where  $\psi$  is the digamma function.

## 3. Evaluation of an integral and numerical check

There is of course another way to express the trapping potential energy for the relative motion:

$$E_{\text{trap}} = \langle \Psi | \frac{1}{2} R^2 | \Psi \rangle. \quad (\text{A15})$$

But the hyperradius is separable [33, 39]:

$$\Psi = \frac{F(R)}{R^2} \phi(\Omega) \quad (\text{A16})$$

where  $\Omega$  denotes the hyperangles [73]. Thus,

$$E_{\text{trap}} = \frac{\int_0^\infty dR R^3 F(R)^2}{2 \int_0^\infty dR R F(R)^2}. \quad (\text{A17})$$

The hyperradial wavefunction is [39]:

$$F(R) = R^{-1} W_{\frac{E}{2}, \frac{s}{2}}(R^2) \quad (\text{A18})$$

where  $W$  is a Whittaker function.

Using [74] we can evaluate the integral in the denominator on the right-hand-side of Eq. (A17):

$$\int_0^\infty dR R F(R)^2 = \frac{\pi \text{Im} \psi \left( \frac{1+s-E}{2} \right)}{\sinh(|s|\pi) \left| \Gamma \left( \frac{1+s-E}{2} \right) \right|^2}. \quad (\text{A19})$$

The numerator on the right-hand-side of Eq. (A17) becomes, from Eq. (A18),

$$\int_0^\infty dR R^3 F(R)^2 = \frac{1}{2} I \quad (\text{A20})$$

where

$$I = \int_0^\infty dx \left[ W_{\frac{E}{2}, \frac{s}{2}}(x) \right]^2. \quad (\text{A21})$$

We did not find this last integral in [75]. But we can evaluate it thanks to the expression of  $E_{\text{trap}}$  which we obtained from the virial theorem. Using Eq. (A14, A17, A19, A20) we get:

$$I = \frac{2 \pi}{\sinh(|s|\pi) \left| \Gamma \left( \frac{1+s-E}{2} \right) \right|^2} \left( E \text{Im} \psi \left( \frac{1+s-E}{2} \right) + |s| \right). \quad (\text{A22})$$

Numerical checks confirm this relation, thereby also confirming the virial theorem.

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