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Corrected Bohr-Sommerfeld Quantum Conditions for Nonseparable Systems*

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For a separable or nonseparable system an approximate solution of the Schrödinger equation is constructed of the form $Ae^{i\hbar^{-1}S}$. From the single-valuedness of the solution, assuming that A is single-valued, a condition on S is obtained from which follows A. Einstein's generalized form of the Bohr-Sommerfeld-Wilson quantum conditions. This derivation, essentially due to L. Brillouin, yields only integer quantum numbers. We extend the considerations to multiple valued functions A and to approximate solutions of the form

$$\sum A_k \exp(i\hbar^{-1}S_k).$$

In this way we deduce the corrected form of the quantum conditions with the appropriate integer, half-integer or other quantum number (generally a quarter integer). Our result yields a classical mechanical principle for determining the type of quantum number to be used in any particular instance. This fills a gap in the formulation of the "quantum theory", since the only other method for deciding upon the type of quantum number—that of Kramers—applies only to separable systems, whereas the present result also applies to nonseparable systems.

In addition to yielding this result, the approximate solution of the Schrödinger equation—which can be constructed by classical mechanics—may itself prove to be useful.

INTRODUCTION

In the "quantum theory" the motion of a system is described by classical mechanics but certain constants of the motion are restricted to be integers. These restrictions are called the quantum conditions and the integers occurring in them are called the quantum numbers. In many cases better agreement between theory and observation is obtained if half-integer quantum numbers are employed instead of integers. However no theoretical principle is available to determine whether an integer, half-integer or other quantum number is to be used in any particular case. It is the purpose of this article to provide such a principle.

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Historically the problem of deciding between integer and half-integer quantum numbers was circumvented by the invention of quantum mechanics, which replaced the "quantum theory". Therefore the discovery of a procedure for deciding between the two kinds of quantum numbers might now be considered to be of purely academic interest. However this is not necessarily the case because the procedure can still be used in the approximate solution of quantum mechanical problems.

A way of deciding between integer and half-integer quantum numbers for separable systems was found by Kramers (*2*) by means of an approximate solution of the Schrödinger equation. His result also showed that for such systems these conditions are consequences of quantum mechanics in the limit as Planck's constant h tends to zero. Another derivation of the quantum conditions from the Schrödinger equation was given by Brillouin (*3*). It was more general than Kramers' since it applied to both separable and nonseparable systems, but it was incorrect since it yielded only integer quantum numbers. Brillouin's argument is essentially the following:

Consider a quantum mechanical system with N coordinate operators q_r, N conjugate momentum operators $p_r \equiv -i\hbar^{-1}(\partial/\partial q_r)$, $r = 1, \cdots, N$, and Hamiltonian operator $H(q_r, p_r, t)$. Let the Schrödinger representor of the state of the system be $\Psi(q_r, t)$. Suppose that Ψ is approximately equal to Ψ_0 defined by

$$\Psi_0 = A(q_r, t, \hbar) \exp[i\hbar^{-1}S(q_r, t, \hbar)]. \tag{1}$$

The function Ψ and hence Ψ_0 must be single valued. Therefore if S is multiple valued and if ΔS denotes the difference between any two of its values, it is necessary that

$$\Delta S = nh. \tag{2}$$

Here n is an integer. This condition guarantees that Ψ_0 will be single valued even if S is not. The quantum conditions with integer quantum numbers follow from (2), as will be shown below. We will also show that (2) is equivalent to the quantum condition postulated by Einstein (*4*) in generalizing the Bohr-Sommerfeld-Wilson conditions to nonseparable systems.

We note that Brillouin's argument assumes that A is single valued. However if A is not single valued then in order for Ψ_0 to be single valued (2) must be replaced by

$$\Delta S = h\left[n + i\frac{\Delta \log A}{2\pi}\right]. \tag{3}$$

Suppose, for example, that two values of A differ only in sign. Then $\Delta \log A = -i\pi$ and (3) yields

$$\Delta S = h[n + \tfrac{1}{2}]. \tag{4}$$

From (4) the quantum condition with a half-integer quantum number follows.

We have just indicated how to modify Brillouin's argument in order to obtain the appropriate integer, half-integer or other quantum number. To complete the argument we must examine the amplitude A. This will be done in the next sections. However we must first make another change in the method. Instead of (1), we will assume that Ψ_0 is a sum of terms given by

$$\Psi_0 = \sum_{k=1}^{M} A_k(q_r, t, \hbar) \exp [i\hbar^{-1} S_k(q_r, t, \hbar)]. \tag{5}$$

This more general form of approximate solution is required in almost all problems in which S is multiple valued. The various functions S_k and A_k will be considered to be different branches of multiple valued functions S and A. We will also make our considerations more definite by assuming that Ψ is asymptotic to Ψ_0 as Planck's constant $\hbar$ tends to zero. This viewpoint was introduced by Birkhoff (*5*).

ASYMPTOTIC SOLUTION OF THE SCHRÖDINGER EQUATION

The function Ψ satisfies the Schrödinger equation

$$H(q_r, p_r, t)\Psi(q_r, t) = i\hbar \frac{\partial \Psi}{\partial t}(q_r, t). \tag{6}$$

Upon inserting the expression (5) for Ψ_0 into (6) and considering the leading terms in $\hbar$ we obtain equations for the A_k and S_k. These equations were derived by Dirac (*6*) when Ψ_0 consists of a single term and the same analysis applies when Ψ_0 is a sum of terms. The result is that each S_k satisfies the classical Hamilton-Jacobi equation

$$H\left(q_r, \frac{\partial S_k}{\partial q_r}, t\right) = -\frac{\partial S_k}{\partial t}. \tag{7}$$

The equation for each A_k, written in terms of $P_k = A_k^2$ and

$$v_r = \frac{\partial H}{\partial p_r}(q_r, \partial S/\partial q_r, t),$$

is

$$\frac{\partial P_k}{\partial t} + \sum_{r=1}^{N} \frac{\partial}{\partial q_r}[v_r P_k] = 0. \tag{8}$$

Equation (8) is the Liouville equation of classical statistical mechanics for the probability distribution P_k of a classical mechanical system with Hamiltonian H. It is a special form because P_k depends only upon q_r and t, but not upon v_r or p_r as is usual in classical mechanics. This is a consequence of the fact that quantum mechanics does not yield joint probability distributions of conjugate

variables. It is to be noted that P_k is not necessarily positive, nor even real, in the present case. We will also permit S_k to be complex.

Let us solve (7) when H is independent of t. Then $H = E$, where the constant E is the total energy of the system. Now if $q_r(t)$, $p_r(t)$ denote a trajectory, then the function S_k is given at any point of the trajectory in terms of its value $S_k(0)$ at some fixed point on the trajectory by

$$\begin{aligned} S_k(q_r, t, \hbar) &= S_k(0) + \int_0^t \sum_{r=1}^{N} p_r(\tau) \frac{dq_r(\tau)}{d\tau} d\tau - Et \\ &= S_k(0) + \int_0^t \sum_{r=1}^{N} p_r \, dq_r - Et. \end{aligned} \tag{9}$$

Equation (8) can also be solved at once if P_k is independent of t, for then it becomes

$$\sum_{r=1}^{N} \frac{\partial}{\partial q_r}[v_r P_k] = 0. \tag{10}$$

Equation (10) asserts that the probability flux is divergenceless, and therefore by applying Gauss' theorem to a tube of trajectories we obtain

$$P_k v = P_k(0) v_0 \frac{d\sigma_0}{d\sigma}. \tag{11}$$

In (11)

$$v = \left[\sum_{r=1}^{N} v_r^2\right]^{1/2}$$

and $d\sigma$ is the normal cross sectional area of the tube of trajectories, both evaluated at the same point at which P_k is evaluated. The corresponding quantities v_0, $d\sigma_0$, and $P_k(0)$ are evaluated at some other point on the same trajectory, and thus (11) merely asserts the conservation of "probability". Actually (11) holds in the limit as $d\sigma_0$ tends to zero, in which case $d\sigma/d\sigma_0$ denotes the Jacobian of the mapping of one cross section onto another by means of trajectories. The problem of Rutherford scattering has been treated by Gordon (*7*) and by the present author (*1*) by means of Eqs. (9) and (11).

THE QUANTUM CONDITIONS

Quantum mechanics requires that Ψ be a single valued function of the q_r and therefore Ψ_0 must satisfy the same condition. Consequently each term in the expression (5) for Ψ_0 must be single valued. As we have shown in the Introduction, this requires that each S_k and the corresponding A_k must satisfy the condition (3). If any A_k is single valued, this condition becomes the simpler condition (2) for the corresponding S_k.

The differences $\Delta S_k(q_r, t)$ and $\Delta \log A_k(q_r, t)$ are expressible as line integrals over some closed curve in q_r space beginning and ending at q_r. In terms of these integrals, (3) becomes, for each value of k,

$$\oint \nabla S \cdot ds = h\left[n + \frac{i}{2\pi} \oint \nabla \log A \cdot ds\right]. \tag{12}$$

Equation (12) must hold for every closed curve in the q_r space, since only then will Ψ_0 be single valued at every point. However the line integrals in (12) have the same value for every two closed curves which are deformable into one another without crossing a singularity of the integrand. For example, they are zero for a curve which can be deformed into a point. There are, in general, only a finite number of classes of independent curves which cannot be deformed into points. Any other curve is deformable into a linear combination of such curves with integer coefficients. Therefore (12) will be satisfied for all curves if it is satisfied by one curve in each of the independent classes of curves. Thus we have, in general, a finite number of quantum conditions, in each of which the integer n is arbitrary.

Since $\nabla S \cdot ds = \sum_r p_r dq_r$, (12) can be rewritten as

$$\oint \sum_r p_r\, dq_r = h\left[n + \frac{i}{2\pi} \oint \nabla \log A \cdot ds\right]. \tag{13}$$

When A_k is single valued, the conditions (13) become exactly the quantum conditions postulated by Einstein (4) for a system in a steady state of constant energy. He pointed out that these quantum conditions are invariant under a contact transformation of variables because $\sum p_r dq_r$ is invariant. If the variables are separable in the Hamilton-Jacobi equation, so that each p_r can be expressed in terms of the corresponding q_r alone, and if A_k is single valued, then these conditions reduce to the well known Bohr-Sommerfeld-Wilson quantum conditions for a separable system in a steady state of constant energy.

In order to clarify the conditions (12) and (13) let us consider a multiple valued solution S of the Hamilton-Jacobi equation. Such a solution generally has infinite multiplicity, i.e., an infinite number of different values or branches. However only a finite number of its branches, say M of them, are essentially distinct. Every other branch differs from one of these branches by an additive constant. Therefore the function ∇S will have only the finite multiplicity M since any two branches differing by a constant yield the same value for ∇S. Let us introduce an M-sheeted q_r space and associate one branch of the function ∇S with each sheet. We will denote each sheet by an integer k and the corresponding branch of ∇S by ∇S_k, with k ranging from one to M. Any two sheets—say sheets j and k—are to be joined together at all points where $\nabla S_j = \nabla S_k$. Furthermore if ∇S is defined in only part of the q_r space then only that part is covered by additional sheets. The M sheeted q_r space so constructed is called the covering space for the function ∇S. Its main property is that on it ∇S is a single valued function. The Riemann surfaces of function theory are examples of such spaces.

The same considerations may be applied to the multiple valued function $\log A$. Its gradient has the same multiplicity M as does ∇S as we see from (8) and its different branches become equal where those of ∇S do. Therefore the same covering space on which ∇S is single valued also serves as the covering space for $\nabla \log A$. Consequently the line integrals in (12) and (13) may be thought of as being evaluated along a closed path on this covering space. Then the omission of the subscript k in (12) and (13) is appropriate since any number of branches may be involved in each integral. Also the question of whether one closed curve is deformable into another becomes clear in this space. Furthermore, the independent closed curves can be recognized as the basis of the fundamental group of the covering space. In this way we see that the topology of the covering space determines the number of quantum conditions. This number is just the number of closed curves in the basis of the fundamental group.

Let us now consider the evaluation of

$$\Delta \log A = \oint \nabla \log A \cdot ds.$$

We will restrict our attention to steady states since then $A^2 = P$ is explicitly given by (11). From this equation we see that P becomes infinite whenever $v d\sigma$ becomes zero. We will call points at which this occurs caustic points, in analogy with optics where points at which $d\sigma = 0$ are so named. A locus of caustic points is called a caustic of the family of trajectories associated with the S function under consideration. Those caustics which correspond to the vanishing of $d\sigma$ are envelopes of the family of trajectories. Therefore ∇S is multiple valued near these surfaces. Consequently such caustics are the loci of points at which two different branches of ∇S become equal. Thus these caustics form the boundaries at which different sheets of the covering space for ∇S are joined together. Those caustics at which $v = 0$ also form part of these boundaries, assuming that each p_r either changes sign along each trajectory on which v vanishes or is identically zero near the caustic. For then ∇S, which has the p_r as components, reverses its direction at the caustic. Thus this type of caustic is also a boundary on which two branches of ∇S join.

We have seen that A becomes infinite on a caustic and that a caustic must be crossed by a path which goes from one sheet of the covering space to another. It is well known in optics that the phase of A is retarded by $\pi/2$ (i.e., A is multiplied by $e^{-i\pi/2}$) on a ray which passes through a caustic on which $d\sigma$ vanishes simply. (The positive direction along a ray is the direction of ∇S.) Furthermore the phase is retarded by π on a ray passing through a focus, which is a caustic point at which $d\sigma$ vanishes to the second order. The usual method for proving these facts

is based upon the asymptotic evaluation of certain double integrals which represent the wave function. These integral representations are deduced from Green's theorem, and the integrals are evaluated by the method of stationary phase. Both of these considerations can be immediately extended to problems such as the present one in which the number of dimensions is N. The result is this: The phase of A is retarded by $m\pi/2$ on a trajectory which passes through a caustic on which $d\sigma$ vanishes to the mth order. We may replace the statement "$d\sigma$ vanishes to the mth order" by the equivalent statement "the dimensionality of the cross section of a tube of trajectories is reduced by m". This result is an analogue for partial differential equations of the Kramers connection formulas which are employed in the WKB treatment of ordinary differential equations. In the present case the caustics play the role of the turning points.

From the foregoing analysis we see that $\log A$ changes by $-im\pi/2$ along a path which passes from one sheet of the covering space to another in the direction of ∇S. Here the positive integer m is the number of dimensions "lost" by a tube of trajectories at the caustic. Obviously m must be replaced by $-m$ if the path is traversed in the opposite direction. Considerations similar to those outlined above show that at the caustics on which v vanishes the phase of A is also retarded by $m\pi/2$, so $\log A$ changes by $-im\pi/2$ where m is the number of p_r which change sign at the caustic.

The total change $\Delta \log A$ along a closed curve is generally just the change associated with the various caustics through which the curve passes. Therefore, in general, we have

$$\frac{i}{2\pi}\,\Delta \log A = \frac{i}{2\pi}\oint \nabla \log A \cdot ds = \frac{m}{4}. \tag{14}$$

Here m denotes the total number of dimensions "lost" by the trajectories at the caustics through which the curve passes plus the number of p_r which change sign at the $v = 0$ caustics through which the curve passes. In evaluating m account must be taken of whether the curve traverses the caustic in the direction of increasing or decreasing S. When (14) is used the quantum conditions (13) finally become

$$\oint \sum p_r\, dq_r = h\left[n + \frac{m}{4}\right]. \tag{15}$$

These are the corrected quantum conditions for separable or nonseparable systems. In each quantum condition the positive integer n is arbitrary but the integer m is determined by the considerations described above.

THE "CLASSICAL Ψ FUNCTION"

We will call the function Ψ_0 given by (5) the "classical Ψ function" because it can be constructed by classical mechanical considerations alone. In spite of this the probabilities computed from $|\Psi_0|^2$ still show quantum mechanical interference effects if the sum in (5) contains more than one term.

If only one term occurs in (5) then $|\Psi_0|^2 = |A|^2 \exp(-2h^{-1}ImS)$, and the probability, as well as Ψ_0 itself, is exponentially damped in regions where $ImS > 0$. The probability in such regions vanishes as h tends to zero, corresponding to the fact that these regions are excluded in classical mechanics. This can be seen from the fact that the solution of the Hamilton-Jacobi equation is not real there. The exponential tail shows that Ψ_0 describes such quantum mechanical effects as "tunneling".

If $ImS = 0$ and $|A|^2 = A^2 = P$, then $|\Psi_0|^2 = P$. Thus as h tends to zero the quantum mechanical probability distribution approaches that given by the Liouville equation of classical statistical mechanics, and we may say that quantum mechanics approaches classical statistical mechanics, as h tends to zero. The customary statement that quantum mechanics approaches classical mechanics is thus not strictly correct, but holds only when the initial data are such that $P = 0$ except on one trajectory, in which case classical statistical mechanics reduces to classical mechanics. Since the classical method of computing differential scattering cross sections is actually based on classical statistical mechanics, the preceding considerations show that the quantum mechanical cross sections will approach them as h tends to zero when only one term occurs in (5).

Finally it is to be noted from (13) or (15) that h and n enter the solution only in the combination $(n + \frac{1}{4}m)h$. In some problems the solution for fixed n does not have the asymptotic behavior assumed in the derivation. However when the limit in which n becomes infinite while h becomes zero and $(n + \frac{1}{4}m)h$ is constant is considered, the assumed asymptotic behavior may result. In such cases the asymptotic solution applies only for high quantum numbers n.

AN EXAMPLE—THE HARMONIC OSCILLATOR

To exemplify the preceding results, let us consider the steady state of a one-dimensional harmonic oscillator of mass m, energy E, frequency ν_0, and momentum p. Recalling that $S_x = p$, we have from the definition of momentum

$$S_x = p = \pm(2mE - m\nu_0 x^2)^{1/2}. \tag{16}$$

We see that $\nabla S = S_x$ is real and double valued in the interval $-x_0 \leqq x \leqq x_0$ where $x_0 = (2E\nu_0^{-1})^{1/2}$. The two branches of S_x become equal at the endpoints of this interval. Thus the covering space for S_x consists of two line segments joined together at their two ends. This space is topologically equivalent to a circle, and there is only one basic closed curve on it. Therefore there is only one quantum condition. The closed curve passes through the two caustics $x = \pm x_0$ at both of which $v = m^{-1}p$ vanishes and p changes sign. Thus in (15) we have $m = 2$ so (15) becomes

$$\int_{-x_0}^{x_0} (2mE - m\nu_0 x^2)^{1/2}\, dx - \int_{x_0}^{-x_0} (2mE - m\nu_0 x^2)^{1/2}\, dx = h\left(n + \frac{1}{2}\right). \quad (17)$$

Equation (17) is just the result given by the usual WKB method in this case. A similar analysis holds for a particle in any one dimensional potential well.

To construct Ψ_0 we note that $d\sigma_0/d\sigma = 1$ in the present case so (11) yields, with A_0 a constant,

$$A = A_0\, v^{-1/2}. \quad (18)$$

Inserting $v = m^{-1}p$ in (18) with p given by (16) we obtain the two results

$$A_+ = A_0 m^{1/4}(2E - \nu_0 x^2)^{-1/4} \quad (19)$$

$$A_- = e^{-i\pi/2} A_0 m^{1/4}(2E - \nu_0 x^2)^{-1/4}. \quad (20)$$

The phase retardation represented by the factor $e^{-i\pi/2}$ in (20) accounts for the phase shift which occurs upon passing through either caustic. In the present example it arises formally when p is negative and the square root of p^{-1} is taken. Of course our previous considerations are necessary to ensure that we take the correct root.

Upon inserting (19), (20), and (16) into (5) and setting $S(x_0) = 0$, we obtain for $\Psi_0(x)$ in the region $|x| \leqq x_0$,

$$\Psi_0(x) = A_0 m^{1/4}(2E - \nu_0 x^2)^{-1/4} \left\{ \exp\left[-ih^{-1} \int_x^{x_0} (2mE - m\nu_0 x^2)^{1/2}\, dx \right] + \exp\left[-i\frac{\pi}{2} + ih^{-1} \int_x^{x_0} (2mE - m\nu_0 x^2)^{1/2}\, dx \right] \right\} \quad (21)$$

$$= e^{-i(\pi/4)} A_0 m^{1/4}(2E - \nu_0 x^2)^{-1/4} \cos\left[h^{-1} \int_x^{x_0} (2mE - m\nu_0 x^2)^{1/2}\, dx - \frac{\pi}{4} \right].$$

This is the usual WKB result. We may obtain the result for a particle in any one dimensional potential $V(x)$ by replacing $\nu_0 x^2$ by $2V(x)$ in (21).

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Mesons and the Structure of Nucleons

Part II. The Nucleon Isobar and Pion Dynamics*

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An "atomic" model of the physical nucleons, previously applied to the nucleon ground states, is extended to describe the excited isobar nucleon state, of angular momentum and isotopic spin 3/2. The model is used to compute the cross sections for resonant photoproduction of pions and Compton scattering of photons on protons. Other, nonresonant processes are taken into account in a phenomenological fashion, and the computed cross sections for the aforementioned processes are compared with available experimental data. The model is also used as a guide for the phenomenological interpretation of other high-energy processes—in particular, photodisintegration of the deuteron in the region of the photomeson threshold, and the resonant $\pi^- - P$ interaction at ~1 Bev.

INTRODUCTION

In an earlier communication (*1*)[1] a model was developed in which the physical nucleons (proton and neutron) were depicted as bound systems of a nucleon-like core and a single pion. The main features of the physical nucleons were seen to be determined by the condition that the core (spin and isotopic spin 1/2) and the pion (spin 0, isotopic spin 1) are bound in a $p_{1/2}$ state of total isotopic spin $T = 1/2$.

In considering, in I, the field-theoretic basis for this model, it was observed that the pion-nucleon forces in the $p_{3/2}$ state with $T = 3/2$ are also expected to be attractive, although less strongly than in the ground state. The existence of such an attraction is manifest in the well-known resonance phenomena associated with p-wave pion scattering and production in the $T = J = 3/2$ state. Indeed, these resonance phenomena are so pronounced as to suggest the existence of a quasi-stationary or virtual state of the nucleon, the so-called[2] (3,3) or "isobar" state.

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[1] Henceforth referred to as I.

[2] It is customary, in this field, to characterize the various states of a single nucleon and