Research Article

Virial Theorem for Nonrelativistic Quantum Fields in D Spatial Dimensions

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The virial theorem for nonrelativistic complex fields in D spatial dimensions and with arbitrary many-body potential is derived, using path-integral methods and scaling arguments recently developed to analyze quantum anomalies in low-dimensional systems. The potential appearance of a Jacobian J due to a change of variables in the path-integral expression for the partition function of the system is pointed out, although in order to make contact with the literature most of the analysis deals with the $J = 1$ case. The virial theorem is recast into a form that displays the effect of microscopic scales on the thermodynamics of the system. From the point of view of this paper the case usually considered, $J = 1$, is not natural, and the generalization to the case $J \neq 1$ is briefly presented.

1. Introduction

The virial theorem has been proven using a variety of methods. Recently, a path-integral derivation of the virial theorem has been developed in the context of quantum anomalies in nonrelativistic 2D systems, or more generally, systems with $SO(2,1)$ classical symmetry [1]. The path integral is most useful in isolating the anomaly contribution to the equation of state so obtained. This method is in fact quite general and applicable for nonrelativistic systems with an arbitrary 2-body potential $V(\vec{x}_1, \vec{x}_2)$ in D spatial dimensions, even when there are no quantum anomalies present. We present such derivation in this note, extending the original derivation, using also diagrammatic analysis, and recasting the virial theorem into a general equation that relates macroscopic thermodynamics variables to the microscopic physics. As it will be shown, there is generically a Jacobian term J that may contribute to the virial theorem, regardless of the existence of a classical scaling symmetry. We will mainly concern ourselves here with the case $J = 1$ (which we term “nonanomalous”). Conclusions and Comments end the paper.

2. Virial Theorem

The work in [1] was based partly on the work by Toyoda et al. [2–4]. They postulated that spatial scalings¹

$$\vec{x}' = \lambda \vec{x}, \quad (1)$$

$$\psi'(t, \vec{x}') = \lambda^{-D/2} \psi(t, \vec{x})$$

leave the particle number density invariant:

$$d^D \vec{x} \psi^\dagger(t, \vec{x}) \psi(t, \vec{x}) = d^D \vec{x}' \psi'^\dagger(t, \vec{x}') \psi'(t, \vec{x}'). \quad (2)$$

Let us consider a nonrelativistic system whose microscopic physics is represented by a generic 2-body interaction²

$$\begin{aligned} \mathcal{L} = & \psi^* \left(i\partial_t + \frac{\nabla^2}{2} \right) \psi - \frac{1}{2} \int d^D \vec{y} \psi^*(t, \vec{x}) \psi(t, \vec{x}) \\ & \cdot V(\vec{x} - \vec{y}) \psi^*(t, \vec{y}) \psi(t, \vec{y}). \end{aligned} \quad (3)$$

Giving our system a macroscopic volume V , temperature β^{-1} , and chemical potential μ and going into imaginary time gives for the partition function

$$Z[V, \beta, \mu] = \int [d\psi^*] [d\psi] \cdot e^{-\int_0^\beta d\tau \int_V d^D \vec{x} [\psi^* (\partial_\tau - \nabla^2/2 - \mu) \psi + (1/2) \int d^D \vec{y} \psi^* (\tau, \vec{x}) \psi(\tau, \vec{x}) V(\vec{x} - \vec{y}) \psi^* (\tau, \vec{y}) \psi(\tau, \vec{y})]} \quad (4)$$

Now consider a new system with the same temperature and chemical potential but at volume $V' = \lambda^D V$:

$$Z[\lambda^D V, \beta, \mu] = \int [d\psi'^*] [d\psi'] e^{-\int_0^\beta d\tau \int_{\lambda^D V} d^D \vec{x}' [\psi'^* (\partial_\tau - \nabla'^2/2 - \mu) \psi' + (1/2) \int d^D \vec{y}' \psi'^* (\tau, \vec{x}') \psi(\tau, \vec{x}') V(\vec{x}' - \vec{y}') \psi'^* (\tau, \vec{y}') \psi'(\tau, \vec{y}')]}. \quad (5)$$

Substituting (1) into (5) gives

$$Z[\lambda^D V, \beta, \mu] = \int [d\psi^*] [d\psi] J e^{-\int_0^\beta d\tau \int_V d^D \vec{x} [\psi^* (\partial_\tau - (1/\lambda^2)(\nabla^2/2) - \mu) \psi + (1/2) \int d^D \vec{y} \psi^* (\tau, \vec{x}) \psi(\tau, \vec{x}) V(\lambda(\vec{x} - \vec{y})) \psi^* (\tau, \vec{y}) \psi(\tau, \vec{y})]}, \quad (6)$$

where J is the Jacobian for the transformation $(\psi'^*, \psi') \rightarrow (\psi^*, \psi)$. As mentioned above, our emphasis will be in the nonanomalous case, and henceforth we assume $J = 1$ (see however Conclusions and Comments). Then $Z[\lambda^D V, \beta, \mu] \equiv Z^\lambda[V, \beta, \mu]$, where the superscript λ represents a microscopic system whose kinetic energy has a factor $1/\lambda^2$ and whose potential is $V(\lambda(\vec{x} - \vec{y}))$. Note that $Z^{\lambda=1}[V, \beta, \mu] = Z[V, \beta, \mu]$.

The pressures corresponding to $Z[\lambda^D V, \beta, \mu]$ and $Z[V, \beta, \mu]$ are equal, since the intensive variables μ and β^{-1} are the same, and they correspond to the same microscopic system. The argument we just made for the pressures being the same is valid in the thermodynamic limit, based on the principle that two intensive variables determine the third via an equation of state, for example, $P = \rho T$, for an ideal gas. However, in the next section we will also provide a diagrammatical proof that the two pressures are the same.

For now assume that the pressures are equal. Then using $Z = e^{\beta PV}$, we get

$$e^{\beta PV'} - e^{\beta PV} = Z[\lambda^D V, \beta, \mu] - Z[V, \beta, \mu], \quad (7)$$

$$\text{or } e^{\beta P \lambda^D V} - e^{\beta PV} = Z^\lambda[V, \beta, \mu] - Z[V, \beta, \mu].$$

Following [1], we set $\lambda = 1 + \eta$ for infinitesimal η :

$$e^{\beta PV} D\eta \beta PV = Z^{\lambda=1}[V, \beta, \mu] + \partial_\lambda Z^\lambda[V, \beta, \mu] \Big|_{\lambda=1} \eta - Z[V, \beta, \mu] = \partial_\lambda Z^\lambda[V, \beta, \mu] \Big|_{\lambda=1} \eta = Z[V, \beta, \mu] \cdot \left\langle \int_0^\beta d\tau \int_V d^D x \left(-\psi^\dagger \nabla^2 \psi - \frac{1}{2} \int d^D \vec{y} \rho(\tau, \vec{y}) \cdot [(\vec{x} - \vec{y}) \cdot \nabla_{\vec{x}} V(\vec{x} - \vec{y})] \rho(\tau, \vec{x}) \right) \right\rangle \eta, \quad (8)$$

where we have defined $\rho(\tau, \vec{x}) \equiv \psi^\dagger(\tau, \vec{x}) \psi(\tau, \vec{x})$. Cancelling the partition functions on both sides, noting that thermal expectation values for the fields at the same τ are independent

of τ so that the τ integral pulls out a β , and denoting the kinetic energy as KE

$$DPV = 2KE - \left\langle \frac{1}{2} \int d^D \vec{x} \int d^D \vec{y} \rho(\tau, \vec{y}) \cdot [(\vec{x} - \vec{y}) \cdot \nabla_{\vec{x}} V(\vec{x} - \vec{y})] \rho(\tau, \vec{x}) \right\rangle, \quad (9)$$

which is the virial theorem in D dimensions (see (3.30) and (2.6) in [3] and [4], resp.).

3. n -Body

It is clear that this method can be generalized to the n -body case. Since by (2) the scaling transformation preserves $\int d^D \vec{x} \psi^\dagger(\tau, x) \psi(\tau, x) (\equiv \int d^D \vec{x} \rho(\tau, \vec{x}))$, an n -body term transforms as

$$\frac{1}{n!} \int \left(\prod_i^n d^D \vec{x}_i \rho(\tau, \vec{x}_i) \right) V(\vec{x}_1, \dots, \vec{x}_n) \rightarrow \frac{1}{n!} \int \left(\prod_i^n d^D \vec{x}_i \rho(\tau, \vec{x}_i) \right) V(\vec{x}'_1, \dots, \vec{x}'_n). \quad (10)$$

Setting $V(\vec{x}_1, \dots, \vec{x}_n) = \tilde{V}(\vec{z}_{\text{COM}}, \vec{z}_2, \dots, \vec{z}_n)$ where $\vec{z}_i \equiv \vec{x}_i - \vec{x}_1$ and $\vec{z}_{\text{COM}}$ is the center of mass of the $\vec{x}_i$'s gives

$$DPV = 2KE - \left\langle \frac{1}{n!} \int \left(\prod_i^n d^D \vec{x}_i \rho(\tau, \vec{x}_i) \right) \cdot [\vec{z}_{\text{COM}} \cdot \nabla_{\vec{z}_{\text{COM}}} \tilde{V}(\vec{z}_{\text{COM}}, \vec{z}_2, \dots, \vec{z}_n)] \right\rangle - \left\langle \frac{1}{n!} \cdot \int \left(\prod_i^n d^D \vec{x}_i \rho(\tau, \vec{x}_i) \right) \cdot \left[\sum_{i=2}^n \vec{z}_i \cdot \nabla_{\vec{z}_i} \tilde{V}(\vec{z}_{\text{COM}}, \vec{z}_2, \dots, \vec{z}_n) \right] \right\rangle. \quad (11)$$

For translationally invariant systems, we can ignore the derivative w.r.t. the center of mass.

4. Diagrammatic Proof of $P = P'$

To prove diagrammatically that the pressure P' corresponding to $Z[\lambda^D V, \beta, \mu]$ is equal to the pressure P corresponding to $Z[V, \beta, \mu]$, it suffices to show that $\Omega[\lambda^D V, \beta, \mu] = \lambda^D \Omega[V, \beta, \mu]$, where Ω is the grand potential. By the cluster expansion, Ω is given by the sum of connected vacuum graphs [5]. Using the Feynman rules, $\Omega[V, \beta, \mu] \propto \delta^D(0) \mathcal{M}(\beta, \mu)$, where $\delta^D(0)$ expresses conservation of momentum of the vacuum and $\mathcal{M}(\beta, \mu)$ is the Feynman amplitude³ which is independent of V , since $\mathcal{M}$ contains expressions like $(\Delta n_1 \cdots \Delta n_D / V) f(2\pi n_i / L)$ which in the continuum limit $\rightarrow (d^D k / (2\pi)^D) f(k_i)$ ⁴. Taking $\delta^D(0) \propto V$, it is clear that $\Omega[V, \beta, \mu] \propto V \mathcal{M}(\beta, \mu)$, so $\Omega[\lambda^D V, \beta, \mu] = \lambda^D \Omega[V, \beta, \mu]$ in the continuum limit.

Alternatively, since $Z[\lambda^D V, \beta, \mu] = Z^\lambda[V, \beta, \mu]$, another way to show $P' = P$ is to show that the grand potential $\Omega^\lambda[V, \beta, \mu]$ of $Z^\lambda[V, \beta, \mu]$ is larger by a factor of λ^D than $\Omega[V, \beta, \mu]$. Then $\Omega^\lambda[V, \beta, \mu] = \Omega[\lambda^D V, \beta, \mu] = \lambda^D \Omega[V, \beta, \mu]$.

The grand potential Ω^λ is given by

$$\Omega^\lambda = -\beta^{-1} \ln Z^\lambda[V, \beta, \mu]. \quad (12)$$

By the cluster expansion, Ω^λ is given by the sum of connected vacuum graphs. $Z^\lambda[V, \beta, \mu]$ and $Z[V, \beta, \mu]$ have the same macroscopic parameters and only differ in that Z^λ 's propagator is

$$\Delta^\lambda = \frac{1}{i\omega_n - k^2/2\lambda^2 - \mu} \quad (13)$$

and that the potential is

$$V^\lambda(\vec{x} - \vec{y}) = V(\lambda(\vec{x} - \vec{y})) \quad (14)$$

instead of $V(\vec{x} - \vec{y})$. Fourier transforming equation (14) gives the relationship

$$V^\lambda(\vec{k}) = \frac{V(\vec{k}/\lambda)}{\lambda^D}. \quad (15)$$

The Feynman rules for the theory say that each vertex contributes its Fourier transform $V^\lambda(\vec{k})$, where $\vec{k}$ is the momentum flowing through the vertex, and each propagator contributes (13). For vacuum graphs, all momenta $\vec{k}$ in the vertices and propagators are integrated over in loop momenta $\int (d^D k / (2\pi)^D)$. Let us make the change of variables $\int (d^D k / (2\pi)^D) = \int (\lambda^D (d^D k / (2\pi)^D \lambda^D)) = \int (\lambda^D (d^D \tilde{k} / (2\pi)^D))$ and relabel $\tilde{k}$ as $\vec{k}$. This will cause $\Delta_\lambda(i\omega, \vec{k}) = \Delta(i\omega, \vec{k}/\lambda) \rightarrow \Delta(i\omega, \vec{k})$ and $V^\lambda(\vec{k}) = V(\vec{k}/\lambda)/\lambda^D \rightarrow V(\vec{k})/\lambda^D$ in the loop integrals.

Therefore, Ω^λ is the same as Ω , except for an overall scale factor of $(1/\lambda^D)^\nu (\lambda^D)^L$, where ν is the number of vertices and L is the number of loops. Topologically, for connected

vacuum graphs of the 2-body potential, $L = \nu + 1$. So the overall scale factor becomes λ^D . Hence, $\Omega^\lambda = \lambda^D \Omega$, and therefore $P' = P$.

This generalizes to translationally invariant n -body potentials and for spontaneous symmetry breaking. Suppose the interaction is of the form

$$\int_{V'} \left(\prod_{i=1}^n d^D \vec{x}'_i \phi'^{m(i)}(\tau, \vec{x}'_i) \right) V(\vec{x}'_1, \dots, \vec{x}'_n) = \frac{\lambda^{Dn}}{\lambda^{DM/2}} \cdot \int_V \left(\prod_{i=1}^n d^D \vec{x}_i \phi^{m(i)}(\tau, \vec{x}_i) \right) V(\lambda \vec{x}_1, \dots, \lambda \vec{x}_n), \quad (16)$$

where $m(i)$ is the number of fields in the interaction with spatial coordinate $\vec{x}_i$, and $M = \sum_{i=1}^n m(i)$. For translationally invariant potentials

$$V^\lambda = \frac{V(k/\lambda)}{\lambda^{D(n-1)}}. \quad (17)$$

So

$$\Omega^\lambda = \left(\frac{\lambda^{Dn}}{\lambda^{DM/2}} \frac{1}{\lambda^{D(n-1)}} \right)^\nu (\lambda^D)^L \Omega. \quad (18)$$

Since $L = (M/2 - 1)\nu + 1$,⁵ this again gives

$$\Omega^\lambda = \lambda^D \Omega. \quad (19)$$

For a diagram with a mixture of vertices of different types, $L = \sum_i (M_i/2 - 1)\nu_i + 1$, where ν_i is the number of vertices of type i and M_i is the number of lines coming out of each vertex:

$$\Omega^\lambda = \left[\prod_i \left(\frac{\lambda^{Dn_i}}{\lambda^{DM_i/2}} \frac{1}{\lambda^{D(n_i-1)}} \right)^{\nu_i} \right] (\lambda^D)^{\sum_i (M_i/2 - 1)\nu_i + 1} \Omega = \lambda^D \Omega. \quad (20)$$

5. Scale Equation

The virial equation (9) can be recast into a different form that illustrates the effect of microscopic scales on the thermodynamics of a system. A simple way to see this is to write the potential as⁶

$$V(|\vec{x} - \vec{y}|) = \frac{f(g_i/|\vec{x} - \vec{y}|^{[g_i]})}{|\vec{x} - \vec{y}|^2}. \quad (21)$$

f is a dimensionless function whose arguments are the ratios of the couplings g_i of V to their length dimension $[g_i]$ expressed in units of $|\vec{x} - \vec{y}| ((\hbar^2/m)(1/|\vec{x} - \vec{y}|^2))$ provides units of energy⁷. Denoting $r = |\vec{x} - \vec{y}|$

$$\begin{aligned} r \frac{dV}{dr} &= -2V(r) + \frac{1}{r} \frac{df(g_i/r^{[g_i]})}{dr} \\ &= -2V(r) - \frac{1}{r^2} [g_i] g_i \frac{\partial f(g_i/r^{[g_i]})}{\partial g_i} \\ &= -2V(r) - [g_i] g_i \frac{\partial V}{\partial g_i}, \end{aligned} \quad (22)$$

where the chain rule was used in line 2. Substituting this into (9) gives

$$\begin{aligned} \text{DPV} &= 2\text{KE} + 2V - \left\langle \frac{1}{2} \int d^D \vec{x} \right. \\ &\quad \cdot \int d^D \vec{y} \rho(\tau, \vec{y}) \left(-[g_i] g_i \frac{\partial V}{\partial g_i} \right) \rho(\tau, \vec{x}) \Big\rangle = 2E \quad (23) \\ &\quad + \left\langle \frac{1}{2} \int d^D \vec{x} \int d^D \vec{y} \rho(\tau, \vec{y}) \left([g_i] g_i \frac{\partial V}{\partial g_i} \right) \rho(\tau, \vec{x}) \right\rangle. \end{aligned}$$

Rearranging

$$\begin{aligned} 2E - \text{DPV} \\ = - \left\langle \frac{1}{2} \int d^D \vec{x} \int d^D \vec{y} \rho(\tau, \vec{y}) \left([g_i] g_i \frac{\partial V}{\partial g_i} \right) \rho(\tau, \vec{x}) \right\rangle. \quad (24) \end{aligned}$$

On the LHS of (24) are macroscopic thermodynamic variables. The RHS is a measure of the microscopic physics of the system. In particular, if the potential has no scales $[g_i] = 0$ and no anomalies (i.e., $J = 1$), you get 0 on the RHS and (24) reduces to the equation of state for a nonrelativistic scale-invariant system [6].

6. Conclusion and Comments

The goal of this paper has been to highlight certain features in the derivation of the virial theorem for nonrelativistic systems, which display a potentially important omission due to the presence of the Jacobian needed in the path-integral derivation developed here. Indeed, while we set $J = 1$ at the outset in order to make contact with the literature (specifically, Toyoda et al.'s work [2–4]), (6) shows that the natural procedure would be to not assume this and keep the contribution of the Jacobian, regardless of whether or not there is a classical scaling symmetry. Obviously, in the latter case, one has to keep the Jacobian in order to incorporate the quantum anomaly as was shown in [1]. The formal mathematical steps in the general case presented here are the same as in that paper, and (24) would become

$$\begin{aligned} 2E - \text{DPV} \\ = - \left\langle \frac{1}{2} \int d^D \vec{x} \int d^D \vec{y} \rho(\tau, \vec{y}) \left([g_i] g_i \frac{\partial V}{\partial g_i} \right) \rho(\tau, \vec{x}) \right\rangle \quad (25) \\ - \frac{1}{\beta} \text{Tr} \left(\hat{\theta}_s \delta(\tau_x - \tau_y) \delta^D(\vec{x} - \vec{y}) I_2 \right), \end{aligned}$$

where $I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\hat{\theta}_s = -(1 + \vec{x} \cdot \vec{\nabla})$, and we have also used the 2×2 matrix notation of [7] (Tr includes both a matrix and functional trace).

As with the work in [1, 7], the key to assess the importance of the Jacobian term rests upon one's ability to compute its contribution in detail, which implies a careful regularization procedure and possibly also renormalization. The actual details will depend on the type of potentials considered. An interesting direction is the relativistic generalization of these ideas. Work on this is currently in progress [8].

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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Endnotes

1. Toyoda et al. introduced an auxiliary external potential that has the effect of confining the system to a volume V and, then, through a series of infinitesimal scalings and algebraic arguments derived what amounts to the equation of state, which they referred to as virial theorem. Unlike them, we are not using an external potential but simply consider a system with a large volume V (so all the typical large-volume thermodynamical considerations apply), but, like them, we are also calling virial theorem the equation of state that will be derived in this paper.
2. In this paper we set $\hbar = m = 1$.
3. $\mathcal{M}$ is the T-matrix, and $\delta^D(0) = \int (d^D x / (2\pi)^D) e^{-i0 \cdot x} \propto V$.
4. For finite volume, momenta are discrete and summed over $k_i = 2\pi n_i / L$. $\Delta n_1 \cdots \Delta n_D$ is a box of unit volume surrounding the discrete lattice point n_i . In the limit of large L , $f(2\pi n_i / L)$ is assumed not to vary much, so any point within $\Delta n_1 \cdots \Delta n_D$ not on the lattice would still contribute the same value of $f(2\pi n_i / L)$. Then $\sum_{n_i} (1/V) f(2\pi n_i / L) = \sum_{n_i} (\Delta n_1 \cdots \Delta n_D / V) f(2\pi n_i / L) \rightarrow \int (dn_1 \cdots dn_D / V) f(2\pi n_i / L) = \int (d^D k / (2\pi)^D) f(k_i)$.
5. M lines come out of each vertex, and each line coming out is $1/2$ of an internal line, so $M\nu/2 = I$ where I is the number of internal lines. The number of loops is the number of independent momenta, $L = I - \nu + 1$. So $L = (M/2 - 1)\nu + 1$.
6. We are now restricting ourselves to radial potentials.
7. As an example, consider $V(|\vec{x} - \vec{y}|) = (k/2)|\vec{x} - \vec{y}|^2 + \lambda|\vec{x} - \vec{y}|$, where the coupling k has length dimension -4 and λ has length dimension -3 . Then $f(k/|\vec{x} - \vec{y}|^{[k]}, \lambda/|\vec{x} - \vec{y}|^{[\lambda]}) = (1/2)(k/|\vec{x} - \vec{y}|^{-4}) + \lambda/|\vec{x} - \vec{y}|^{-3}$. The couplings k and λ provide the characteristic length scales.

References

- [1] C. R. Ordóñez, “Path-integral Fujikawa’s approach to anomalous virial theorems and equations of state for complex 2D bosonic fields with contact interactions, and for other systems with $\text{SO}(2,1)$ symmetry,” <http://arxiv.org/abs/1503.01384>.
- [2] T. Toyoda, “Canonical generator of conformal transformations in nonrelativistic quantum many-body systems at finite temperatures,” *Physical Review A*, vol. 48, no. 5, pp. 3492–3498, 1993.

- [3] T. Toyoda and K.-I. Takiuchi, “Quantum field theoretical reformulation of the virial theorem,” *Physica A: Statistical Mechanics and Its Applications*, vol. 261, no. 3-4, pp. 471–481, 1998.
- [4] K. Takiuchi, M. Okada, H. Koizumi, K. Ito, and T. Toyoda, “Exact relations for two-dimensional electron gas spin correlation functions,” *Physica E: Low-Dimensional Systems and Nanostructures*, vol. 6, no. 1–4, pp. 810–812, 2000.
- [5] S. Weinberg, *The Quantum Theory of Fields*, vol. 1-2, Cambridge University Press, Cambridge, UK, 2005.
- [6] F. Mancarella, G. Mussardo, and A. Trombettoni, “Energy-pressure relation for low-dimensional gases,” *Nuclear Physics B*, vol. 887, pp. 216–245, 2014.
- [7] C. L. Lin and C. R. Ordóñez, “Path-integral derivation of the nonrelativistic scale anomaly,” *Physical Review D*, vol. 91, no. 8, Article ID 085023, 6 pages, 2015.
- [8] C. L. Lin and C. R. Ordóñez, In progress.