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On the duality of hypervirial and conservation theorems

W. G. SULLIVAN†
Mathematical Institute, Oxford University
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Abstract. Hypervirial theorems are treated from the point of view of observables and states. This technique yields an extension of the classical results and a new proof for the quantum case, and it makes explicit their intimate relationship to conservation theorems.

1. Introduction

Hirschfelder (1960) introduced a family of generalizations of the virial theorem which he designated hypervirial theorems. Interest has been mainly in the quantum-mechanical case, but classical analogues have also been cited. The quantum forms are relations which are satisfied by eigenfunctions of the Hamiltonian. It has also been shown that functions which satisfy a sufficient family of hypervirial relations must be eigenfunctions of the Hamiltonian (Hirschfelder 1960, Coulson 1965, Sullivan 1967).

In this paper the hypervirial theorems are treated from the statistical point of view of observables and states. In this context the hypervirial theorems are naturally dual to the conservation theorems, the former characterizing invariant states and the latter invariant observables. Furthermore, the parallel between classical and quantum results is underlined. The Liouville theorem is a hypervirial theorem. Also this treatment leads directly to the result that the stationary states are exactly those which satisfy the hypervirial theorems.

2. Abstract formalism

A detailed discussion of the observables and states point of view can be found in von Neumann (1955).

We assume the physical system to be described by the set O of observables, the set S of states, the operation $\langle o, s\rangle$ giving the expectation value of the observable o in the state s, and the dynamical evolution operator T_t. It is assumed that T_t is parameterized by the real line, but other parameterization could be employed. We require the following:

(i) $\langle , \rangle$ is bilinear in O and S when these have linear or convex structures.

(ii) No two distinct observables take on equal expectation values in every state, and no two distinct states give equal expectation values to each observable.

(iii) T_t can be regarded as acting either on observables or on states. Its actions are automorphisms. For o in O we write the action of T_t as $T_t{}^*o$; for s in S, $T_{t*}s$. We have $\langle T_t{}^*o, s\rangle = \langle o, T_{t*}s\rangle$ for all o, s and t.

Next we define invariance.

Definition. An observable o is called invariant if $T_t{}^*o = o$ for all t. A state s is called invariant if $T_{t*}s = s$ for all t.

Now the straightforward application of (ii) and (iii) gives the following theorems.

Abstract conservation and hypervirial theorems in integrated form. An observable o is invariant if, and only if, $\langle o, T_{t*}s\rangle = \langle o, s\rangle$ for each state s and all t. A state s is invariant if, and only if, $\langle T_t{}^*o, s\rangle = \langle o, s\rangle$ for each observable o and all t.

3. Classical mechanics

Configuration space is taken to be R^n with phase space R^{2n}, a point of which being indicated by $(q_1, ..., q_n; p_1, ..., p_n)$. Time evolution is given by $T_t : R^{2n} \rightarrow R^{2n}$, which is related to the Hamiltonian $H(q_1, ..., q_n; p_1, ..., p_n; t)$ by the system of differential equations

$$\frac{d}{dt}\{T_t(q_1, \ldots, q_n; p_1, \ldots, p_n)\} = \left(\frac{\partial H}{\partial p_1}, \ldots, \frac{\partial H}{\partial p_n}; -\frac{\partial H}{\partial q_1}, \ldots, -\frac{\partial H}{\partial q_n}\right)$$

† National Science Foundation graduate fellow.

subject to the initial condition that T_0 is the identity operator. Further, we assume that $T_t : R^{2n} \to R^{2n}$ is invertible for each t and that both T_t and T_t^{-1} are C^∞ jointly in t and phase-space variables.

Now, we take for observables the set $\mathscr{D}$ of all C^∞ functions on R^{2n} with compact supports, as described by Schwartz (1950). For the observable f in $\mathscr{D}$ we define the action of T_t by

$$T_t^*f(q_1, \ldots, q_n; p_1, \ldots, p_n) = f(T_t(q_1, \ldots, q_n; p_1, \ldots, p_n)).$$

For each fixed t, T_t^*f is in $\mathscr{D}$. Considered as a function of both t and phase-space variables, T_t^*f is jointly C^∞.

For states the set $\mathscr{D}'$, the topological vector space dual of $\mathscr{D}$, is employed. $\langle , \rangle$ is composition of functions with linear functionals. It is usual for physical reasons to restrict the set of states to probability measures, but it is convenient mathematically to have the additional resources of $\mathscr{D}'$. The action of T_t on $\mathscr{D}'$ is defined to be the adjoint of T_t^*, so that (iii) will be satisfied:

$$\langle f, T_{t*}m \rangle = \langle T_t^*f, m \rangle, \qquad f \in \mathscr{D}, m \in \mathscr{D}'.$$

Let us consider the case that m in $\mathscr{D}'$ can be represented by integration with respect to the probability measure denoted by $\mathbf{m}$, i.e.

$$\langle f, m \rangle = \int f \, d\mathbf{m}.$$

In this case the action of T_t on $\mathbf{m}$ is usually defined to be

$$T_{t*}\mathbf{m}(B) = \mathbf{m}\{T_t^{-1}(B)\}$$

for the Borel set B. By a well-known result of measure theory (see Halmos 1950)

$$\int f \, d(\mathbf{m}T_t^{-1}) = \int f \circ T_t \, d\mathbf{m}$$

which implies that our definition agrees with the usual one. This transfer of the action of T_t from states to observables is the difficult step in the treatment of hypervirial theorems. The rest is just an application of the abstract theorem using the differentiability assumed for T_t.

It is convenient to express the time derivative of T_t^* in terms of the Poisson bracket (see Landau and Lifshitz 1960)

$$\{H, f\} = \sum \frac{\partial H}{\partial p_j}\frac{\partial f}{\partial q_j} - \sum \frac{\partial H}{\partial q_j}\frac{\partial f}{\partial p_j}.$$

For f in $\mathscr{D}$ we have

$$\frac{d}{dt}(T_t^*f) = \{H, f\}.$$

For f in $\mathscr{D}$ and m in $\mathscr{D}'$, $\langle T_t^* f, m \rangle$ is a C^∞ function of t, and Schwartz (1950) shows that differentiation within $\langle , \rangle$ is valid. Thus

$$\frac{d}{dt}\langle T_t^*f, m \rangle = \langle \{H, f\}, m \rangle.$$

Classical conservation and hypervirial theorems for C^∞ time development. An observable f in $\mathscr{D}$ is invariant if, and only if, $\langle \{H, f\}, m \rangle = 0$ for all m in $\mathscr{D}'$ and all t. A state m in $\mathscr{D}'$ is invariant if, and only if, $\langle \{H, f\}, m \rangle = 0$ for all f in $\mathscr{D}$ and all t.

Proof. $\langle T_t^* f, m \rangle$ is a C^∞ function of t and hence is constant if, and only if, its time erivative is zero.

The Liouville theorem that Lebesgue measure in phase space is invariant is an easy corollary of the above result. Integration by parts yields that the Lebesgue integral of $\{H, f\}$ is identically zero for all f in $\mathscr{D}$.

To obtain the standard classical mechanical virial theorem we use $\mathscr{E}$ and $\mathscr{E}'$ for observables and states instead of $\mathscr{D}$ and $\mathscr{D}'$. $\mathscr{E}$ is the space of C^∞ functions with unrestricted supports and $\mathscr{E}'$ its topological vector space dual defined by Schwartz (1950). It is assumed that $H = T(p)+V(q)$, with T a homogeneous quadratic and V a homogeneous function of degree k. Then $\Sigma p_j q_j$ is in $\mathscr{E}$ and

$$\{H, \sum p_j q_j\} = 2T - kV$$

by Euler's theorem on homogeneous functions. Thus for any invariant state m in $\mathscr{E}'$

$$2\langle T, m\rangle = k\langle V, m\rangle.$$

In particular, the time average over a bounded orbit in phase space is an invariant element of $\mathscr{E}'$, which is the particular case given by Landau and Lifshitz (1960). The existence and invariance of such time averages in the probability measure case are problems of ergodic theory, but the results used here are elementary applications of distribution theory.

4. Quantum mechanics

The underlying structure of our quantum system is assumed to be a complex Hilbert space. The Hamiltonian H is assumed to be a *bounded* self-adjoint operator. The time evolution T_t of a vector ϕ in the space is given by $T_t\phi = e^{-iHt}\phi$. The set O of observables is taken to be the set of all bounded linear operators. The set S of states is taken to be the set of all trace-class operators. For physical reasons the states are often restricted to positive operators of unit trace, but this restriction is not enforced here. $\langle , \rangle$ is given by

$$\langle A, P\rangle = \mathrm{tr}(AP) \quad \text{for } A \in O, P \in S.$$

The actions of T_t are

$$T_t^* A = e^{iHt} A\, e^{-iHt}, \qquad T_{t*} P = e^{-iHt} P\, e^{iHt}.$$

The time derivative of the actions of T_t can conveniently be expressed in teıms of the commutator bracket:

$$[H, A] = HA - AH.$$

We have

$$\frac{d}{dt} T_t^* A = i[H, A], \qquad \frac{d}{dt} T_{t*} P = i[P, H].$$

Quantum conservation and hypervirial theorems for bounded Hamiltonian. An observable A is invariant if, and only if, $\mathrm{tr}(A[P, H]) = 0$ for all states P. A state P is invariant if, and only if, $\mathrm{tr}([H, A]P) = 0$ for all observables A.

Proof. The proof is by differentiation of $\mathrm{tr}((T_t^* A)P)$ with respect to t. Analytic justification for formal differentiation is found by Schatten (1960).

Let θ be an eigenvector of H. The original form of the hypervirial theorems is that the matrix element $([H, A]\theta, \theta)$ is zero for each observable A. Let P be the projector of the subspace spanned by the normalized vector ϕ. Then

$$([H, A]\phi, \phi) = \mathrm{tr}([H, A]P) = \mathrm{tr}(A[P, H])$$

which shows the relation to the theorem presented above. The so-called off-diagonal hypervirial theorems (Coulson 1965, Chen 1964) are not immediate consequences of the above theorem, but a simple modification of the techniques used above can cover this case.

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