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ON THE QUANTIZATION CONDITION OF SOMMERFELD AND EPSTEIN

by A. Einstein

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Translator's Notes

In the past decade a great deal of attention has been focused on the problem of semiclassical quantization of nonseparable but integrable Hamiltonian systems. This paper of Einstein's, published in 1917, postulates quantization conditions for systems of this nature. In this translation I have used "modern" language and notation. A few connective sentences/phrases have been added to improve the logical flow. The note added in proof, which in the original German suffers from poor construction, has been substantially rewritten, with the words "local" and "global" used to clarify Einstein's meaning. I have also added some footnotes and references to clarify this work in light of more recent developments. However, no attempt has been made to be exhaustive; references to recent numerical implementations of these ideas have been omitted.

I wish to acknowledge the critical reading of early versions of this translation by W. P. Reinhardt, H. H. Jaffé and M. Strand. W. P. Reinhardt has made numerous editorial revisions in the final version of the manuscript. This translation has also been compared (with permission) to the unpublished literal translation of W. Jakubetz and J. N. L. Connor which was brought to our attention by R. A. Marcus. This work was supported, in part, by grants CHE77-16307 and PHY76-04761 from the National Science Foundation.

Charles Jaffé

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§1. The Existing Formalism

It is clear that, for periodic mechanical systems of one degree of freedom, the quantization condition is[1]

$$\int p\,dq = \int p \frac{dq}{dt}\,dt = nh \quad . \tag{1}$$

The integration is performed over the entire period of the motion; q denotes the coordinate, p the conjugate momentum of the system. Further, the theoretical work of Sommerfeld demonstrates that for systems with ℓ degrees of freedom, the single quantization condition must be replaced by ℓ quantization conditions. According to Sommerfeld these ℓ conditions are

$$\int p_i\,dq_i = n_i h \quad . \tag{2}$$

This formulation is not independent of the choice of coordinates, so it can only be proven correct for certain choices of coordinates. It is only when such a choice has been made and the q_i are periodic functions of time that the conditions of Eq. (2) are applicable.

The more recent work of Epstein (and Schwarzschild) provides a fundamental improvement to this theory by providing criteria by which to choose the coordinates. Epstein bases his choice of coordinates on Jacobi's theorem.[2] Let $H = H(q_i, p_i, t)$ be the Hamiltonian of the system, which appears in the canonical equations

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{3}$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \tag{4}$$

and which — provided it does not contain time explicitly — is identical with the energy E.* If $S(q_1,\ldots,q_\ell,\alpha_1,\ldots,\alpha_\ell,t)$ is a total integral (Hamilton's Principal Function) of the Hamilton-Jacobi partial differential equation[3]

$$\frac{\partial S}{\partial t} + H\left(q_i\ ,\ \frac{\partial S}{\partial q_i}\right) = 0 \quad , \tag{5}$$

then the solutions of the canonical equations are

$$\frac{\partial S}{\partial \alpha_i} = \beta_i \tag{6}$$

$$\frac{\partial S}{\partial q_i} = p_i \quad . \tag{7}$$

If the Hamiltonian does not contain time explicitly, which is assumed in what follows, then Eq. (5) may be satisfied by use of the Ansatz[4]

$$S = W - Et \quad ,$$

where E is a constant and W (Hamilton's Characteristic Function) does not depend explicitly upon time. Equations (5), (6) and (7) are then replaced by

$$H\left(q_i\ ,\ \frac{\partial W}{\partial q_i}\right) = E \tag{5a}$$

$$\left.\begin{aligned} \frac{\partial W}{\partial \alpha_i} &= \beta_i \\ \frac{\partial W}{\partial E} &= t - t_0 \end{aligned}\right\} \tag{6a}$$

$$\frac{\partial W}{\partial q_i} = p_i \quad . \tag{7a}$$

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*In this case one has

$$\frac{dH}{dt} = \sum_i \frac{\partial H}{\partial q_i}\dot{q}_i + \sum_i \frac{\partial H}{\partial p_i}\dot{p}_i \quad .$$

Now the first equation in Eq. (6a) represents ℓ-1 equations, in the last equation α_ℓ is replaced by the constant E, and β_n by the constant t_o.

Epstein showed that if the coordinates are chosen so that Hamilton's Characteristic Function has the form

$$W = \sum_i W_i(q_i) \quad , \tag{8}$$

where W_i is a function of only q_i and not the other q_j's, then Sommerfeld's quantization condition, Eq. (2), will be valid provided the coordinates are periodic functions.

In spite of the success of Sommerfeld's and Epstein's generalization of the quantum principle in treating systems of several degrees of freedom, it still remains unsatisfactory in that according to Eq. (8) it is dependent upon a separation of variables. Such a separation of variables is not related to the quantum problem. This paper proposes a small modification of the Sommerfeld-Epstein condition in order to avoid this drawback. I will briefly outline the basic thoughts in the next section, and then in the following carry them out more precisely.

§2. The Modified Formalism

For systems of one degree of freedom, pdq is an invariant, that is, independent of the choice of the coordinate. However, for systems of several degrees of freedom, the individual products $p_i dq_i$ are not invariants; consequently the quantization conditions (2) do not lead to an invariant result. Only the sum $\sum_i p_i dq_i$, which extends over all ℓ degrees of freedom, is invariant. One can derive a set of invariant quantization conditions (from the single invariant sum) in the following manner: Let us consider the p_i as functions of the q_i. Then one can consider the p_i as a vector (covariant in character) on the ℓ-dimensional space of the q_i. If one then draws an arbitrary closed curve, in coordinate space, which need not be a "trajectory" of the mechanical system, the line integral

$$\int \sum p_i dq_i \quad , \tag{9}$$

performed over this curve, is an invariant. If the p_i are any arbitrary functions of the q_i, then in general the integral (9) will have a different value for each closed curve. However, if

$$\frac{\partial p_i}{\partial q_k} - \frac{\partial p_k}{\partial q_i} = 0 \quad , \tag{10}$$

which follows if the p_i are derivable from a function,[5] W, as

$$p_i = \frac{\partial W}{\partial q_i} \quad , \tag{10a}$$

then the integral (9) has the same value for all closed curves which can be continuously deformed into each other.[6] Further, the integral (9) vanishes for all curves that can be contracted into a single point by a continuous change. Now if the coordinate space, with its associated momentum vector field is multiply connected, then there are closed paths that cannot be contracted to a point by means of a continous change.[7] If this is the case, W is not a single valued (but an infinitely multivalued) function of the q_i, and in general the integral (9) will be different from zero for such a curve. Moreover, there will exist a finite number of closed curves, C_ℓ, in q-space, to which, by means of a continuous change, all closed curves are reducible. In this sense one can prescribe a finite number of quantization conditions

$$\int_{C_\ell} \sum_i p_i dq_i = n_\ell h \quad . \tag{11}$$

In my opinion these must replace the quantization conditions (2). We would expect that the number of equations (11), which cannot be reduced into one another, are equal to the number of degrees of freedom of the system. If it is smaller, then we have a case of "degeneracy."

The basic idea, which has been investigated above, will be explained in somewhat more detail in the following.

§3. A Descriptive Derivation from the Hamilton-Jacobi Differential Equation

If a point, P, in the coordinate space, with the coordinate q_i and associated with the canonical momentum coordinate p_i, is given, then the motion is completely determined by the canonical equations (3) and (4).* As a result, corresponding to every point on a trajectory L, there is a definite velocity, that is, the p_i are determined as functions of the q_i on L. If for each point P on a $(\ell-1)$ dimensional "surface" in coordinate space, the q_i and p_i are given, then associated with every point in coordinate space is such a trajectory L. If the p_i on the surface are continuous functions of the q_i, then these trajectories will continuously fill the coordinate space (or a part thereof). There will be a specific trajectory passing through every point (q_i) of the coordinate space; thus each of these points will also be associated with a specific momentum coordinate. From this it is clear that there is a vector field p_i associated with coordinate space. We wish to formulate the law of this vector field.

*It is again assumed that H does not depend explicitly on time.

If we consider the p_i, in the canonical system of equations (3), as functions of the q_i, we then must replace the left-hand sides by

$$\sum_k \frac{\partial p_i}{\partial q_k}\frac{\partial q_k}{\partial t} \quad ,$$

which by (4) may in turn be replaced by

$$\sum \frac{\partial p_i}{\partial q_k}\frac{\partial H}{\partial p_k} \quad .$$

Thus in place of (3) we obtain

$$\frac{\partial H}{\partial q_i} + \sum_k \frac{\partial H}{\partial p_k}\frac{\partial p_i}{\partial q_k} = 0 \quad . \qquad (12)$$

It is this system of ℓ linear differential equations that defines the p_k's as functions of q_k's.

Now we ask whether there exists a function W from which one can derive the momentum vector field, and for which the conditions (10) and (10a) are fulfilled. If this is the case, Eq. (12) takes the form

$$\frac{\partial H}{\partial q_i} + \sum_k \frac{\partial H}{\partial p_k}\frac{\partial p_k}{\partial q_i} = 0 \quad .$$

This equation shows that H is independent of the q_i. Thus functions W of the desired kind exist, e.g., the W's that satisfy the Hamilton-Jacobi equation (5a), or the S that satisfies equation (5).

It has been shown that equation (3) can be replaced by equation (7a) and (5a), or by (7) and (5). We shall now demonstrate that the system of equations (4) are fulfilled by (6a) or (6), even though this is of no importance for the subsequent discussion. After integration of (5a) one can express the p_i as functions of the q_i by virtue of (7a). The equations (4) form a system of

...tal differential equations which determines the q_i's as functions of time. According to the theory of differential equations of first order, this system of total differential equations is equivalent to the partial differential equation

$$\sum_k \frac{\partial H}{\partial p_r} \frac{\partial \phi}{\partial q_k} + \frac{\partial \phi}{\partial t} = 0 \quad . \tag{13}$$

Equation (13) is satisfied by $\phi = \partial S/\partial \alpha_i$, provided S is a complete integral of (5). This can be seen by placing this value of ϕ in the left-hand side of (13), thus obtaining, using (7),

$$\sum_k \frac{\partial H}{\partial(\partial J/\partial q_k)} \frac{\partial^2 S}{\partial q_k \partial \alpha_i} \frac{\partial^2 S}{\partial t \partial \alpha_i}$$

or

$$\frac{\partial}{\partial \alpha_i} \left\{ H\left(q_k , \frac{\partial S}{\partial \alpha_k}\right) + \frac{\partial S}{\partial t} \right\}$$

which vanishes because of (5). From this it follows that equation (4) is integrable by means of (6) and (6a).

§4. The p_i-Field of a Unique Trajectory

Having shown, in §3, that there exist momentum fields p_i such that $\int \sum p_i dq_i$ is path independent, we now come to an essential point, which I have intentionally omitted in the previous sketch of basic thoughts in §2. In the arguments of §3, we have explored the p_i-field by the means of $(\ell-1)$ infinites of trajectories, which fill the classically allowed region of coordinate space. We now follow the undisturbed motion of an isolated system through an infinitely long time and trace the trajectory in the q_i-space. Two cases may occur:

1) in the course of time, the trajectory comes arbitrarily close to every point in the classically allowed region of coordinate space, or

2) the trajectory is confined in a continuum of fewer than ℓ dimensions. (An example is the case of exactly closed orbits.)

Case 1 represents the general situation while Case 2 is a specialization. As an example of 1, we imagine the motion of a point mass under the influence of a central force, described by two coordinates that determine the position of the point in the plane of motion. Case 2 occurs, for example, when the attractive force law is exactly proportional to $1/r^2$, and when the deviation from the Kepler motion arising from the relativistic theory is ignored; the orbit is then closed, and its points form a continuum of only one dimension. Considered in three dimensional space, the central motion is always a motion of type 2, since the trajectory can be accommodated in a continuum of two dimensions. In working with three dimensions, one must consider the central motion as a special case of a more complicated (non-central) force law (for example that of Epstein's study of motion in the Stark effect).

The following argument is based on the general case 1. Consider an element $d\tau$ of q_i-space. A trajectory will pass through this element infinitely often. Corresponding to each such crossing is a momentum vector. <u>A priori</u>, two fundamentally different types of trajectories are possible.[8] Type a): the p_i-vector repeats itself, so that only a finite number of p_i-vectors belong in $d\tau$. In this case the p_i are single or multivalued functions of q_i. Type b): there appear infinitely many p_i-systems at the point considered. In this case the p_i cannot be represented as a function of q_i.

One notices immediately that type b) excludes the quantization condition formulated in §2. Classical statistical mechanics on the other hand describe essentially only type b); only in this case is the microcanonical ensemble equivalent to the time averaged ensemble.*

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*In the microcanonical ensemble there exist systems which for given q_i arbitrary (with the proper energy) p_i exist.

Summarizing, we note that application of the quantization condition (11) requires that (i) trajectories be of type a) and, ii) that the individual trajectories determine a function W from which the momentum field can be derived. (However, see "Note added in proof," Ed.)

§5. The Rational Coordinate Space

It has already been mentioned that the p_i are, in general, multivalued functions of the q_i. We consider, as a simple example, the circular motion of a point under the attractive force of a fixed center. The point moves in such a way that its distance from the attractive center oscillates periodically between a minimum value r_1 and a maximum value r_2. If one considers a point in the space of q_i, that is, a point on the coordinate space annulus whose limits are both of the circles with radii r_1 and r_2, then in the course of time the trajectory will come infinitely close to it, or -- less precisely -- pass through it. However, for the passage of a portion of the orbit with increasing r, or a portion of the orbit with decreasing r, the radial component of the velocity has different signs; the p_ν are double-valued functions of q_ν.

The inconvenience for visualization caused by this fact is best removed by means of the well-known method introduced into function theory by Riemann. We imagine that we double the surface of a circular ring, so that two congruent, circular ring-shaped sheets lie on top of each other. On the upper annulus we imagine the orbit sections with positive dr/dt together with the associated vector p_ν, and on the lower annulus those sections with negative dr/dt together with the associated vector p_ν. At both circumferences we imagine the two sheets are connected, since the orbit must cross from one circular sheet to the other whenever the trajectory touches one of the boundary circumferences. It is easily seen that along the circles the p_ν on both sheets are equal. Interpreted on this double surface, the p_ν are not only continuous but also single valued functions of the q_ν.

On this double surface there are obviously two types of closed paths, which can neither be contracted to a point by a continuous change, nor be reduced to each other. Figure 1 shows an example of each of the two (L_1 and L_2) types; the parts of the path which lie on the lower sheet are drawn dotted. All other closed paths may, by a continuous change on the doubled surface, either be contracted into a point or deformed into one or more paths of types L_1 and L_2. The quantum condition (11) would here have to be applied to the two path types L_1 and L_2.

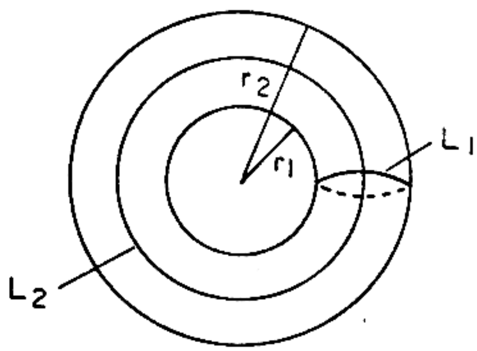

Fig. 1

It is clear that this consideration generalizes for all motion that fulfills the condition of §4. One has to imagine the phase space is respectively divided into a number of "sheets" which are connected along $(\ell-1)$ dimensional "surfaces" in such a way that in order to interpret the resulting structure the p_i are single valued and (with respect to crossing from one [sheet] to another) continuous functions. This auxiliary geometrical construction we will denote as the "rational phase space." The quantum principle (11) ought to be applicable to all contours, which are closed in rational coordinate space.

In order for the quantum principle in this formulation to have an exact meaning, the integral $\int \sum p_i dq_i$, performed over all closed curves in rational q_i-space that can be transformed continuously into one another, must have the same value. The proof is to be carried out according to the familiar scheme. Let L_1 and L_2 be closed curves in rational q_i-space (see Fig. 2), which, maintaining the direction of motion can be continuously transformed into one another. Then the line plotted in the figure is a closed curve which can be contracted continuously into a point. From this it follows, due to (10), that the integral, performed over the plotted line, vanishes. If one bears in mind that the integrals, performed over the infinitely adjacent joining lines $\overline{A_1A_2}$ and $\overline{B_1B_2}$, are equal to one another as a result of the single valuedness of the p_i in the rational q_i-space, it follows that the integrals performed over L_1 and L_2 are equal.

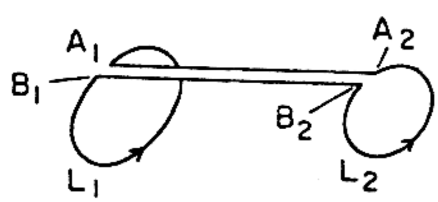

Fig. 2

Finally, we note that the function W is infinitely multivalued even in the rational q_i-space. However, according to the quantum principle this multivaluedness is the simplest conceivable. That is, if W has the value W* at a particular point in rational q_i-space, then the remaining values of the function are W* + nh, where n is an integer.

...te added in proof

Further reflection on condition (ii) given at the end of §4 for the applicability of the quantization condition (11) reveals that it is always satisfied. That is, the following principle is true: If the motion determines a momentum field then there exists a function from which this field may be obtained by Eq. (10a).

According to Jacobi's principle, every motion of a system can be derived from a total integral W of (5a). Thus there exists locally at least one function W of the q_i, from which the p_i of a system can be computed

$$p_i = \frac{\partial W}{\partial q_i} \quad .$$

We must now remember that W is obtained with the help of a partial differential equation. Thus if we want to know how W changes for a system in the course of its motion, we must integrate the differential equation along the trajectory to obtain the continuation of W. Now if the orbit, after a certain (VERY long) time, closely approaches the vicinity of a point P, through which the orbit has previously passed, then $\partial W/\partial q_i$ produces that momentum for both times.

There are however two cases. Corresponding to motion of type "b" (see §4), on each return to P one should not expect to return to the previous values of $\partial W/\partial q_i$. On the contrary, one should expect to encounter a new value of p_i each time the orbit returns to P. Consequently it is not possible to find a global representation of the p_i (or W) as a function of the q_i. Corresponding to motion of type "a," however, the p_i-vectors eventually reappear as the coordinate configuration repeats, then the $\partial W/\partial q_i$ can be represented globally as (multiple valued) functions of q_i. Thus if a p_i-field exists for the infinitely continued motion, then a function W $(\bar{q})$ exists.

We restate our conclusions as follows: If there exist ℓ integrals of the equations of motion of the form

$$R_k(q_i, p_i) = \text{const.} \quad , \tag{14}$$

where the R_k's are algebraic functions of the p_i, then $\sum p_i dq_i$ is always a total differential. The quantization condition states that the integral $\oint \sum p_i dq_i$, performed over an irreducible curve, should be a multiple of h. The quantization condition coincides with the Sommerfeld-Epstein condition if, specifically, every p_i depends only upon the associated q_i. If there exist fewer than ℓ integrals of type (14), as Poincare has proven for the three-body problem, then the p_i cannot be represented (globally) as functions of the q_i, and even the modified form of the Sommerfeld-Epstein quantization condition [i.e., that of Eq. (11)] fails.

Footnotes

[1]Subsequent work by Brillouin (1926), Keller (1958), and Maslov (1972) has shown that even the one-dimensional quantization conditions must be modified to read

$$\int p dq = (n + \alpha/4)h \quad ,$$

where the value of the parameter α is determined by counting the number of caustics (i.e., boundaries connecting the sheets or surfaces on which the p are single valued in the q_i) which the integration path crosses. For further discussion of this parameter the reader is referred to the work of Berry and Mount (1972), Percival (1976), and Voros (1976).

[2]See Goldstein (1950), Chapter 9, for a clear and informative discussion of Hamilton-Jacobi theory. I have changed the notation in this paper to correspond to Goldstein's notation.

[3]Both S and W are generating functions, which are usually chosen to be of type $F_2(q,P)$, using the notation of Goldstein (1950). If we make this choice and then choose the constants, α_i's, to be the action variables, then the β_i's are the angle variables and develop linearly in time, i.e.,

$$\beta_i = \omega_i t + \delta_i \quad .$$

[4]This is a Legendre transformation from the time-dependent representation of classical mechanics to the time-independent formulation.

[5]Einstein calls W a "potential," I have translated this as "function."

[6]It should be noted that these results are analogous to Cauchy's theorem with regard to integration in the complex plane.

[7]By continuous change, Einstein means any deformation of the closed path on the surface of the invariant torus which does not require the path to be broken.

[8]A pedagogical discussion of the nature of these regular and irregular types of classical motion is given by Berry (1978), and references therein.

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