Non-strictly canonical transformations and a generalisation of the Virial Theorem

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Geometry of Manifolds and Mathematical Physics, Krakow, 27th June - 1st July, 2011

Abstract

The Virial's theorem both in the classical and in the quantum frameworks is revisited from a geometric approach, what enables us to loook at the Virial's Therem from a modern geometric perspective. The theory of one-parameter groups of non-strictly canonical transformations is shown to play a relevant role.

This is a collaboration with: M. F. RAÑADA

Outline

Introduction: The standard virial's theorem

Inspired by the work of Carnot on heat engines, R. J. E. Clausius began a long study of the mechanical nature of heat in 1851

Twenty years later, in a lecture delivered on June 13 of 1870, in the Association for Natural and Medical Sciences of the Lower Rhine: On a Mechanical Theorem Applicable to Heat, Claussius stated the theorem as The mean vis viva of the system is equal to its virial.

vis viva integral is the total kinetic energy of the system

Latin word virias (the plural of vis) meaning forces was used by Clausius to coin the word virial as the scalar quantity represented in terms of the forces $\mathbf{F}_i$ acting on the system as

$$\frac{1}{2}\langle\langle\sum_i \mathbf{F}_i \cdot \mathbf{r}_i\rangle\rangle$$

and it can be shown to be 1/2 the average potential energy of the system.

The quantum mechanical version of the Theorem is due to M. Born, W. Heisenberg, and P. Jordan (Zeitschrift für Physik A Hadrons and Nuclei **35**, 557 (1926)).

A generalisation of the Theorem is due to Lord Rayleigh in 1903 and more recent contributions are due to:

H. Poincaré, *Lectures on Cosmological Theories*, Hermann, Paris, 1911.

E. Parker, Phys. Rev. **96**, 1686-1689 (1954) .

S. Chandrasekhar and N.R. Lebovitz, Ap.J. **136**, 1037–1047 (1962)

P. Ledoux developed a variational form of the virial theorem to obtain pulsational periods for stars and investigate their stability (Ap. J. **102**, 134–153 (1945))

S. Chandrasekhar and E. Fermi extended the virial theorem in 1953 to include the presence of magnetic fields (Ap. J. **118**, 116 (1953)).

Remark that in order to replace the time averages with something observable we can use the ergodic theorem to replace time averages by phase space averages

The important point is the wide range of applicability of the virial theorem:

a) it is applicable to dynamical and thermodynamical systems,

b) it can also be formulated to deal with relativistic (in the sense of special relativity) systems,

c) it is applicable to systems with velocity dependent forces and viscous systems,

d) it provides less information that the equations of motion but it is simpler to apply and then it can provide information concerning systems whose complete analysis may defy description

e) In astronomy, the virial theorem finds applications in 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.

Consider a particle of mass m under the action of a force $\mathbf{F}$.

Clausius introduced in 1870 the virial function

$$G(\mathbf{x}, \dot{\mathbf{x}}) = m\,\mathbf{x}\cdot\dot{\mathbf{x}} = \frac{d}{dt}\left(\frac{1}{2}m\,\mathbf{x}\cdot\mathbf{x}\right).$$

The time evolution of such function is given by:

$$\frac{dG}{dt} = m\,\dot{\mathbf{x}}\cdot\dot{\mathbf{x}} + \mathbf{x}\cdot\mathbf{F},$$

where use has been made of Newton second law: $\mathbf{F} = m\,\ddot{\mathbf{x}}$.

When integrating this expression between $t = 0$ and $t = T$ and dividing by the total time interval T we find

$$\frac{1}{T}[G(T) - G(0)] = \frac{2}{T}\int_0^T E_c(\dot{\mathbf{x}})\,dt + \frac{1}{T}\int_0^T \mathbf{x}\cdot\mathbf{F}(\mathbf{x})\,dt = \langle\langle 2\,E_c(\dot{\mathbf{x}})\rangle\rangle + \langle\langle \mathbf{x}\cdot\mathbf{F}\rangle\rangle,$$

where E_c denotes the kinetic energy and $\langle\langle A\rangle\rangle$ means time average.

If the motion is periodic of period T or the possible values of the function G are bounded and we take the limit of T going to infinity:

$$0 = \langle\langle 2\,E_c(\dot{\mathbf{x}})\rangle\rangle + \langle\langle \mathbf{x}\cdot\mathbf{F}\rangle\rangle.$$

In the particular case of a conservative force, $\mathbf{F} = -\boldsymbol{\nabla} V$, the dynamical evolution of G is given by

$$\frac{dG}{dt} = m\,\dot{\mathbf{x}}\cdot\dot{\mathbf{x}} + \mathbf{x}\cdot\mathbf{F} = 2\,E_c(\dot{\mathbf{x}}) - \mathbf{x}\cdot\boldsymbol{\nabla} V,$$

and with an analogous integration from $t = 0$ to $t = T$

$$\frac{1}{T}[G(T)-G(0)] = \frac{2}{T}\int_0^T E_c(\dot{\mathbf{x}})\,dt - \frac{1}{T}\int_0^T (\mathbf{x}\cdot\boldsymbol{\nabla} V)\,dt = \langle\langle 2\,E_c(\dot{\mathbf{x}})\rangle\rangle - \langle\langle \mathbf{x}\cdot\boldsymbol{\nabla} V\rangle\rangle.$$

When the motion is periodic of period T or the possible values of G are bounded and we take the limit of T going to infinity:

$$0 = \langle\langle 2\,E_c(\dot{\mathbf{x}})\rangle\rangle - \langle\langle \mathbf{x}\cdot\boldsymbol{\nabla} V\rangle\rangle.$$

If the potential V is homogeneous of degree k, Euler's theorem of homogeneous functions implies that $\mathbf{x}\cdot\boldsymbol{\nabla} V = k\,V$, and therefore,

$$2\,\langle\langle E_c(\dot{\mathbf{x}})\rangle\rangle = k\,\langle\langle V(\mathbf{x})\rangle\rangle,$$

i.e. if E is the total energy,

$$\langle\langle E_c(\dot{\mathbf{x}})\rangle\rangle = \frac{k\,E}{k+2}, \qquad \langle\langle V(\mathbf{x})\rangle\rangle = \frac{2\,E}{k+2}.$$

For instance in the harmonic oscillator case, $k = 2$,

$$\langle\langle E_c(\dot{\mathbf{x}})\rangle\rangle = \langle\langle V(\mathbf{x})\rangle\rangle = \frac{1}{2}E,$$

and in the Kepler problem, $k = -1$,

$$\langle\langle E_c(\dot{\mathbf{x}})\rangle\rangle = -E, \qquad \langle\langle V(\mathbf{x})\rangle\rangle = 2\,E.$$

Relevant questions are: Where does the virial function G comes from?

Why the relation is simpler for power law potentials?

Why is the reason for the values of the coefficients?

Is there any generalisation?

What about a quantum mechanical counterpart?

Virial's theorem in Hamiltonian systems

Let us analyse the problem in the frame of Hamiltonian systems (M, ω, H).

Here ω is a symplectic form, i.e, a non-degenerated closed 2-form in M.

We restrict ourselves to the case of time-independent systems. We will show that the preceding case is but a particular case of a more general result.

Let X_F be the Hamiltonian vector field defined with Hamiltonian function F, defined by

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

In particular the dynamics is given by the vector field X_H defined by

$$i(X_H)\omega = dH.$$

For any two functions in M the Poisson bracket is given by

$$\{F, G\} = \omega(X_F, X_G) = X_G F = -X_F G.$$

Let ϕ_t denote the flow of X_H. Such a flow commutes with X_H, and having in mind that, for any $f \in C^\infty(M)$,

$$X_H \phi_t^* f = \phi_t^* X_H f = \frac{d}{ds}[\phi_s^*(\phi_t^* f)]_{|s=0} = \frac{d}{ds}(\phi_{s+t}^* f)_{|s=0} = \frac{d}{du}[\phi_u^* f]_{|u=t},$$

we see that if we choose as f an observable function $f = G$,

$$\frac{d}{dt}(\phi_t^* G) = \phi_t^*(\{G, H\}) = -\phi_t^*(X_G H).$$

If we integrate both sides of this relation with respect to t from $t = 0$ to $t = T$,

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

This result is sometimes known as Hypervirial Theorem: If the function remains bounded in its time evolution, taking the limit when T goes to infinity:

$$\langle\langle \{G, H\} \rangle\rangle = 0.$$

When $M = T^*\mathbb{R}^3$ endowed with its canonical symplectic structure and consider the function $G(\mathbf{x}, \mathbf{p}) = \mathbf{x} \cdot \mathbf{p}$, the corresponding Hamiltonian vector field X_G is

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

i.e. it is the dilation generator, and if H is given by

$$H(\mathbf{x},\mathbf{p}) = \frac{1}{2m}\mathbf{p}\cdot\mathbf{p} + V(\mathbf{x}) = H_0(\mathbf{p}) + V(\mathbf{x}),$$

we recover from

$$(X_G H)(\mathbf{x},\mathbf{p}) = -2H_0(\mathbf{p}) + \mathbf{x}\cdot\boldsymbol{\nabla}V,$$

the standard result in the Hamiltonian framework:

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

and taking the limit of T going to infinity:

$$\langle\langle 2H_0\rangle\rangle = \langle\langle \mathbf{x}\cdot\boldsymbol{\nabla}V\rangle\rangle.$$

A very important particular case is that of the Hamiltonian system defined by a regular Lagrangian: (TQ,ω_L,E_L).

The virial theorem reduces to

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

and if the function remains bounded in its time evolution, taking the limit when T goes to infinity:

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

In the very simple case in which $Q = \mathbb{R}^3$ and

$$L(\mathbf{x}, \dot{\mathbf{x}}) = \frac{1}{2} m\, \dot{\mathbf{x}} \cdot \dot{\mathbf{x}} - V(\mathbf{x}) \Longrightarrow E_L(\mathbf{x}, \dot{\mathbf{x}}) = \frac{1}{2} m\, \dot{\mathbf{x}} \cdot \dot{\mathbf{x}} + V(\mathbf{x}),$$

then $\omega_L = m\, d\mathbf{x} \wedge d\dot{\mathbf{x}}$, and when G is the observable function $G(\mathbf{x}, \dot{\mathbf{x}}) = m\, \mathbf{x} \cdot \dot{\mathbf{x}}$, then

$$X_G(\mathbf{x}, \dot{\mathbf{x}}) = \mathbf{x} \cdot \boldsymbol{\nabla}_{\mathbf{x}} - \dot{\mathbf{x}} \cdot \boldsymbol{\nabla}_{\dot{\mathbf{x}}},$$

and consequently, we recover the original virial's theorem:

$$X_G E_L(\mathbf{x}, \dot{\mathbf{x}}) = \mathbf{x} \cdot \boldsymbol{\nabla} V(\mathbf{x}) - m\, \dot{\mathbf{x}} \cdot \dot{\mathbf{x}} \Longrightarrow \langle\langle 2\, E_c(\dot{\mathbf{x}}) \rangle\rangle = \langle\langle \mathbf{x} \cdot \boldsymbol{\nabla} V \rangle\rangle.$$

A very important example is that of Lagrangian systems of mechanical type. Such Lagrangians are defined by a Riemannian metric g in the base, the configuration space Q. The corresponding kinetic energy is then given by

$$T = \frac{1}{2}\, \widetilde{g}(D, D)$$

for any choice of the SODE vector field D. Here $\widetilde{g}$ denotes the pull-back of g to TQ.

Non-strictly canonical transformations

A diffeomorphism $\phi : M \to M$ push forward tensorial fields and those diffeomorphisms leaving invariant a tensor field are called symmetries of such a tensor field. For covariant tensors ϕ_* means $(\phi^{-1})^*$.

So: If $\Gamma \in \mathfrak{X}(M)$, its symmetries are diffeomorphisms of M such that $\phi_*\Gamma = \Gamma$.

If ω is a symplectic structure in M, its symmetries (to be called symplectomorphisms) are diffeomorphisms of M such that $\phi_*\omega = \omega \Longleftrightarrow \phi^*\omega = \omega$.

The symmetries of $H \in C^\infty(M)$ are the diffeomorphisms ϕ such that $\phi_* H = H \Longleftrightarrow \phi^* H = H$.

The remarkable point is that

$$i(X_H)\omega = dH \Longleftrightarrow i(\phi_* X_H)(\phi_*\omega) = d(\phi_* H).$$

Therefore symplectomorphisms that are symmetries of H are also symmetries of X_H.

However, THERE ARE SYMMETRIES OF X_H that are not symplectomorphisms

One-parameter subgroups of symmetry transformations of tensor fields are characterized by the vanishing of the Lie derivative of the tensor field with respect to the vector field generating the one-parameter subgroup:

$$[X, \Gamma] = 0, \quad \text{for vector fields.}$$
$$\mathcal{L}_X \omega = 0, \quad \text{for symplectic forms.}$$
$$XH = 0, \quad \text{for functions.}$$

Given a Hamiltonian system (M, ω, H) one usually look for vector fields whose flows are symplectomorphisms that are also symmetries of H and, therefore, symmetries of X_H. Then for each $G \in C^\infty(M)$, the relation

$$X_H G = \{G, H\} = -X_G H$$

shows that X_G is a symmetry of H if and only if G is a constant of motion (Noether's theorem).

A diffeomorphism $\phi : M \to M$ is said to be a canonoid transformation for a Hamiltonian system (M, ω, H) when $\phi_* X_H \in \mathfrak{X}_H(M, \omega)$ or equivalently $X_H \in \mathfrak{X}_H(M, \phi^*\omega)$. Of course, as ω is closed such condition is equivalent to $d(i(X_H)\phi^*\omega) = 0$.

Canonical tranformations are those transformations of M that are canonoid for each Hamiltonian, i.e. such that $\phi_*(\mathfrak{X}_H(M, \omega)) \subset \mathfrak{X}_H(M, \omega)$.

If there exists a nonzero real number $r \in \mathbb{R}$ such that $\phi^*\omega = r\,\omega$, the transformation ϕ is canonical. The number λ is called valence of the canonical transformation.

The inverse property is true and one can show the existence for each canonical of a factor r, such that $\phi^*\omega = r\,\omega$.

In summary, symplectomorphisms are STRICTLY CANONICAL TRANSFORMATIONS but ....

There exist more general canonical transformations such that

$$\phi^*\omega = r\,\omega, \quad r \in \mathbb{R}.$$

In the case of a vector field X whose flow is made up by canonical transformations if there exists a function $r(\epsilon)$ such that $\phi_\epsilon^*\omega = r(\epsilon)\,\omega$. Therefore $r(\epsilon) = e^{a\epsilon}$ and

$$\mathcal{L}_X\omega = a\,\omega, \qquad (a = r'(0)).$$

Note that a diffeomorphism of M such that

$$\phi_*\omega = r\,\omega, \qquad \phi_*H = r\,H.$$

is a symmetry of X_H (leaves invariant the Hamiltonian vector field X_H).

At the infinitesimal level, if $\mathcal{L}_X\omega = a\,\omega$ and $XH = a\,H$, then $[X_H, X] = 0$, because using $(\mathcal{L}_X i_{X_H} - i_{X_H}\mathcal{L}_X)\omega = i([X, X_H])\omega$, we obtain from

$$\mathcal{L}_X dH - a\,i(X_H)\omega = d(a\,H) - a(dH) = 0 = (\mathcal{L}_X i_{X_H} - i_{X_H}\mathcal{L}_X)\omega$$

that

$$i([X, X_H])\omega = 0 \Longrightarrow [X, X_H] = 0.$$

In the case of a Hamiltonian dynamical system defined by a regular Lagrangian L, (TQ, ω_L, dE_L), for diffeomorphisms ϕ of TQ defined from diffeomorphism φ of the base, i.e. $\phi = \varphi_* = T\varphi$, it happens that

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

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, $Y \in \mathfrak{X}(Q)$,

$$\mathcal{L}_X\theta_L = \theta_{XL}, \qquad XE_L = E_{XL}.$$

On the other side, it can be shown that L' defines the same Hamiltonian system as L (i.e. $\omega_L = \omega_{L'}$ and $E_L = E_{L'}$) when there exists a closed 1-form α in Q such that

$$L' = L + \widehat{\alpha},$$

where $\widehat{\alpha}$ is the function in TQ defined by $\widehat{\alpha}(U) = \alpha(\tau_*(U))$.

Therefore $X = Y^c$ is a symmetry of the Hamiltonian dynamical system defined by the function L if there exists a closed form α in Q such that

$$XL = \widehat{\alpha}.$$

We can at least locally write $\alpha = d\widetilde{h}$ where h is a function in Q. Note that in this case

$$\widehat{dh} = \Gamma(\widetilde{h}), \quad \forall\ \texttt{SODE}\ \Gamma.$$

Theorem: Let $X = Y^c$ be such that $XL = a\,L + \widehat{dh}$, where $a \in \mathbb{R}$ and L is a regular Lagrangian function. Then,

i) X is a symmetry of the dynamical vector field Γ (recall that $i(\Gamma)\omega_L = dE_L$).

ii) The function $G = i(X)\theta_L - \widetilde{h}$ is such that $\Gamma G = a\,L$.

Proof.- First of all $\theta_{XL} = a\,\theta_L + \widetilde{dh}$ and therefore $\omega_{XL} = a\,\omega_L$. Furthermore, $E_{XL} = a\,E_L$. Consequently $\mathcal{L}_X\omega_L = a\,\omega_L$ and $\mathcal{L}_X E_L = a\,E_L$, and we have seen that this implies that $[\Gamma, X] = 0$.

Moreover, from

$$\mathcal{L}_\Gamma(i(X)\theta_L) = i(X)\mathcal{L}_\Gamma\theta_L = i(X)dL = a\,L + \widehat{dh} = a\,L + \Gamma(h),$$

we see that

$$\Gamma(G) = \Gamma(i(X)\theta_L - h) = a\,L.$$

From this expression we obtain a virial type relation:

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

and consequently

$$\lim_{t_1\to-\infty, t_2\to\infty} \frac{1}{t_2 - t_1}[G(t_2) - G(t_1)] = a\,\langle\langle L\rangle\rangle.$$

For instance, in the particular case of the harmonic oscillator, dilations are such that $a = 2$:

$$Y = \mathbf{x}\cdot\boldsymbol{\nabla} \Longrightarrow X = \mathbf{x}\cdot\boldsymbol{\nabla} + \dot{\mathbf{x}}\cdot\boldsymbol{\nabla}_{\dot{\mathbf{x}}}$$

and then

$$XL = X\left(\frac{1}{2}m\dot{\mathbf{x}}\cdot\dot{\mathbf{x}} - \frac{1}{2}m\omega\,\mathbf{x}\cdot\mathbf{x}\right) = 2\,L,$$

and we obtain

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

Let X be the vector field in $\mathbb{R}$ given by

$$X = \xi(q)\frac{\partial}{\partial q}$$

and therefore its complete lift is

$$X^c(q,v) = \xi(q)\frac{\partial}{\partial q} + v\frac{\partial \xi}{\partial q}\frac{\partial}{\partial v}$$

If the Lagrangian $L(q,v)$ is given by

$$L(q,v) = \frac{1}{2}m(q)v^2 - V(q),$$

then

$$X^c L(q,v) = \frac{1}{2}\,\xi\, m'(q)v^2 - \xi\, V'(q) + v\,\xi'(q)\, m(q)\, v,$$

and therefore the condition $X^c L = a\, L$ is written

$$\begin{cases} \quad 2\xi'(q) + \xi\,\mu(x) = a, \\ \quad \xi\, V'(q) = a\, V(q) \end{cases}$$

where $\mu = m'(q)/m(q)$.

The first equation is an inhomogeneous linear one and its general solution is

$$\xi(q) = \frac{1}{\sqrt{m(q)}}\left(\frac{a}{2}\int^q \sqrt{m(q')}\, dq'\right).$$

The potential energy $V(q)$ is then

$$V(q) = C \exp\left(\int^q \frac{a}{\xi(q')}\, dq'\right)$$

As an example consider the equation for a 1-dimensional nonlinear oscillator studied in 1974 by Mathews and Lakshmanan

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

The general solution takes the form $x = A\sin(\omega\, t + \phi)$, 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 Lagrangian:

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

We can also allow negative values for λ, but when $\lambda < 0$ the values of x are limited by the condition $|x| < 1/\sqrt{|\lambda|}$.

The system can be seen as a deformation of the harmonic oscillator or as an oscillator with a position-dependent effective mass which depends on λ: $m_\lambda = \frac{1}{1+\lambda\, x^2}$

Coming back to the Hamiltonian framework, let $(M, \omega = -d\theta)$ be an exact symplectic manifold. We denote X_1 the vector field such that

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

Note that such a vector field is such that

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

and therefore

$$\mathcal{L}_{X_1}\omega = -\omega,$$

because

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

Given a vector field X generating a one-parameter group of non-strictly canonical transformations, we know that there exists a real number a such that $\mathcal{L}_X\omega = a\,\omega$ and therefore the vector field $X + a\,X_1$ is locally Hamiltonian, because

$$\mathcal{L}_{X+a\,X_1}\omega = a\,\omega - a\,\omega = 0.$$

That means that there exists a closed 1-form α such that

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

Conversely, given a closed 1-form α the preceding relation defines a vector field X generating a one-parameter (local) subgroup of non-strictly canonical transformations ϕ_ϵ with valence $e^{a\epsilon}$.

In a Darboux chart for which

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

if we choose

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

we find that X_1 is a 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

$$X = X_\phi - a \, X_1$$

Therefore,

$$X H = \{H, \phi\} - a \, X_1 H,$$

In particular, if there exists $b \in \mathbb{R}$ such that $XH = b\,H$:

$$\{H, \phi\} - a\,X_1 H = b\,H$$

Using a Darboux chart, if we assume that $H(q,p) = T(p) + V(q)$, we find

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

and taking into account that

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

we obtain.

$$XH = \left\{H, \phi + \frac{a}{2}\sum_{i=1}^{n} q^i p_i\right\} + 2\,a\,T$$

As before, when integrating in time from $t = 0$ to $t = T$ we obtain in the limit of T going to infinity (or when the motion is periodic)

$$2\,a\,\langle\langle T\rangle\rangle = \langle\langle XH\rangle\rangle,$$

and when $XH = b\,H$,

$$2\,a\,\langle\langle T\rangle\rangle = b\,E.$$

The virial's theorem in Quantum Mechanics

A separable complex Hilbert space $(\mathcal{H}, \langle\cdot,\cdot\rangle)$ can be considered as a real linear space, to be then denoted $\mathcal{H}_{\mathbb{R}}$. The norm in $\mathcal{H}$ defines a norm in $\mathcal{H}_{\mathbb{R}}$, where $\|v\|_{\mathbb{R}} = \|v\|_{\mathbb{C}}$.

The linear real space $\mathcal{H}_{\mathbb{R}}$ is endowed with a natural symplectic structure as follows:

$$\omega(u, v) = 2\,\mathrm{Imag}\,\langle u, v\rangle.$$

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

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

$$\chi_v(w)f = \frac{d}{dt} f(v + t\,w)_{|t=0},$$

where $f \in C^\infty(v)$. This is an isomorphism $\chi_v : \mathcal{H}_\mathbb{R} \to T_v\mathcal{H}_\mathbb{R}$ of $\mathcal{H}_\mathbb{R}$ with $T_v\mathcal{H}_\mathbb{R}$. The identification corresponds to the one given by the free transitive action of the Abelian group of translations.

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

$$\theta(v)[\chi_v(w)] = -\mathrm{Imag}\,\langle v, w\rangle,$$

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

$$\omega(v)(\chi_v(u), \chi_v(w)) = 2\,\mathrm{Imag}\,\langle u, w\rangle.$$

A *continuous* vector field in $\mathcal{H}_\mathbb{R}$ is a *continuous* map $X\colon \mathcal{H}_\mathbb{R} \to \mathcal{H}_\mathbb{R}$. For instance for each $v \in \mathcal{H}$, the constant vector field X_v defined by

$$X_v(w) = \chi_w(v) = v.$$

It is the generator of the one-parameter subgroup of transformations of $\mathcal{H}_\mathbb{R}$ given by

$$\Phi(t, w) = w + t\,v\,,$$

i.e. with the natural identification of $T\mathcal{H}_{\mathbb{R}}$ with $\mathcal{H}_{\mathbb{R}} \times \mathcal{H}_{\mathbb{R}}$,

$$X_v : w \mapsto (w, v) \, .$$

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

Similarly, for each vector $v \in \mathcal{H}_{\mathbb{R}}$ there is a constant 1-form in $\mathcal{H}_{\mathbb{R}}$, α_v, 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

$$\alpha_{v_1 + \lambda\, v_2} = \alpha_{v_1} + \lambda \alpha_{v_2} \, , \quad \lambda \in \mathbb{R} \, .$$

The 1-form θ defined above satisfies

$$\theta(X_v) = -\mathrm{Imag} \, \langle \cdot, v \rangle \, ,$$

because according to the definition of the 1-form θ,

$$[\theta(X_v)](w) = \theta(w)[X_v(w)] = \theta(w)[\chi_w(v)] = -\mathrm{Imag} \, \langle w, v \rangle \, .$$

One can see that $X_w[\theta(X_v)]$ takes a constant value:

$$X_w[\theta(X_v)](u) = \frac{d}{dt}\left[\theta(X_v)(u+tw)\right]_{|t=0} = -\mathrm{Imag}\,\frac{d}{dt}\langle u{+}tw, v\rangle_{|t=0} = -\mathrm{Imag}\,\langle w, v\rangle\,.$$

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

$$-d\theta(X_v, X_w) = -X_v\,\theta(X_w) + X_w\theta(X_v) = -2\,\mathrm{Imag}\,\langle w, v\rangle = \omega(X_v, X_w)\,.$$

As another particular example of vector field consider the vector field X_A defined by the $\mathbb{C}$-linear map $A : \mathcal{H} \to \mathcal{H}$, and in particular when A is skew-selfadjoint.

With the natural identification natural of $T\mathcal{H}_{\mathbb{R}} \approx \mathcal{H}_{\mathbb{R}} \times \mathcal{H}_{\mathbb{R}}$, 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, $\Delta = X_I$, usually denoted Δ given by $\Delta(v) = (v, v)$.

Given a selfadjoint 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.,

$$a = \langle \Delta, X_A \rangle \,.$$

Then,

$$\begin{aligned} da_v(w) &= \frac{d}{dt} a(v + tw)_{|t=0} = \frac{d}{dt} \left[\langle v + tw, A(v + tw) \rangle \right]_{|t=0} \\ &= 2\,\mathrm{Re}\,\langle w, Av \rangle = 2\,\mathrm{Imag}\,\langle -iAv, w \rangle = \omega(-iAv, w). \end{aligned}$$

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

$$X_a(v) = -i\,Av\,.$$

Therefore if A is the Hamiltonian H of a quantum system, the Schrödinger equation describing time-evolution plays the rôle 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

$$\dot{v} = X_h(v) = -i\,Hv\,.$$

The real functions $a(v) = \langle v, Av \rangle$ and $b(v) = \langle v, Av \rangle$ corresponding to two selfadjoint operators A and B satisfy

$$\{a, b\}(v) = -i \langle v, [A, B]v \rangle \,,$$

because

$$\{a, b\}(v) = [\omega(X_a, X_b)](v) = \omega_v(X_a(v), X_b(v)) = 2\,\mathrm{Imag}\,\langle Av, Bv \rangle \,,$$

and taking into account that

$$2\,\mathrm{Imag}\,\langle Av, Bv \rangle = -i\,[\langle Av, Bv \rangle - \langle Bv, Av \rangle] = -i\,[\langle v, ABv \rangle - \langle v, BAv \rangle] \,,$$

we find the above result.

In particular on the integral curves of the vector field X_h defined by a Hamiltonian H,

$$\dot{a}(v) = \{a, h\}(v) = -i \langle v, [A, H]v \rangle \,,$$

what is usually known as Ehrenfest theorem:

$$\frac{d}{dt} \langle v, Av \rangle = -i \langle v, [A, H]v \rangle \,.$$

This is the starting point for the Virial Theorem in Quantum Mechanics.

If the state v is stationary is obviously true, 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

$$\langle\langle\langle v, [A,H]v\rangle\rangle\rangle = 0,$$

which is the quantum Virial's Theorem.

Suppose that the Hamiltonian of a quantum system is

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

Let now G be given by

$$G = \frac{1}{2}\left(\mathbf{X}\cdot\mathbf{P} + \mathbf{P}\cdot\mathbf{X}\right).$$

We first remark that as $\mathbf{X}\cdot\mathbf{P} - \mathbf{P}\cdot\mathbf{X} = i\,\hbar$, $[\mathbf{X}\cdot\mathbf{P}, H] = [\mathbf{P}\cdot\mathbf{X}, H]$.

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

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

while

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

and therefore

$$\langle v, [\mathbf{X} \cdot \mathbf{P}, H]v \rangle = i\,\hbar\,(\langle v, \mathbf{P} \cdot \mathbf{P} v \rangle - \langle v, (\mathbf{X} \cdot \boldsymbol{\nabla} V(\mathbf{X}))v \rangle)\,.$$

and we obtain that

$$\langle v, \mathbf{P} \cdot \mathbf{P} v \rangle - \langle v, (\mathbf{X} \cdot \boldsymbol{\nabla} V(\mathbf{X}))v \rangle = 0,$$

which is the quantum version of the standard virial theorem

$$\langle v, \mathbf{P} \cdot \mathbf{P} v \rangle = \langle v, (\mathbf{X} \cdot \boldsymbol{\nabla} V(\mathbf{X}))v \rangle$$

Note that $G = \frac{1}{2}\,(\mathbf{X} \cdot \mathbf{P} + \mathbf{P} \cdot \mathbf{X})$ is the generator fo the dilation subgroup.

If a Lie group G acts on M on the left, then if μ is a G-invariant volume, we can define the so called quasi-regular unitary representation in $(\mathcal{L}^2(M), \mu)$ as follows:

$$(U(g)\psi)(gx) = \psi(g^{-1}x).$$

When μ is not G-invariant but quasi–invariant, in order to get an 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 given by.

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

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

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

and its generator comes form

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

from where we see that the generator of such action is

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

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

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

or in terms of the parameter α,

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

from where we see that the generator of such action is

$$G = \frac{3}{2} + \mathbf{x}\cdot\boldsymbol{\nabla} = \frac{1}{2}\left(\mathbf{x}\cdot\boldsymbol{\nabla} + \boldsymbol{\nabla}\cdot\mathbf{x}\right).$$

Finally, some comments on Fock approach to the Virial's Theorem in Quantum Mechanics:

Starting with an arbitrary wave function ϕ we consider the one-parameter family of trial functions $\{\phi^\lambda = U(\lambda)\phi \mid \lambda \in \mathbb{R}_*\}$.

The expectation value of the kinetic term is homogeneous of degree -2 and the potential is assumed to be homogeneous of degree k:

$$\langle \phi^\lambda, T\phi^\lambda \rangle = \lambda^{-2} \langle \phi, T\phi \rangle, \qquad \langle \phi^\lambda, V\phi^\lambda \rangle = \lambda^k \langle \phi, V\phi \rangle,$$

therefore

$$E_\lambda = \langle \phi^\lambda, T\phi^\lambda \rangle = \lambda^{-2} \langle \phi, T\phi \rangle + \lambda^k \langle \phi, V\phi \rangle.$$

The best approach to an eigenvalue in the family will be by a value of λ such that

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

In particular, if ϕ is actually an eigenvector, then the extremal is found for $\lambda = 1$,

$$2\,\langle \phi, T\phi \rangle = k\,\langle \phi, V\phi \rangle,$$

and we reobtain in this way the Virial's theorem for eigenstates of H.

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