A geometric approach to a generalized virial theorem

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Received 9 April 2012, in final form 12 August 2012
Published 13 September 2012
Online at stacks.iop.org/JPhysA/45/395210

Abstract
The virial theorem, introduced by Clausius in the field of statistical mechanics
and later applied in both classical mechanics and quantum mechanics, is studied
by making use of symplectic formalism as an approach, in the case of both the
Hamiltonian and Lagrangian systems. The possibility of establishing virial-like
theorems from one-parameter groups of non-strictly canonical transformations
is analysed; the case of systems with a position-dependent mass is also
discussed. Using the modern symplectic approach to quantum mechanics, we
arrive at the quantum virial theorem in full analogy with the classical case.

PACS numbers: 02.40.Yy, 45.20.Jj, 03.65.Ca
Mathematics Subject Classification: 37J05, 70H05, 70G45, 81Q70

1. Introduction
In 1870 (see [1] for an historical account), Clausius introduced the virial function for a
one-particle system

\[ G(r, v) = m \cdot v \]  

for studying the motion of a particle of mass \( m \) under the action of a force \( F \). Then, using such
a function and the Newton second law, he proved that when either the motion is periodic of
period \( T \), or the motion is not periodic but the possible values of the function \( G \) are bounded
and we take the limit of \( T \) going to infinity, the time average over a time interval \( T \) of the
kinetic energy \( E_k(v) \) is given by

\[ \langle \langle E_k(v) \rangle \rangle = -\frac{1}{2} \langle \langle r \cdot F \rangle \rangle, \]  

so that, in the particular case of a conservative force, he obtained

\[ \langle \langle E_k(v) \rangle \rangle = \frac{1}{2} \langle \langle r \cdot \nabla V \rangle \rangle. \]
If the potential $V$ is homogeneous of degree $k$, Euler’s theorem of homogeneous functions implies that $r \cdot \nabla V = k V$, and therefore, $2 \langle\langle E_c(v)\rangle\rangle = k \langle\langle V(r)\rangle\rangle$, that leads to the following values for the averages of the kinetic energy and the potential

$$\langle\langle E_c(v)\rangle\rangle = \frac{kE}{k + 2}, \quad \langle\langle V(r)\rangle\rangle = \frac{2E}{k + 2},$$

where $E$ is the total energy [2]. For instance in the harmonic oscillator case, with $k = 2$, and in the Kepler problem with negative energy, with $k = -1$, we obtain, respectively,

$$\langle\langle E_c(v)\rangle\rangle = \langle\langle V(r)\rangle\rangle = \frac{1}{2}E,$$

$$\langle\langle E_c(v)\rangle\rangle = -E, \quad \langle\langle V(r)\rangle\rangle = 2E.$$

The virial theorem was originally introduced in classical statistical mechanics (studied by Clausius) but later became important in many other different branches of physics. The quantum mechanical version of the theorem is due to Born, Heisenberg and Jordan [3] and presently it is a tool frequently used in many body quantum mechanics (e.g. systems of fermions) and in molecular physics; in addition, this matter has also been related to certain fundamental questions arising in nonrelativistic quantum mechanics as the Hellmann–Feynman theorem (see [4–18] and the references therein). We also mention the importance of the virial theorem in solar and stellar astrophysics [19]. The important point therefore is the wide range of applicability of the virial theorem with applications ranging from dynamical (even relativistic) and thermodynamical systems, to the dust and gas of interstellar space, as well as cosmological considerations of the universe as a whole and in other discussions concerning the stability of clusters, galaxies and clusters of galaxies [20], or giving information on the masses of bound systems being the main reason we think that dark matter exists [21, 22]. Of course this virial theorem provides less information than the equations of motion but it is simpler to apply and gives us some information on systems whose complete analysis may defy description.

After this standard approach to the virial theorem several questions appear. For instance, the role played by the function $G$ and also the reason why the relation is simpler for power law potentials. There are more general results known as hypervirial theorems introduced in [5] whose natural framework is the theory of locally Hamiltonian dynamical systems. Moreover, quantum mechanics is also a particular case of this more general theory which suggests to us to analyse the problem from this new perspective, that then enables us to develop the corresponding theorem in quantum mechanics. The main point is that the standard theory is always related to scaling and dilation transformations [10, 11, 4, 23, 24]; there is no room for such transformations when the configuration space is no longer a linear space but there exist, for example, holonomic constraints.

Concerning the last question, the search for generalizations is a matter that has been studied by different authors from different viewpoints (in fact the quantum mechanical virial for the expectation values of a quantized system can be considered as a generalization of the original virial theorem). Here we mention a version for discrete maps [25] or a virial theorem in a spherical geometry [26]. An interesting result is that it has been related with Noether’s theorem and with the invariance properties of the Lagrange function [27, 28].

The main aim of this paper is to develop a deeper analysis of the virial theorem, both in classical and quantum mechanics, using the modern theory of Hamiltonian systems in symplectic manifolds as an approach, and therefore including Lagrangian formulations.

The paper is organized as follows. In section 2, a generalized virial theorem is established in the framework of the theory of Hamiltonian systems in symplectic manifolds. In section 3, the virial theorem is related with the Lagrangian formalism by considering the Lagrangian systems as Hamiltonian systems in tangent bundle manifolds; we prove that not only
point symmetries of $L$ are useful in classical mechanics but more general transformations modifying Lagrangian formalism by a factor, can be used to establish virial type relations. Two generalizations of the virial theorem are studied in sections 4 and 5. In section 4 we consider the case of systems with a position-dependent mass and in section 5 we relate the theorem with the theory of non-strictly canonical transformations. We study in section 6 the virial theorem in quantum mechanics using quantum symplectic formalism as an approach. Finally, in section 7 we make some comments and present some open questions.

2. Virial theorem for Hamiltonian systems in symplectic manifolds

To make the paper self-contained and to introduce the notation, we recall some concepts of the geometrical approach to the theory of Hamiltonian systems. Then we consider the virial theorem from a geometric perspective.

If $(M, \omega)$ is a symplectic manifold, the Hamiltonian vector field $X_F$ defined by the function $F$ on $M$ is the solution of the equation

$$i(X_F)\omega = dF.$$ 

A dynamic is given by choosing a Hamiltonian $H$ through the corresponding Hamiltonian vector field $X_H$. For instance, the phase space $M$ of the Hamiltonian systems studied in classical mechanics is the cotangent bundle $T^*Q$ of the configuration space $Q$ [29–32]. They are endowed with a canonical exact symplectic structure $\omega_0$ that in cotangent bundle coordinates $(q_i, p_i)$, $i = 1, \ldots, n$, is given by $\omega_0 = dq_i \wedge dp_i$, i.e. $\omega_0 = -d\theta$, with $\theta = p_i dq_i$, where the summation on repeated indices is understood. The Lagrangian formulation for regular Lagrangian functions $L$ is also an example. The manifold is the tangent bundle $M = TQ$ and the symplectic structure is not canonical but depends on the choice of the function $L$.

The Poisson bracket of two functions $F_1$ and $F_2$ in a symplectic manifold $(M, \omega)$ is defined as the symplectic product of the corresponding Hamiltonian vector fields

$$\{F_1, F_2\} = \omega_0(X_{F_1}, X_{F_2}) = X_{F_2}F_1.$$ 

It can be verified that, when written in Darboux coordinates, the integral curves of $X_H$ are solutions of the Hamilton equation and for the Poisson brackets we recover the expression usually given in classical mechanics.

The flow of the Hamiltonian vector field $X_H$ on a symplectic manifold $(M, \omega)$ commutes with the action of $X_H$; thus, if $F$ is a function in $M$ we have

$$\phi^*_t(X_HF) = X_H(\phi^*_tF) = \frac{d}{ds}[\phi^*_s(\phi^*_tF)]|_{s=0} = \frac{d}{ds}(\phi^*_sF)|_{s=0} = \frac{d}{ds}[\phi^*_tF]|_{s=0}.$$ 

For a given function $G$ which is going to play the role of the function (1) we obtain

$$\frac{d}{dt}(\phi^*_tG) = \phi^*_t(\{G, H\}) = -\phi^*_t(X_GH),$$ 

and integrating this relation with respect to the time from $t = 0$ to $t = T$, we arrive at

$$\frac{1}{T} [G \circ \phi_T - G] = -\frac{1}{T} \int_0^T (X_GH) \circ \phi_t dt = \frac{1}{T} \int_0^T \{G, H\} \circ \phi_t dt.$$ (4)

This result is sometimes known as the hypervirial theorem [5]: if either the motion is periodic of period $T$, or when $G$ remains bounded in its time evolution, taking the limit $T \to \infty$:

$$\langle \{G, H\} \rangle = 0.$$ (5)
Actually a family of hypervirial theorems was introduced in [5] with an especial emphasis on homogeneous first-degree functions in momenta, but the formulation is still valid for any choice of the function $G$.

In the particular case $Q = \mathbb{R}^3$ the phase space is the cotangent bundle $M = T^*\mathbb{R}^3$ which is endowed with its canonical symplectic structure $\omega_0$. Then the Hamiltonian vector field $X_G$ of the Clausius function $G$ given by $G(r, p) = r \cdot p$, takes the form

$$X_G = \sum_{i=1}^{3} \left( x^i \frac{\partial}{\partial x^i} - p_i \frac{\partial}{\partial p_i} \right),$$

and represents the generator of dilations in $M = T^*\mathbb{R}^3$: the infinitesimal dilations in $Q = \mathbb{R}^3$ are generated by $D = \sum_{i=1}^{3} x^i \partial / \partial x^i$ and its cotangent lift to the phase space as an infinitesimal generator of point transformations, gives us $X_G$.

When $H$ is a natural Hamiltonian (kinetic term plus a potential)

$$H(r, p) = \frac{1}{2m} p^2 + V(r) = H_0(p) + V(r),$$

the action of $X_G$ on $H$ becomes $(X_GH)(r, p) = -2H_0(p) + r \cdot \nabla V$. Therefore, the relation (4) is

$$\frac{1}{T} [G \circ \phi_T - G] = \langle\langle 2H_0 \rangle\rangle \neq \langle\langle r \cdot \nabla V \rangle\rangle,$$

and, in a periodic motion of period $T$, or in the limit $T \to \infty$ when $G$ remains bounded in its time evolution, (5) reduces to the standard result in the Hamiltonian framework

$$\langle\langle 2H_0 \rangle\rangle = \langle\langle r \cdot \nabla V \rangle\rangle.$$

Summarizing, the standard virial and hypervirial theorems can be considered as particular cases of more general properties stated for Hamiltonian systems in symplectic manifolds.

3. The virial theorem in Lagrangian formalism

It has been shown (see [33, 34]) that a (regular) Lagrangian system is a particular case of a Hamiltonian system on a symplectic manifold, on the tangent bundle $TQ$ of the configuration space $Q$ and with a symplectic structure depending on the Lagrangian function. We can therefore translate the theory developed in Hamiltonian formalism to a Lagrangian framework.

Two important geometric ingredients are the Liouville vector field $\Delta$, that is the generator of dilations along the fibres, and the vertical endomorphism $S$. Given a differentiable function $L$ on $TQ$, we can construct a semibasic 1-form $\theta_L \in \bigwedge^1(TQ)$, an exact two-form $\omega_L \in \bigwedge^2(TQ)$ and an energy function by

$$\theta_L = S^*(dL), \quad \omega_L = -d\theta_L, \quad E_L = \Delta(L) - L.$$

If the Lagrangian $L$ is regular then $\omega_L$ is symplectic and the Lagrangian dynamics are given by the uniquely determined vector field $X_L$ solution of the equation

$$i(X_L)\omega_L = dE_L.$$

$X_L$ satisfies the second-order property $S(X_L) = \Delta$, and the curves on $Q$ that are a projection of the integrals curves of $X_L$ in $TQ$, satisfy the second-order Euler–Lagrange equations.

To summarize, a regular Lagrangian $L$ determines a symplectic structure $\omega_L$ in $TQ$ and the Lagrangian formalism is an instance of the theory of Hamiltonian dynamical systems. The virial theorem reduces in this case to

$$\frac{1}{T} [G \circ \phi_T - G] = \frac{1}{T} \int_0^T (X_G(E_L)) \circ \phi_t \, dt = \frac{1}{T} \int_0^T \{G, E_L\}_L \circ \phi_t \, dt,$$  

(6)
where $X_G$ is the vector field such that $i(X_G)\omega_L = dG$, and $[G, E_L]_L = \omega_L(X_G, X_L)$. If the motion is periodic of period $T$, or if the function $G$ remains bounded in its time evolution, when taking the limit of $T$ going to infinity we obtain

$$\langle \langle X_G(E_L) \rangle \rangle = 0.$$  

(7)

Let us consider the simple case of a natural Lagrangian defined in $Q = \mathbb{R}^3$

$$L(r, v) = \frac{1}{2}mv^2 - V(r).$$

The energy function and the symplectic form are given by

$$E_L(r, v) = \frac{1}{2}mv^2 + V(r), \quad \omega_L = m \, dr \wedge dv,$$

and when $G$ is the observable function $G(r, v) = m \cdot v$, then

$$X_G = \sum_{\ell=1}^3 \left( x^\ell \frac{\partial}{\partial x^\ell} - v^\ell \frac{\partial}{\partial v^\ell} \right),$$

or written in a simpler way

$$X_G(r, v) = r \cdot \nabla_r - v \cdot \nabla_v.$$

Note that here the minus sign shows that $X_G$ is the Hamiltonian vector field defined by $G$ but it is not the lift to the tangent bundle $TQ$ of the infinitesimal generator of dilations in $Q = \mathbb{R}^3$, but $X_G$ depends on the function $L$. Then we have

$$X_G(E_L) = r \cdot \nabla V(r) - v \cdot (mv),$$

and we thus recover the original virial theorem (3).

One-parameter groups of point symmetries of the Lagrangian lead to constants of motion but infinitesimal transformations that are not symmetries of $L$ can also play a role in establishing virial theorems. Next we give a geometric approach to a result of [27], which is a particular case of a more general result to be given in the next section where one-parameter groups of non-strictly canonical transformations are to be considered.

It is important to remember that if $\phi$ is a diffeomorphism in $TQ$ that is obtained from a diffeomorphism $\varphi$ in the base $Q$, that is $\phi = T \varphi$, then the following two properties [34] are satisfied

$$\phi^* \theta_L = \theta_{\phi^*L}, \quad \phi^* E_L = E_{\phi^*L}.$$  

Correspondingly, at the infinitesimal level, for a vector field $X \in \mathfrak{X}(TQ)$ that is a complete lift, $X = Y^c$, of a vector field in the base, $Y \in \mathfrak{X}(Q)$, we have

$$\mathcal{L}_X \theta_L = \theta_{X(L)}, \quad X(E_L) = E_{X(L)},$$

where $\mathcal{L}_X$ denotes the de Lie derivative with respect to $X$.

In the following, given a 1-form $\alpha \in \bigwedge^1(Q)$ we denote by $\tilde{\alpha}$ a function on $TQ$ that is linear in the fibres defined by $\tilde{\alpha}(q, v) = \langle \alpha_q, v \rangle$. Then, as $\theta_L$ is the pull-back of $\alpha$ and $E_{\tilde{\alpha}} = 0$, $L' = L + \tilde{\alpha}$ defines the same Hamiltonian system on $TQ$ as $L$ if (and only if) $\alpha$ is closed. Hence a vector field $X = Y^c$, $Y \in \mathfrak{X}(Q)$, such that $X(L) = \tilde{\alpha}$, with $\alpha$ a closed form in $Q$, is a symmetry of the Hamiltonian dynamical system $(TQ, \omega_L, E_L)$ defined by $L$. We can at least locally write $\alpha = d\tilde{h}$ where $\tilde{h}$ is the pullback through the tangent bundle projection of a function $h$ in $Q$. Note that, making use of this notation, the property $d\tilde{h} = \Gamma(\tilde{h})$, true for any vector field $\Gamma$ on $TQ$ satisfying the second order differential equation $v^b$ condition, $S(\Gamma) = \Delta$.

**Theorem 1.** Let $L$ be a regular Lagrangian and $X = Y^c$ a vector field on $TQ$ such that $X(L) = aL + \tilde{h}$, with $a \in \mathbb{R}$. Then:
(i) the vector field $X$ is a symmetry of the dynamical vector field $X_L$;
(ii) the function $G = i(X)\theta_L - \tilde{h}$ is such that $X_L(G) = aL$.

Proof.

(i) First, we have $\theta_{X(L)} = a\theta_L + d\tilde{h}$, and therefore $\omega_{X(L)} = a\omega_L$. Furthermore, the energy $E_{X(L)}$ is given by $E_{X(L)} = aE_L$. Consequently $L_X\omega_L = \omega_{X(L)} = \omega_L$ and $L_XE_L = E_{X(L)} = aE_L$. Then we have

\[ i[X, X_L] = L_X(i[X_L] \omega_L) - i(X_L)(L_X\omega_L) = L_X(dE_L) - i(X_L)(a\omega_L) = 0. \]

Hence $[X, X_L]$ is in the kernel of $\omega_L$ and, as $\omega_L$ is symplectic (and therefore regular), the kernel is trivial and we arrive at $[X, X_L] = 0$.

(ii) Since $X$ commutes with $X_L$, we then have $L_X(i(X)\theta_L) = i(X)(L_X\theta_L)$. Therefore

\[ L_X(i(X)\theta_L) = i(X)(L_X\theta_L) = i(X)dL = X(L) = aL + \tilde{h} = aL + X_L(h), \]

and from here we get

\[ X_L(G) = X_L(i(X)\theta_L - \tilde{h}) = aL. \]

The result of this theorem can be used to obtain the following virial type relation

\[ \frac{1}{t_2 - t_1}[G(t_2) - G(t_1)] = \frac{a}{t_2 - t_1} \int_{t_1}^{t_2} X_L(G) \, dt = \frac{a}{t_2 - t_1} \int_{t_1}^{t_2} L \, dt, \]

and consequently, in a periodic motion of period $T$ we can take $t_1 = 0$ and $t_2 = T$ and obtain $\langle \langle L \rangle \rangle = 0$. In the more general case,

\[ \frac{1}{t_2 - t_1}[G(t_2) - G(t_1)] = a\langle \langle L \rangle \rangle, \]

where $L$ is averaged in $t \in [t_1, t_2]$ and we can also take the limit when $t_1 \rightarrow -\infty, t_2 \rightarrow \infty$.

As an example we consider the vector field $X$ that is the complete lift of the vector field $Y$ generating dilations in $Q$, given by

\[ X = Y^c = \sum_{i=1}^{3} \left( x^i \frac{\partial}{\partial x^i} + v^i \frac{\partial}{\partial v^i} \right). \]

Then the action of $X$ on the Lagrangian $L$ of the harmonic oscillator is given by

\[ X(L) = X \left( \frac{1}{2} m v^2 - \frac{1}{2} m \omega^2 x^2 \right) = 2L, \]

so that $X$ is a symmetry of dynamical vector field of the harmonic oscillator with $a = 2$. Hence we have the following property

\[ \frac{1}{t_2 - t_1} \left[ \sum_{i=1}^{3} x^i \frac{\partial L}{\partial x^i} \right]_{t_1}^{t_2} = 2 \langle \langle L \rangle \rangle, \]

where on the right-hand side $L$ is averaged in $t \in [t_1, t_2]$. Once again we can particularize the time interval $t_2 - t_1$ for a periodic $T$ of the system (this result is also true for the limit $t_2$ going to infinity, since the motion is always bounded and periodic).

This example can be obtained as a particular case when starting with the general one-dimensional case of a natural Lagrangian $L$ given by

\[ L(x, v) = \frac{1}{2} m v^2 - V(x). \]
Let $Y$ be the vector field in $\mathbb{R}$ given by
\[ Y = \xi(x) \frac{\partial}{\partial x}, \] (9)
whose complete lift $X$ is given by
\[ X(x, v) = Y^c(x, v) = \xi(x) \frac{\partial}{\partial x} + \left(v \frac{\partial \xi}{\partial x}\right) \frac{\partial}{\partial v}, \] (10)
then we have
\[ (X(L))(x, v) = -\xi(x)V'(x) + mv\xi'(x)v, \]
and therefore the condition $Y^cL = aL$, with $a \in \mathbb{R}$ is written
\[ \begin{cases} 2\xi'(x) = a, \\ \xi(x)V'(x) = aV(x) \end{cases} \]
from where we obtain
\[ \xi(x) = \frac{1}{2}ax + C, \quad V(x) = C_2(x + C_1)^2, \]
and we recover, as a particular case for $a = 2$, the above mentioned harmonic oscillator.

### 4. The virial theorem for position-dependent mass systems

The study of systems with position-dependent mass has received a lot of attention recently, with the non-commutativity of mass and momentum being a difficulty to be taken into account in the quantization process [35–37]. From the classical point of view the situation corresponds to systems for which the kinetic energy is defined from a non-Euclidean metric. Therefore, the systems are not invariant under dilation and one should look for alternative functions giving rise to a virial-like theorem. The more general theory we have developed here allows us to deal with this more general case.

We now consider the one-dimensional case of a Lagrangian $L$ given by
\[ L(x, v) = \frac{1}{2} m(x) v^2 - V(x), \] (11)
where $m(x)$ is a positive differentiable function.

According to the formalism presented in the preceding section, we must look for a vector field $Y$ in $\mathbb{R}$ given by (9) and its corresponding complete lift $X = Y^c$ (10) such that $X(L) = aL$, with $a \in \mathbb{R}$. Then as we have
\[ (X(L))(x, v) = \frac{1}{2}\xi(x)m'(x)v^2 - \xi(x)V'(x) + v\xi'(x)m(x)v, \]
the mentioned condition leads to
\[ \begin{cases} 2\xi'(x) + \xi(x)\mu(x) = a, \\ \xi(x)V'(x) = aV(x) \end{cases} \]
where $\mu(x) = m'(x)/m(x)$.

The first equation is an inhomogeneous linear differential equation with a general solution:
\[ \xi(x) = \frac{1}{\sqrt{m(x)}} \left( C_1 + \frac{a}{2} \int_0^x \sqrt{m(\xi)} \, d\xi \right). \] (12)
Consequently, the vector field $Y$ is a sum of two vector fields. The first one $Y_1$, which is obtained putting $a = 0$ in the preceding expression, preserves the kinetic term $T$ and it therefore represents a Killing vector of the associated metric. The second one $Y_2$ is given by
\[ Y_2 = \frac{a}{2} \frac{1}{\sqrt{m(x)}} \left( \int_0^x \sqrt{m(\xi)} \, d\xi \right) \frac{\partial}{\partial x}. \]
The potential energy $V(x)$ is then given by

$$V(x) = C_2 \exp \left( \int_a^x \frac{a}{\xi(\zeta)} \, d\zeta \right),$$

while the function $G$ is

$$G(x, v) = m(x) \xi(x) v = \sqrt{m(x)} \left( C_1 + \frac{a}{2} \int_0^x \sqrt{m(\zeta)} \, d\zeta \right) v,$$

and the virial theorem provides the relation

$$\langle \langle X_L(G) \rangle \rangle = a \langle \langle L \rangle \rangle.$$

As an example we can consider the differential equation for a one-dimensional nonlinear oscillator studied in 1974 by Mathews and Lakshmanan [38]

$$(1 + \lambda q^2) \ddot{q} - \lambda \dot{q}^2 q + \alpha^2 q = 0, \quad \lambda > 0.$$

The general solution takes the form $q(t) = A \sin(\omega t + \phi)$, with the following additional restriction linking frequency and amplitude

$$\omega^2 = \frac{\alpha^2}{1 + \lambda A^2}.$$

The system admits a Lagrangian formulation with the Lagrangian:

$$L_\lambda(q, \dot{q}) = \frac{1}{2} \frac{1}{1 + \lambda q^2} (q^2 - \alpha^2 q^2).$$

It is a system with nonlinear oscillations with a frequency (or period) showing amplitude dependence. We can also allow negative values for $\lambda$, but when $\lambda < 0$ the values of $x$ are limited by the condition $|x| < 1/\sqrt{\lambda}$ [39].

In the limit $\lambda \to 0$ we recover the equation of motion and the Lagrangian of the harmonic oscillator. It can also be considered as an oscillator with a position-dependent effective mass which depends on $\lambda$, $m_\lambda(q) = (1 + \lambda q^2)^{-1}$. A quantum version of this model was studied in [39], a superintegrable generalization to several degrees of freedom in classical mechanics was proposed in [40] and the corresponding quantum version was studied in [41–43].

In order to deal simultaneously with all possible values of $\lambda$, it is convenient to introduce the following $\kappa$-trigonometric functions where $\kappa \in \mathbb{R}$:

$$C_\kappa(x) = \begin{cases} \cos \sqrt{\kappa}x & \text{if } \kappa > 0, \\ 1 & \text{if } \kappa = 0, \\ \cosh -\sqrt{-\kappa}x & \text{if } \kappa < 0, \end{cases}$$

$$S_\kappa(x) = \begin{cases} \frac{1}{\sqrt{\kappa}} \sin \sqrt{\kappa}x & \text{if } \kappa > 0, \\ x & \text{if } \kappa = 0, \\ \frac{1}{\sqrt{-\kappa}} \sinh \sqrt{-\kappa}x & \text{if } \kappa < 0, \end{cases}$$

and the $\kappa$-dependent tangent function $T_\kappa(x)$ defined in the natural way, $T_\kappa(x) = S_\kappa(x)/C_\kappa(x)$. The fundamental properties of these curvature-dependent trigonometric-hyperbolic functions are

$$C_\kappa^2(x) + \kappa S_\kappa^2(x) = 1,$$

and

$$C_\kappa(2x) = C_\kappa^2(x) - \kappa S_\kappa^2(x), \quad S_\kappa(2x) = 2 S_\kappa(x) C_\kappa(x).$$

It can also verified that the derivatives of these functions are given by

$$\frac{d}{dx} S_\kappa(x) = C_\kappa(x), \quad \frac{d}{dx} C_\kappa(x) = -\kappa S_\kappa(x).$$
as well as
\[ \frac{d}{dx} T_\kappa (x) = \frac{1}{C_\kappa^2 (x)}, \quad \frac{d}{dx} T_\kappa^{-1} (x) = \frac{1}{1 + \kappa x^2}. \]

In the case we are considering, the position-dependent mass \( m(q) \) is given by \( m(q) = (1 + \lambda q^2)^{-1} \) and the function \( \xi(q) \) becomes
\[ \xi(q) = \sqrt{1 + \lambda q^2} \left( C_1 + \frac{a}{2} \int_q^u \frac{dq'}{\sqrt{1 + \lambda q'^2}} \right). \]

Under the change of variables \( q = S_\kappa (u) \) with \( \kappa = -\lambda \), and therefore \( \sqrt{1 + \lambda q^2} = C_\kappa (u) \), we obtain
\[ \xi(u) = C_\kappa (u) \left( C_1 + \frac{a}{2} u \right), \]
or rewritten in terms of the original variables
\[ \xi(q) = \sqrt{1 + \lambda q^2} \left( C_1 + \frac{a}{2} S_\kappa^{-1}(q) \right). \]

The potential energy \( V(q) \) is then given by the integral
\[ V(q) = C \exp \left( \int_q^u \frac{a}{\xi(\zeta)} d\zeta \right) = C \exp \left( \int_0^u \frac{a}{C_1 + \frac{a}{2} \zeta} d\zeta \right), \]
that leads to the value
\[ V(q) = C \left( 1 + \frac{a}{2C_1} u \right)^2 = C \left( 1 + \frac{a}{2C_1} S_\kappa^{-1}(q) \right)^2. \]

For such a potential the function \( G \) is given by
\[ G(q, v) = \frac{v}{\sqrt{1 + \lambda q^2}} \left( C_1 + \frac{a}{2} S_\kappa^{-1}(q) \right), \]
and the virial theorem provides the relation
\[ \langle (X_L(G)) \rangle = a \langle (L) \rangle. \]

We close this section with a comment on the general case of the Lagrangian (11). If we introduce a new coordinate \( u \) given by the relation
\[ u(x) = \int_0^x \sqrt{m(\zeta)} d\zeta \]
and such that \( du/dx = \sqrt{m(x)} \), then the expression for the function \( \xi(x) \) becomes
\[ \xi = \frac{1}{\sqrt{m(x)}} \left( C_1 + \frac{1}{2} u(x) \right), \]
and the potential \( V(x) \) is just a quadratic function in the function \( u(x) \)
\[ V(x) = C_2 \left( 1 + \frac{a}{2C_1} u(x) \right)^2. \]
5. The virial theorem and non-strictly canonical transformations

In classical mechanics a transformation that preserves the Poisson brackets up to a multiplicative constant, called the valence of the transformation, is said to be a canonical transformation [44] (if the valence is the unity then the transformation is strictly canonical, otherwise it is non-strictly canonical). In differential geometric terms, a vector field $X$ on a symplectic manifold $(M, \omega)$ is the generator of a one-parameter group of non-strictly canonical transformations if there exists a real number $a \neq 0$ such that $\mathcal{L}_X \omega = a \omega$.

Given such a vector field $X$, let us choose a vector field $X_1$ such that

$$i(X_1)\omega = \theta,$$

because then

$$\mathcal{L}_{X_1} \omega = i(X_1) d\theta + d(i(X_1) \theta) = -i(X_1) \omega + d(i(X_1) \theta) = -\theta + d(i(X_1) \theta),$$

and therefore

$$\mathcal{L}_{X_1} \omega = -\mathcal{L}_{X_1} (d\theta) = -d\mathcal{L}_{X_1} \theta = d\theta = -\omega.$$ 

Note, however, that manifolds exist that do not admit exact symplectic forms, because of topological obstructions. For instance, there is no exact volume form in a compact manifold $M$, as a consequence of the Stokes theorem, while if $\omega$ is an exact symplectic form in a $2n$-dimensional manifold $M$, then $\omega^n$ would be an exact volume form in $M$.

Anyway, if $X_1$ satisfies (15), then $X + aX_1$ is a locally-Hamiltonian vector field since it satisfies

$$\mathcal{L}_{X+aX_1} \omega = a\omega - a\omega = 0.$$ 

That means the existence of a closed 1-form $\alpha$ such that

$$i(X)\omega + ai(X_1)\omega = \alpha.$$ 

Conversely, given a closed 1-form $\alpha$ the preceding relation defines a vector field generating a one-parameter (local) group of non-strictly canonical transformations $\phi_\epsilon$ with valence $e^a \epsilon$.

In a Darboux chart for which

$$\omega = \sum_{i=1}^n dq^i \wedge dp_i,$$

we can choose as $\theta$ (such that $\omega = -d\theta$) the 1-form given by

$$\theta = \frac{1}{2} \sum_{i=1}^n \left( p_i dq^i - q^i dp_i \right),$$

and then the vector field $X_1$ is the dilation generator

$$X_1 = -\frac{1}{2} \sum_{i=1}^n \left( q^i \frac{\partial}{\partial q^i} + p_i \frac{\partial}{\partial p_i} \right).$$

If $\alpha = d\phi$ (at least locally), then we can write $X$ as follows

$$X = \phi_\epsilon - aX_1,$$

and then the action of $X$ on the Hamiltonian is given by

$$X(H) = [H, \phi] - aX_1(H).$$
Using a Darboux chart, if we assume that $H(q, p) = H_0(p) + V(q)$, with $H_0$ a quadratic function, we find

$$X_1(H) = -\frac{1}{2} \left( 2H_0(p) + \sum_{i=1}^{n} q_i \frac{\partial V}{\partial q} \right)$$

and taking into account that

$$\{ H, \sum_{k=1}^{n} q_k p_k \} = \sum_{k=1}^{n} q_k \frac{\partial V}{\partial q_k} - \sum_{k=1}^{n} p_k \frac{\partial H_0}{\partial p_k} = \left( \sum_{k=1}^{n} q_k \frac{\partial V}{\partial q_k} \right) - 2H_0(p)$$

we obtain

$$X(H) = \{ H, \phi \} + a \sum_{i=1}^{n} q_i p_i + 2aH_0.$$ 

Now integrating in time from $t = 0$ to $t = T$ and, as according to (5) the average of the Poisson bracket vanishes, we obtain, in the limit of $T$ going to infinity (or when the motion is periodic with periodic $T$), the following equality

$$2a\langle\langle H_0 \rangle\rangle = \langle\langle X(H) \rangle\rangle.$$ 

Finally, if there exists $b \in \mathbb{R}$ such that $X(H) = bH$, then $\{ H, \phi \} - aX_1(H) = bH$, and we arrive at

$$2a\langle\langle H_0 \rangle\rangle = bE.$$ 

As a concrete example, let us consider a homogeneous potential of degree $d \neq 2$, i.e.

$$\sum_{k=1}^{n} q_k^d \frac{\partial V}{\partial q^d} = dV, \quad d \neq 2,$$

and the one-parameter group of transformations generated by

$$X_a = \sum_{i=1}^{n} \left( \frac{a - 1}{2} q_i \frac{\partial}{\partial q_i} + \frac{a + 1}{2} p_i \frac{\partial}{\partial p_i} \right).$$

One immediately computes

$$\mathcal{L}_{X_a} \omega = a\omega$$

and, therefore, $X_a$ generates non-strictly canonical transformations. Besides, if we chose $a = (d + 2)/(d - 2)$ we have

$$X_a(H) = \frac{2d}{d - 2}H,$$

i.e. $b = 2d/(d - 2)$, and we are in the situation described before. Hence, using the previous result we have

$$(d + 2)\langle\langle H_0 \rangle\rangle = dE,$$

or equivalently

$$2\langle\langle H_0 \rangle\rangle = d\langle\langle V \rangle\rangle,$$

which is the standard form of the virial theorem for homogeneous potentials. Another example, combining the scaling of momenta with translations in coordinates, was used for the Toda lattice in [28].

Finally, it is to be remarked that the case we considered in the preceding section of infinitesimal groups of point transformations such that $X(L) = aL$ (up to a gauge term) is only a particular case (with $a = b$) of the preceding situation for the Hamiltonian system ($TQ, \omega_L, E_L$).
6. The virial theorem in quantum mechanics

There has been an increasing interest in the geometric formulation of quantum mechanics as a particular case of a Hamiltonian dynamical system (see e.g. [45–47] and the references therein), the main difference with the classical mechanics case being that the symplectic manifold is a (maybe infinite-dimensional) Hilbert space seen as a real Banach space. More specifically, a separable complex Hilbert space \((\mathcal{H}, \langle \cdot, \cdot \rangle)\) can be considered as a real linear space, then denoted \(\mathcal{H}_R\). The norm in \(\mathcal{H}\) defines a norm in \(\mathcal{H}_R\), where \(\|v\|_R = \|v\|_C\). Of course, more accurately one knows that the pure states in quantum mechanics are rays rather than vectors, but this fact can also be taken into account by replacing the Hilbert space for the corresponding projective Hilbert space.

The real linear space \(\mathcal{H}_R\) is endowed with a natural symplectic structure as follows:

\[
\omega(u, v) = 2\text{Im} \langle u, v \rangle.
\]

In fact, \(\omega\) is a skew-symmetric real bilinear map and the \(\mathbb{R}\)-linear map \(\hat{\omega} : \mathcal{H}_R \rightarrow \mathcal{H}_R^*\) defined by \(\hat{\omega}(u)v = \omega(u, v)\) is not only injective but it is also an isomorphism, because if \(\hat{\omega}(u) = 0\), then \(\hat{\omega}(u)(iu) = 2\langle u, u \rangle = 0\), and consequently \(u = 0\). Riesz theorem can be used to prove that the map is also surjective.

The Hilbert space \(\mathcal{H}_R\) can be considered as a real manifold modelled by a Banach space admitting a global chart. Moreover, for each \(v \in \mathcal{H}_R\) the tangent space \(T_v \mathcal{H}_R\) is canonically isomorphic to the own \(\mathcal{H}_R\): we associate with \(w \in \mathcal{H}_R\) the vector in the tangent space \(T_v \mathcal{H}_R\) defined by

\[
\chi_v(w)f = \frac{d}{dt} f(v + tw)_{t=0},
\]

where the function \(f\) is differentiable in the neighbourhood of the vector \(v\), \(f \in C^\infty(v)\). This is an isomorphism \(\chi_v : \mathcal{H}_R \rightarrow T_v \mathcal{H}_R\) providing us with an identification which corresponds to the one given by the free transitive action of the Abelian group of translations on \(\mathcal{H}_R\).

One can prove (see later on) that the constant symplectic structure \(\omega\) in \(\mathcal{H}_R\), considered as a Banach manifold, is exact, i.e. there exists a 1-form \(\theta \in \bigwedge^1(\mathcal{H}_R)\) such that \(\omega = -d\theta\). Such a 1-form \(\theta \in \bigwedge^1(\mathcal{H}_R)\) is, for instance, the one defined by

\[
\theta(v)[\chi_v(w)] = -\text{Im}\langle v, w \rangle,
\]

because then \(\omega = -d\theta\) is a symplectic 2-form such that

\[
\omega(v)(\chi_v(u), \chi_v(w)) = 2\text{Im}\langle u, w \rangle.
\]

A continuous vector field in \(\mathcal{H}_R\) is a continuous map \(X : \mathcal{H}_R \rightarrow \mathcal{H}_R\). For instance, for each \(v \in \mathcal{H}_R\), the constant vector field \(X_v\) defined by

\[
X_v(w) = \chi_w(v),
\]

is the generator of the one-parameter subgroup of transformations of \(\mathcal{H}_R\) given by

\[
\Phi(t, w) = w + tv,
\]

i.e. with the natural identification of \(T\mathcal{H}_R\) with \(\mathcal{H}_R \times \mathcal{H}_R\),

\[
X_v : w \mapsto (w, v).
\]

The values at a point of such vector fields generate the tangent space at the point.

Similarly, for each vector \(v \in \mathcal{H}_R\) there is a constant 1-form \(\alpha_v\) in \(\mathcal{H}_R\), given by

\[
\alpha_v : w \mapsto \langle v, w \rangle.
\]

Obviously,

\[
\alpha_{v_1}(X_{v_2}) = \langle v_1, v_2 \rangle.
\]
and therefore
\[ \alpha_{v_1 + \lambda v_2} = \alpha_{v_1} + \lambda \alpha_{v_2}, \quad \forall \lambda \in \mathbb{R}. \]
The 1-form \( \theta \) defined above satisfies
\[ \theta(X_v) = -\text{Im} \langle \cdot , v \rangle, \]
because according to the definition of the 1-form \( \theta \),
\[ \theta(X_v)(w) = \theta(w)(X_v)(w) = \theta(w)(\chi_w(v)) = -\text{Im} \langle w, v \rangle. \]
One can see that \( X_w \theta(X_v) \) takes a constant value:
\[ X_w \theta(X_v)(u) = \frac{d}{dt} \theta(X_v)(u + tw) \bigg|_{t=0} = -\text{Im} \frac{d}{dt} \langle u + tw, v \rangle \bigg|_{t=0} = -\text{Im} \langle w, v \rangle. \]
This allows us to check that \( \omega = -d \theta \), because for any pair \( v, w \) \( \in \mathcal{H} \), as \( X_v \) and \( X_w \) commute,
\[ [X_v, X_w] = 0, \]
we have
\[ -d\theta(X_v, X_w) = -X_v \theta(X_w) + X_w \theta(X_v) = -2 \text{Im} \langle w, v \rangle = \omega(X_v, X_w). \]
As another particular example of a vector field, consider the vector field \( X_A \) defined by the \( \mathbb{C} \)-linear map \( A : \mathcal{H} \rightarrow \mathcal{H} \), and in particular when \( A \) is self-adjoint. With the natural identification of \( TH_{\mathbb{R}} \cong \mathbb{R} \times \mathbb{H} \), \( X_A \) is given by
\[ X_A : v \mapsto (v, Av) \in \mathcal{H} \times \mathcal{H}. \]
When \( A = I \) the vector field \( X_I \) is the Liouville generator of dilations along the fibres, usually denoted \( \Delta = X_I \) and given by \( \Delta(v) = (v, v) \).

Given a self-adjoint operator \( A \) in \( \mathcal{H} \) we can define a real function in \( \mathcal{H}_{\mathbb{R}} \) by
\[ a(v) = \langle v, Av \rangle, \]
i.e. the evaluation map, which can be rewritten
\[ a = \langle \Delta, X_A \rangle. \]
Then,
\[ da_v(w) = \frac{d}{dt} a(v + tw) \bigg|_{t=0} = \frac{d}{dt} \langle v + tw, A(v + tw) \rangle \bigg|_{t=0} = 2 \text{Re} \langle w, Av \rangle = 2 \text{Im} \langle -iAv, w \rangle = \omega(-iAv, w). \]
If we recall that the Hamiltonian vector field defined by the function \( a \) is such that for each \( w \in T_v \mathcal{H} = \mathcal{H} \),
\[ da_v(w) = \omega(X_a(v), w), \]
we see that
\[ X_a(v) = -iAv. \]
Therefore, if \( A \) is the Hamiltonian \( H \) of a quantum system, the Schrödinger equation describing time-evolution plays the role of ‘Hamilton equations’ for the Hamiltonian dynamical system \( (\mathcal{H}, \omega, h) \), where \( h(v) = \langle v, Hv \rangle \): the integral curves of \( X_h \) satisfy
\[ \dot{v} = X_h(v) = -iHv. \]
The real functions \( a(v) = \langle v, Av \rangle \) and \( b(v) = \langle v, Av \rangle \) corresponding to two self-adjoint operators \( A \) and \( B \) satisfy
\[ \{a, b\}(v) = -i(v, [A, B]v). \]
because
\[ \{a, b\}(v) = [\omega(X_a, X_b)](v) = \omega(\mathbf{X}_a(v), \mathbf{X}_b(v)) = 2 \Im \langle Av, Bv \rangle, \]
and taking into account that
\[ 2 \Im \langle Av, Bv \rangle = -i(\langle Av, Bv \rangle - \langle Bv, Av \rangle) = -i(\langle v, ABv \rangle - \langle v, BAv \rangle), \]
we find the above result.

In particular, on the integral curves of the vector field \( X_\alpha \) defined by a Hamiltonian \( H \),
\[ \dot{a}(v) = [a, H](v) = -i(v, [A, H]v), \]
that can be rewritten as
\[ \frac{d}{dt}(v, Av) = -i(v, [A, H]v), \quad (16) \]
and is usually known as the Ehrenfest theorem. This is the starting point for the virial theorem in quantum mechanics.

Note that in the derivation of (16) we have used that \( Av \) belongs to the domain of \( H \).
This is not a restriction if \( H \) is defined in the whole Hilbert space, but in many occasions the self-adjoint Hamiltonian has a domain that is only dense in \( \mathcal{H} \) and if \( A \) does not preserve this domain, extra boundary terms should be added to the standard Ehrenfest theorem, see [49–51] where the occurrence of this kind of anomaly in quantum mechanics has been studied. In this paper we shall assume that we have no boundary effects or, in other words, the anomaly is absent and (16) holds. Also note that identity (16) does not require that \( A \) be self-adjoint.

Finally, for the sake of completeness, we must comment that if we want to consider the projective Hilbert space, one can start with the open submanifold \( \mathcal{H} - \{0\} \) of \( \mathcal{H} \) and the action of the two-dimensional Lie group \( \mathbb{C}^* = \mathbb{C} - \{0\} \), which is an Abelian Lie group isomorphic to the direct product \( \mathbb{R}_+ \otimes U(1) \) of \( \mathbb{R}_+ = \{\lambda \in \mathbb{R} | \lambda > 0\} \) and \( U(1) = \{e^{i\varphi} | \varphi \in \mathbb{R}\} \). The corresponding vector fields are \( X_\theta \) and \( X_\phi \) given by
\[ X_\theta(v) = \frac{d}{d\theta} e^{-i\theta} v|_{\theta=0} = -v, \]
\[ X_\phi(v) = \frac{d}{d\phi} e^{i\phi} v|_{\phi=0} = -iv. \]
Let \( \Psi \) be the map,
\[ \Psi : \mathcal{H} - \{0\} \rightarrow \mathbb{R}_+ \times S\mathcal{H}, \quad \Psi(v) = \left( \|v\|, \frac{v}{\|v\|} \right), \quad (17) \]
where \( S\mathcal{H} \) is the subset of unit vectors of \( \mathcal{H} \)
\[ S\mathcal{H} = \{v \in \mathcal{H} | \langle v, v \rangle = 1\}, \quad (18) \]
and denote \( \text{pr}_1 : \mathbb{R}_+ \times S\mathcal{H} \rightarrow \mathbb{R}_+ \) and \( \text{pr}_2 : \mathbb{R}_+ \times S\mathcal{H} \rightarrow S\mathcal{H} \) the projections of \( \Psi(\mathcal{H} - \{0\}) = \mathbb{R}_+ \times S\mathcal{H} \) on each factor. The map \( \text{pr}_1 \circ \Psi : v \mapsto \|v\| \) identifies \( (\mathcal{H} - \{0\})/\mathbb{R}_+ \) with \( S\mathcal{H} \), \( (\mathcal{H} - \{0\})/\mathbb{R}_+ \approx S\mathcal{H} \), and we obtain in this way a reduced space which can be seen as a submanifold \( j_{S\mathcal{H}} : S\mathcal{H} \rightarrow \mathcal{H} \), endowed with the 2-form \( \omega_{S\mathcal{H}} = j_{S\mathcal{H}}^* \omega \), which is an exact \( (\omega_{S\mathcal{H}} = -d\theta_{S\mathcal{H}}, \text{with } \theta_{S\mathcal{H}} = j_{S\mathcal{H}}^* \theta) \) but degenerate 2-form.
As a second step in the reduction process as the symplectic action of the Abelian group \( U(1) = \{e^{i\varphi} | \varphi \in \mathbb{R}\} \), on \( \mathcal{H} \), preserves the submanifold \( S\mathcal{H} \), the set of orbits is \( S\mathcal{H}/U(1) \) is the projective Hilbert space \( P\mathcal{H} = (\mathcal{H} - \{0\})/\mathbb{C}^* \). Note that the momentum map \( J : \mathcal{H} \rightarrow \mathbb{C}^* \) can be found to be given by
\[ \langle J(v), i\lambda \rangle = \lambda \langle v, v \rangle, \]
i.e. $J(v) = \langle v, v \rangle$ and therefore $J^{-1}(1) = \mathcal{H}$ is endowed with a presymplectic form $\omega_\mathcal{H}$ that is the pull-back of $\omega$. Its kernel is generated by the fundamental vector field corresponding to $i \mathfrak{a} \in \mathfrak{u}(1)$. Consequently the Marsden and Weinstein reduction process leads to a uniquely determined reduced symplectic form in the quotient space, the projective Hilbert space. Note, however, that such a symplectic form is not exact and recall that if the dimension of $\mathcal{H}$ is finite, then its projective Hilbert space is compact. Of course the evaluation maps $a$ associated with the self-adjoint operator $A$ are not projectable and must be replaced by the expectation value function $[48]
abla e_A(v) = \frac{\langle v, Av \rangle}{\langle v, v \rangle},$

which coincides with the evaluation map at points $v \in \mathcal{H}$. The dynamical vector field obtained in this way is projectable and gives us the dynamics in the projective Hilbert space.

If the state $v$ is stationary then the above equation (16) becomes an identity since both sides are zero. In a generic state, if we integrate between 0 and $T$ we obtain

$$\langle v(T), Av(T) \rangle - \langle v(0), Av(0) \rangle = -i \int_0^T \langle v(t), [A, H]v(t) \rangle \, dt,$$

and if $\langle v(t), Av(t) \rangle$ remains bounded, taking the limit when $T$ goes to infinity of the quotient of both sides by $T$ we find

$$\lim_{T \to \infty} \frac{\langle \langle \langle v, [A, H]v \rangle \rangle \rangle}{T} = 0,$$

which is the quantum hypervirial theorem when no anomaly, due to boundary terms, is present [51].

Suppose that the Hamiltonian of a quantum system is

$$H = \frac{1}{2}P \cdot P + V(X),$$

where $P = -i \nabla$ and natural units are used. Let $A$ now be given by

$$A = \frac{i}{2}(X \cdot P + P \cdot X).$$

We first remark that $[X \cdot P, H] = [P \cdot X, H]$ because of $X \cdot P - P \cdot X = 3i$.

Taking into account the algebraic relation $[AB, C] = A[B, C] + [A, C]B$ one can see that

$$\left[ X \cdot P, \frac{1}{2}P \cdot P \right] = \frac{1}{2} \sum_{i=1}^3 X_i[P_i, P \cdot P] + \frac{1}{2} \sum_{i=1}^3 [X_i, P \cdot P]P_i = iP \cdot P,$$

while

$$[X \cdot P, V(X)] = \sum_{i=1}^3 X_i[P_i, V(X)] = -iX \cdot \nabla V(X),$$

and therefore

$$\langle v, [X \cdot P, H]v \rangle = i\left( \langle v, P \cdot Pv \rangle - \langle v, (X \cdot \nabla V(X))v \rangle \right),$$

and we obtain the standard quantum virial theorem

$$\lim_{T \to \infty} \frac{\langle \langle \langle v, P \cdot Pv \rangle \rangle \rangle}{T} - \langle \langle \langle v, (X \cdot \nabla V(X))v \rangle \rangle \rangle = 0.$$

Note that $A = \frac{i}{2}(X \cdot P + P \cdot X)$ is the generator for the dilation subgroup. Recall that if a Lie group $G$ acts on $M$ on the left, then if $\mu$ is a $G$-invariant volume, we can define the so called quasi-regular unitary representation in $(\mathcal{L}^2(M), \mu)$ as follows:

$$(U(g)\psi)(x) = \psi(g^{-1}x).$$
When $\mu$ is not $G$-invariant but quasi-invariant, in order to get a unitary representation we must correct the right-hand side by the square root of the Radon–Nikodym derivative.

In the case of dilations in the one-dimensional case, $M = \mathbb{R}$, and if $G$ is the dilation group there is no invariant measure. The quasi-regular representation then turns out to be

$$[U(\lambda)\psi](x) = \lambda^{-1/2}\psi(\lambda^{-1}x).$$

The expression so defined is a one-parameter group of transformations with canonical parameter $\alpha$ such that $\lambda = e^\alpha$,

$$[U(\alpha)\psi](x) = e^{-\alpha/2}\psi(e^{-\alpha}x),$$

and its generator comes from

$$\left.\frac{\partial e^{-\alpha/2}\psi(e^{-\alpha}x)}{\partial \alpha}\right|_{\alpha=0} = -\frac{1}{2}\psi(x) - \frac{x}{\lambda} \frac{\partial \psi}{\partial x},$$

from where we deduce that the generator of this action is

$$A = \frac{1}{2} + \frac{x}{\lambda} \frac{\partial}{\partial x} = \frac{1}{2} \left( \frac{x}{\lambda} \frac{\partial}{\partial x} + \frac{\partial}{\partial x} \right).$$

For $M = \mathbb{R}^3$, the quasi-regular representation is

$$[U(\lambda)\psi](x) = \lambda^{-3/2}\psi(\lambda^{-1}x),$$

or in terms of the parameter $\alpha$,

$$\left.\frac{\partial e^{-\alpha/2}\psi(e^{-\alpha}x)}{\partial \alpha}\right|_{\alpha=0} = -\frac{3}{2}\psi(x) - x \cdot \nabla \psi,$$

and the generator of the action can be written

$$A = \frac{3}{2} + x \cdot \nabla = \frac{1}{2} (x \cdot \nabla + \nabla \cdot x).$$

In order to better understand the geometric properties of the virial theorem in quantum mechanics, it is interesting to study the quantum version of the system with position-dependent mass, introduced in section 4. Its quantization has been studied in detail in [39], where it was shown that the appropriate description of the system implies the introduction of a non-trivial metric $g = m(x) dx \otimes dx$ in $\mathbb{R}$. Consequently, the Hilbert space is $L^2(\mathbb{R}, d\mu)$ with $d\mu = \sqrt{m(x)} dx$ and then the norm of a function $\Psi$ is given by

$$||\Psi||^2 = \int_{-\infty}^{\infty} |\Psi(x)|^2 \sqrt{m(x)} dx. \quad (19)$$

The Hamiltonian operator of the system reads

$$H = H_0 + V(x) = \frac{1}{2}P^2 + V(x)$$

where

$$P = \frac{i}{\sqrt{m(x)}} \frac{\partial}{\partial x},$$

is symmetric with respect to the scalar product induced by (19) and self-adjoint when appropriate boundary conditions are chosen. Note also that $P$ is a Killing vector of the metric, i.e. $L_P g = 0$, and it is, up to a factor $i$ the generator of the translation group in this non-homogeneous space.

In order to apply the virial theorem, we introduce the generator of the dilation group $A = \xi(x)\partial_x$, with the property

$$[P, A] = \frac{a}{2} P.$$
The general solution was obtained in (12) and is given by

\[ \xi(x) = \frac{1}{\sqrt{m(x)}} \left( C_1 + \frac{a}{2} \int_0^x \sqrt{m(\zeta)} \, d\zeta \right). \]  

(20)

Notice that the name of dilation group is justified because of the commutation relation of its generator with that of translations and also because of the action on the metric, i.e.

\[ \mathcal{L}_\lambda g = ag, \]

that corresponds to a conformal transformation.

We consider now the potential

\[ V(x) = C_2 \exp \left( -\int_b^x \xi(\zeta) \, d\zeta \right), \]  

(21)

that verifies

\[ [V, A] = bV. \]

With all these ingredients we have

\[ \langle v, [H, A]v \rangle = a\langle v, H_0v \rangle + b\langle v, Vv \rangle, \]

and consequently

\[ a\langle \langle \langle v, H_0v \rangle \rangle \rangle + b\langle \langle \langle v, Vv \rangle \rangle \rangle = 0. \]

Finally, some comments on the Fock approach to the virial theorem in quantum mechanics [52]: starting with an arbitrary wavefunction \( \phi \) we consider the one-parameter family of trial functions \( \{ \phi_\lambda = U(\lambda)\phi \mid \lambda \in \mathbb{R}_+ \} \), where \( U \) is a linear representation of the dilation group.

When \( d = 1 \) the expectation value of the kinetic term \( H_0 \) is homogeneous of degree \(-2\) and the potential \( V \) is assumed to be homogeneous of degree \( k \):

\[ \langle \phi_\lambda, H_0\phi_\lambda \rangle = \lambda^{-2} \langle \phi, H_0\phi \rangle, \quad \langle \phi_\lambda, V\phi_\lambda \rangle = \lambda^k \langle \phi, V\phi \rangle, \]

therefore

\[ E_\lambda = \langle \phi_\lambda, H\phi_\lambda \rangle = \lambda^{-2} \langle \phi, H_0\phi \rangle + \lambda^k \langle \phi, V\phi \rangle. \]

The best approach to an eigenvalue in the family will be by a value of \( \lambda \) such that

\[ \frac{dE_\lambda}{d\lambda} = -2\lambda^{-3} \langle \phi, H_0\phi \rangle + k\lambda^{k-1} \langle \phi, V\phi \rangle = 0. \]

In particular, if \( \phi \) is actually an eigenvector, then the extremal is found for \( \lambda = 1 \),

\[ 2\langle \phi, H_0\phi \rangle = k\langle \phi, V\phi \rangle, \]

and we reobtain in this way the virial theorem for eigenstates of \( H \).

7. Final comments

The standard theory of the virial theorem has been revisited from the perspective of the theory of Hamiltonian systems in symplectic manifolds. This allows us to consider the classical counterpart of the usually called hypervirial theorem and clarify that the theory is not related in the general case with the group of scale transformations. In this way we have found room for dealing with systems whose configuration spaces are not linear spaces. The geometric formalism is valid not only in the Hamiltonian approach (cotangent bundle with the canonical two-form) but also in the Lagrangian case (tangent bundle with a \( L \)-dependent symplectic form); we have shown the usefulness of some infinitesimal point transformations that are not
symmetries of the Lagrangian for establishing virial-like relations. The example of position-dependent mass has been used to illustrate the theory and the particular example of a nonlinear oscillator is explicitly studied.

The use of the modern symplectic approach to quantum mechanics enables us to prove in the second part of the paper that the virial theorem in quantum mechanics appears in full similarity with the analogous classical case. We only need to take into account the point of view of symplectic geometry in infinite dimensional linear spaces. We hope this analogy will be helpful for dealing with various quantum cases.

Acknowledgments

This work was supported by the research projects FPA-2009-09638, MTM-2009-11154 (MEC, Madrid) and DGA-E24/1, DGA-E24/2 (DGA, Zaragoza).

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