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Integral invariants and quantum hypotheses

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H. Poincaré (¹) introduced the important concept of integral invariant into celestial mechanics. Since some aspects of it might also have some significance in quantum theory, I would like to derive their most important properties.

Let:

$$\frac{dx_k}{dt} = X_k (x_1, x_2, ..., x_n, t) \qquad (k = 1, 2, ..., n)$$

be a system of ordinary differential equations, in which *t* is the independent variable ("time"), and $x_1, x_2, ..., x_n$ are the dependent variables ("coordinates"). If we call system of values of $x_1, x_2, ..., x_n$ a point in *n*-dimensional space then every point at the moment t_0 will be associated a point at the moment *t* by solving the differential equations. If we imagine a *k*-dimensional manifold M_0 in *n*-dimensional space at the moment *t*, i.e., the point-set that is defined by the equations:

$$x_i = \varphi_i (u_1, ..., u_k) \quad (i = 1, 2, ..., n) \quad (k \le n),$$

in which the *u*-values are restricted by only one or more *inequalities*. That manifold will go to another, likewise *k*-dimensional, *M* at time *t*. Now, let:

$$\int \cdots \int \sum A \, d\omega$$

be a *k*-fold integral, in which *A* is a function of $x_1, x_2, ..., x_n$, and *t*, and $d\omega$ is a k^{th} -order combination of differential $dx_1, ..., dx_n$. When the value of that integral at the moment t_0 when it is extended over M_0 is the same as the value that it will have at the moment *t* when it is extended over *M*, we say that the integral is an *integral invariant* of the differential system. It can happen that when k < n, the integral will keep its value only when the manifold M_0 (so *M* as well) is closed. One then speaks of a *relative integral invariant*.

⁽¹⁾ H. Poincaré, Les méthodes nouvelles de la mécanique céleste, t. III, Gauthier-Villars, Paris, 1899, pp. 1

Here, we shall not speak of the *general* theory of integral invariants, but only of the ones that are assigned to each mechanical system. We can write down one of them immediately. Namely, let $q_1, q_2, ..., q_f$ be the generalized coordinates and let $p_1, p_2, ..., p_f$ be the impulses of a mechanical system. We will then have:

$$J = \int p_1 \, dq_1 + p_2 \, dq_2 + \dots + p_f \, dq_f$$

as an integral invariant relative to *closed* curves. One can see that this integral keeps its value under any canonical substitution (contact transformation) with no calculation. Namely, let P_k be the new impulses, while Q_k are the new coordinates. It is then known that:

$$P_1 dQ_1 + P_2 dQ_2 + \dots + P_f dQ_f - p_1 dq_1 - p_2 dq_2 - \dots - p_f dq_f = dS$$

is a total differential for every canonical substitution. Thus:

$$\int P_1 dQ_1 + P_2 dQ_2 + \dots + P_f dQ_f = \int p_1 dq_1 + p_2 dq_2 + \dots + p_f dq_f + \int dS.$$

Naturally, the last term will vanish for every closed curve. Now, according to **Hamilton** and **Jacobi**, the coordinates and impulses at two different time-points t and t_0 are connected by a canonical substitution, namely:

$$p_1 dq_1 + \ldots + p_f dq_f - p_{10} dq_{10} - \ldots - p_{f_0} dq_{f_0} = dS$$
,

in which S is **Hamilton**'s action function that includes time as a parameter.

Conversely, it is easy to show that a system of differential equations that has J as a relative integral invariant is canonical (¹).

Assuming that, let:

$$\frac{dJ}{dt} = \int \dot{p}_1 dq_1 + \dots + \dot{p}_f dq_f + p_1 d\dot{q}_1 + \dots + p_f d\dot{q}_f$$

be equal to zero for every closed curve. One must then have that:

$$\dot{p}_1 dq_1 + \dots + \dot{p}_f dq_f + p_1 d\dot{q}_1 + \dots + p_f d\dot{q}_f$$

is a total differential. Now, one has:

$$p_k d\dot{q}_k = d\left(p_k \dot{q}_k\right) - \dot{q}_k dp_k,$$

so:

$$\dot{p}_1 dq_1 + \dots + \dot{p}_f dq_f - \dot{q}_1 dp_1 - \dots - \dot{q}_f dp_f$$

⁽¹⁾ E. T. Whittaker, Anal. Dynamics, Cambridge, 1904, pp. 266.

will be a total differential -dH. Therefore:

$$\dot{p}_k = -\frac{\partial H}{\partial q_k}, \qquad \dot{q}_k = \frac{\partial H}{\partial p_k}.$$
 Q. E. D.

From that relative invariant, we can find a second-order absolute invariant with the help of the analogue of **Stokes**'s theorem for multidimensional space $(^1)$:

$$J_1 = \iint dp_1 \, dq_1 + \dots + dp_f \, dq_f \, .$$

The integral extends over an arbitrary open two-dimensional manifold in 2f-dimensional space.

We prefer to show that this integral remains invariant under any canonical substitution directly. We imagine that we have represented the two-dimensional manifold by giving the p_k , q_k as functions of two parameters u, v, so:

$$J_1 = \iint \sum_{k=1}^f dp_k \, dq_k = \iint \sum \frac{\partial(p_k, q_k)}{\partial(u, v)} du \, dv.$$

The integral over the parameters u and v is now an ordinary double integral.

Let:

$$J_1' = \iint dP_1 dQ_1 + \dots + dP_f dQ_f = \iint \sum_{k=1}^f \frac{\partial(P_k, Q_k)}{\partial(u, v)} du dv.$$

If we introduce Q_k , q_k as new variables in J_1 in place of p_k , q_k with the help of the canonical substitution:

$$P_k = \frac{\partial S}{\partial Q_k}, \qquad p_k = -\frac{\partial S}{\partial q_k} \qquad (k = 1, 2, ..., f)$$

then we will have:

$$J_{1} = \iint \sum_{i} \left| \frac{\partial p_{i}}{\partial u} \quad \frac{\partial q_{i}}{\partial u}}{\partial v} \right| du \, dv = \iint \sum_{i} \left| -\sum_{k} \frac{\partial^{2}S}{\partial q_{i} \partial Q_{k}} \quad \frac{\partial Q_{k}}{\partial u} \quad \frac{\partial q_{i}}{\partial u}}{\partial v} \right| du \, dv$$
$$= \iint \sum_{i,k} \frac{\partial^{2}S}{\partial q_{i} \partial Q_{k}} \quad \frac{\partial Q_{k}}{\partial v} \quad \frac{\partial q_{i}}{\partial v} \right| du \, dv.$$

^{(&}lt;sup>1</sup>) **H. Poincaré**, *loc. cit.*, pp. 43.

We likewise introduce q_k , Q_k as new variables in J'_1 in place of P_k , Q_k :

$$J_{1}' = \iiint \sum_{i} \left| \frac{\partial P_{i}}{\partial u} \quad \frac{\partial Q_{i}}{\partial u} \right| du \, dv = \iiint \sum_{i} \left| \frac{\sum_{k} \frac{\partial^{2} S}{\partial q_{k} \partial Q_{i}} \frac{\partial q_{k}}{\partial u} \quad \frac{\partial Q_{i}}{\partial u}}{\sum_{k} \frac{\partial^{2} S}{\partial q_{k} \partial Q_{i}} \frac{\partial q_{k}}{\partial v} \quad \frac{\partial Q_{i}}{\partial v}} \right| du \, dv$$
$$= \iiint \sum_{i,k} \frac{\partial^{2} S}{\partial q_{k} \partial Q_{i}} \left| \frac{\partial q_{k}}{\partial u} \quad \frac{\partial Q_{i}}{\partial v} \right| du \, dv.$$

Upon switching two columns in the determinants, one will see that:

$$J_1 = J_1'$$

With that, we have also proved that J_1 is independent of time, as above (¹). One likewise proves that:

$$J_2 = \iiint \int dp_1 dp_2 dq_1 dq_2 + \dots + dp_{f-2} dp_{f-1} dq_{f-1} dq_f,$$

in which each combination of two indices occurs, is an integral invariant. The same thing is true of:

$$J_3 = \int \cdot (6) \cdot \int dp_1 dp_2 dp_3 dq_1 dq_2 dq_3 + \dots + dp_{f-2} dp_{f-1} dp_f dq_{f-2} dq_{f-1} dq_f ,$$

in which each combination of three indices occurs, etc. The last integral in that series is:

$$J_f = \int (2f) \cdot \int dp_1 dp_2 \cdots dp_f dq_1 dq_2 \cdots dq_f$$

The fact this is independent of time is known to be the content of Liouville's theorem.

I would now like to show what sort of meaning those integral invariants have in quantum theory. I assert that the static paths are determined by the equations:

$$J_1 = \iint dp_1 dq_1 + \dots + dp_f dq_f = (n_1 + n_2 + \dots + n_f) h ,$$

⁽¹⁾ The independence of time is also easy to show with the help of the equations $\frac{\partial \dot{p}_k}{\partial p_k} + \frac{\partial \dot{q}_k}{\partial q_k} = 0$.

$$J_{2} = \iiint dp_{1} dp_{2} dq_{1} dq_{2} + \dots + dp_{f-2} dp_{f-1} dq_{f-1} dq_{f} = (n_{1} n_{2} + \dots + n_{f-1} n_{f}) h^{2},$$

$$J_{f} = \int (2f) \cdot \int dp_{1} dp_{2} \cdots dp_{f} dq_{1} dq_{2} \cdots dq_{f} = n_{1} n_{2} \dots n_{f} h^{f},$$

in which $n_1, n_2, ..., n_f$ are positive whole numbers (¹). However, those equations will become meaningful only when the domain of integration has been given. We assume that the motion is required to be periodic, i.e., that the coordinates and impulses can be represented as *f*-fold Fourier series in the angle coordinates $w_1, ..., w_f$, which are themselves linear functions of time. We then introduce new variables $w_1, ..., w_f$ and their associated impulses $\alpha_1, ..., \alpha_f$ by a canonical substitution. As we saw above, $J_1, ..., J_f$ will remain invariant. We now determine the domain of integration for $J_1, J_2, ..., J_f$ by projecting onto the two-dimensional manifold α_k, w_k (fourdimensional manifold $\alpha_i, \alpha_k, w_i, w_k$, etc.) such that they will be mutually independent for each pair α_k, w_k . However, $J_1, ..., J_f$ will decompose into sums and products of individual integrals $\iint d\alpha_k dw_k$, and the solution of the system of equations will give:

$$\iint d\alpha_k \, dw_k = n_k \, h \qquad (k = 1, 2, \dots, f),$$

which is the usual formulation for the quantization condition according to Schwarzschild.

If am deeply grateful to Herrn Prof. Born for his continuing interest and encouragement.

Göttingen, Theor.-phys. Institut, July 1921.

^{(&}lt;sup>1</sup>) In regard to them, I should point out that the introduction of elementary symmetric functions of the quantum numbers as an Ansatz was on the recommendation of my friend **P. Csillag**.