Quasi-Classical Theory of the Nonspinning Electron*

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We develop a modified Hamiltonian-Jacobi theory of classical mechanics following the early work of Van Vleck. This modified Hamiltonian-Jacobi theory, or quasi-classical theory, permits us to exhibit in classical mechanics many features that in the past have been exclusively associated with quantum mechanics. We deal with classical wave functions, classical operators, classical "eigenvalue" equations, a classical "sum over paths" formulation of classical mechanics, and with classical creation and destruction operators. Following Van Vleck, one can derive the WKB approximate solutions to the Schrödinger equation from the solutions of the classical Hamilton-Jacobi equation. If we apply the methods of Keller to the nonrelativistic and relativistic Kepler problem, we derive eigenvalues from the requirement of single-valuedness imposed on the WKB solutions. It turns out that the energy eigenvalues are those given by the Schrödinger equation and the Klein-Gordon equation, respectively. In the particular case of the harmonic oscillator there exists a canonical transformation which transforms the quasi-classical equation into an exact equation of quantum mechanics. We conjecture that if the WKB approximation and the Schrödinger equation predict the same eigenvalues, then there always exists a canonical transformation which transforms the quasi-classical equation into the corresponding Schrödinger equation. Finally we derive the quasi-classical equations in momentum space.

I. INTRODUCTION

THE WKB approximation is a well-known procedure in quantum mechanics for passing from the wave theory to classical mechanics. The ensembles of particles described by the Schrödinger equation are replaced in this approximation by ensembles of particles constructed from the solutions of the classical Hamilton-Jacobi equation. These WKB solutions are asymptotic solutions of the wave equation, except in the neighborhood of the classical turning points where they become infinite.

A more deeply founded version of the WKB approximation was presented by Van Vleck[1] in 1928. Van Vleck showed that, without direct reference to the Schrödinger theory, the WKB wave solutions could be constructed from the solutions of the classical Hamilton-Jacobi equation. His solutions, tied as they are to the Hamilton-Jacobi theory, transform in a determinate way under canonical transformation.

If no additional conditions are imposed on these WKB solutions they approximate true wave functions with large-valued quantum numbers in regions of space distant from the classical turning points. We may gain an improved approximation to the Schrödinger functions by demanding that the classical wave functions satisfy additional requirements characteristic of a wave theory. Wave functions defined in ordinary configuration space have to be bounded, continuous, and single-valued. In bound-state problems these requirements quantize the theory, as they lead to discrete eigenvalues for the classical integrals of the motion.

These quantized WKB solutions we call quasi-classical solutions, and we shall hereafter refer to Van Vleck's version of the WKB theory, together with the requirements for quantization, as the quasi-classical theory.[2]

The Van Vleck formalism also permits us to construct exact solutions of the Schrödinger equation from the solutions of the Hamilton-Jacobi theory. Classical wave functions describing ensembles of particles originating from a point source are such exact solutions. The success of Feynman's "sum over paths" formulation of the quantum theory is based on the existence of these classical wave functions which satisfy the Schrödinger equation. Given such a solution, all equivalent solutions of the Schrödinger equation may be found by unitary transformation.

In addition to the point-source solutions there exist other WKB wave functions which are solutions of the Schrödinger equation. We have found such a solution in the case of the one-dimensional harmonic oscillator in the configuration space of classical creation operators.

Van Vleck's formulation of the WKB theory also provides us with a means of enriching our description of classical mechanics so that its mathematical form corresponds more closely to that of quantum mechanics. We shall show the existence of classical differential operators, classical "eigenvalue" equations, a classical "sum over paths" formalism, classical "creation operators," etc. The appearance in classical physics of mathematical elements which in the past have been associated exclusively with quantum mechanics does not imply that we have reduced the quantum theory to classical mechanics. In a wave theory the wave functions must provide a meaningful description of wave phenomena. One must therefore require that these functions be bounded, continuous, and single-valued. These requirements lead to such typical features of the quantum theory as quantized energy

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[1] J. H. Van Vleck, Proc. Natl. Acad. Sci. U. S. 14, 178 (1928).

[2] Although in principle we have made a distinction between the classical and quantized solutions to the same equation, in practice we shall use the terms classical and quasi-classical (the latter implying quantized) interchangeably. No confusion can result since all the solutions we exhibit in this paper are derived from classical mechanics, and it will be quite clear to the reader when we pass over to the quantum theory.

levels and barrier penetration. On the other hand, the basic principles of classical mechanics would be violated if we adopted similar requirements for classical systems.

II. MODIFIED HAMILTON-JACOBI THEORY

The Hamilton-Jacobi equation for a classical system of particles is

$$\partial S/\partial t+H\left(q^k,\frac{\partial S}{\partial q^k},t\right)=0. \tag{1}$$

H is the Hamiltonian and the q_k ($k=1,2,\cdots,N$) are the generalized coordinates of the dynamical system. The dependent variable S is known as Hamilton's principal function.

Since Eq. (1) is a partial differential equation of the first order which does not depend explicitly on S, a complete integral of the equation is of the form,

$$S=S(q^k,\alpha^k,t)+c,$$

where the α^k and c are constants. In this paper we shall assume that the additive constant c vanishes unless otherwise noted. The constants α^k are chosen so that the determinant $\|\partial^2S/\partial q^i\partial\alpha^k\|$ nowhere vanishes. The $2N$ variables, q^i and α^i, then cover the $2N$-dimensional phase space available to the dynamical system.

Van Vleck[1] first showed that from a solution of the Hamilton-Jacobi equation one could derive a conserved density in configuration space This density is the Van Vleck determinant, D,

$$D=\left\|\frac{\partial^2S}{\partial q^i\partial\alpha^k}\right\|. \tag{2}$$

D satisfies the equation

$$\frac{\partial D}{\partial t}+\frac{\partial}{\partial q^i}(Dv^i)=0, \tag{3}$$

where

$$v^i=\frac{\partial H}{\partial(\partial S/\partial q^i)}.$$

We shall rederive this equation of continuity by generalizing a procedure due to Pauli.[3] Pauli restricted his derivation to a very small class of classical ensembles; those which correspond to the so-called kernels of the Schrödinger equation when that equation is written in terms of cartesian coordinates. In our discussion we deal with the most general Hamilton-Jacobi ensembles in the spirit of Van Vleck's original work.

We differentiate the Hamilton-Jacobi equation twice, once with respect to the α^i, and then with respect to q^k, and we find

$$\frac{\partial}{\partial t}\left(\frac{\partial^2S}{\partial\alpha^i\partial q^k}\right)+\frac{\partial}{\partial q^k}\left(\frac{\partial H}{\partial(\partial S/\partial q^l)}\frac{\partial^2S}{\partial q^l\partial\alpha^i}\right)=0. \tag{4}$$

We now introduce the matrix $\phi_{li}=\partial^2S/\partial\alpha^i\partial q^l$. This matrix must possess an inverse since we have assumed that the determinant $D=\|\phi_{li}\|$ nowhere vanishes. The inverse matrix ϕ^{ij} is defined by the relations,

$$\phi^{ji}\phi_{il}=\phi^{ij}\phi_{li}=\delta_l{}^j.$$

The rule for differentiating a determinant gives

$$dD=D\phi^{ji}d\phi_{ij}. \tag{5}$$

If we multiply Eq. (4) by ϕ^{ij}, and make use of Eq. (4), we find that D satisfies the relation,

$$\frac{\partial D}{\partial t}+\frac{\partial}{\partial q^l}\left(D\frac{\partial H}{\partial(\partial S/\partial q^l)}\right)=0. \tag{3}$$

With the two functions S and D we define a classical complex "wave function," Ψ_C,

$$\Psi_C=R\exp(iS/\hbar), \tag{6}$$

where $R=(Dg^{-\frac{1}{2}})^{\frac{1}{2}}$, and g is the determinant of the metric g_{ik} of the configuration space. $\hbar$ is an arbitrary constant with the dimensions of angular momentum and it is introduced to keep the phase of Ψ_C dimensionless. In a classical theory $\hbar$ need not be identified with Planck's constant.

If the classical Hamiltonian takes the form

$$H=\frac{1}{2}\left(\frac{\partial S}{\partial q^i}-\frac{e_i}{C}A_i\right)\left(\frac{\partial S}{\partial q^k}-\frac{e_k}{C}A_k\right)g^{ik}+V,$$

then Ψ_C satisfies the Schrödinger-type equation

$$i\hbar\frac{\partial\Psi_C}{\partial t}=\frac{g^{-\frac{1}{2}}}{2}\left(i\hbar\frac{\partial}{\partial q^i}+\frac{e_i}{C}A_i\right)(g^{\frac{1}{2}}g^{ik})\left(i\hbar\frac{\partial}{\partial q^k}+\frac{e_k}{C}A_k\right)\Psi_C$$
$$+V\Psi_C+\frac{\hbar^2}{2}\frac{g^{-\frac{1}{2}}}{R}\frac{\partial}{\partial q^i}\left(g^{\frac{1}{2}}g^{ik}\frac{\partial R}{\partial q^k}\right)\Psi_C. \tag{7}$$

Equation (7) is a classical equation, a consequence of the Hamilton-Jacobi equation.[4] The constant $\hbar$ occurring in (7) does not appear in the Eqs. (1) and (3), so that it is not a dynamical element in the original classical theory.

In classical mechanics there are nonphysical solutions to the Hamilton-Jacobi equation and its modified form, Eq. (7). These solutions are defined in regions of the configuration space where the classical momentum becomes imaginary. Such solutions are to be ignored in classical dynamics, but they must be included in a wave theory where continuity requirements prevail.

[3] W. Pauli, *Feldquantisierung* (Akad. Buchgenossenschaft, Zurich, 1957), 2nd ed., p. 139.

[4] Since we are ultimately interested in quantizing Eq. (7), we shall characterize it as the "quasi-classical" equation, even when we deal with its classical properties. See reference 2.

III. CLASSICAL ENSEMBLES IN CONFIGURATION SPACE

A. Ensembles in the Hamilton-Jacobi Theory

The classical Hamilton-Jacobi equation describes ensembles of particles. A particular ensemble is constructed as follows: We assume that Hamilton's principal function S is a function of the N coordinates q^i and the N constants of the motion α^i. The constants α^i are determined by some experimental arrangement which fixes these constants and no others. The particles of the ensemble are then distributed uniformly over all possible values of the remaining N constants of the motion $\beta_i=\partial S/\partial\alpha^i$. The β_i are the variables conjugate to the α_i. The existence of the density D satisfying Eq. (3) reflects the conservation of particles in our ensemble.

We prove the above assertions as follows[5]: Assume that we have an arbitrary constant of the motion, f, which depends on the constants α^i and β_i. We now ask for the average value of f assuming that the constants β_i have uniform distribution. This average is

$$f=\int f(\alpha,\beta)d\beta_1 d\beta_2\cdots d\beta_N. \tag{8}$$

The constants β_i appearing in the integrand on the right in Eq. (8) may be written in terms of q^i, α^i, and t. If we make this replacement in Eq. (8), we find that $f(\alpha,\beta)$ becomes $F(\alpha,q,t)$ and

$$f=\int F(\alpha,q,t)\left\|\frac{\partial^2 S}{\partial\alpha\partial q}\right\|dq\,dq^2\cdots dq^N. \tag{9}$$

Since the average defined in Eq. (9) depends only on constants of the motion, its value should not change in the course of time. If we differentiate (9) with respect to time, and assume that surface integrals vanish, we immediately verify that the average value of f remains constant, provided the determinant $D\equiv\|\partial^2 S/\partial q\partial\alpha\|$ satisfies the equation of continuity

$$\frac{\partial D}{\partial t}+\frac{\partial}{\partial q^i}(Dv^i)=0. \tag{3}$$

B. Generalized Classical Ensembles

If we assume that our classical ensembles are to be described by the solutions of Eq. (7), without direct reference to the original solutions of the form $\Psi_C=R\exp(iS/\hbar)$, we can find more complex classical ensembles than the uniform distributions described by the Van Vleck determinant. If the classical action is real then Eq. (7) defines a conservation law:

$$\partial\rho/\partial t+\nabla\cdot\mathbf{j}=0, \tag{10}$$
$$\rho=\Psi^*\Psi,\quad \mathbf{j}=(\hbar/2i)(\Psi^*\nabla\Psi-\nabla\Psi^*\Psi)-(e/c)\mathbf{A}.$$

[5] We follow a proof due to Van Vleck, reference 1.

If $\Psi_C=R\exp(iS/\hbar)$, then Eq. (10) reduces to Eq. (3). It turns out, however, that there are solutions of Eq. (7) which are not in the original form $\Psi_C=R\exp(iS/\hbar)$.

One such solution arises in the classical one-dimensional problem of a single particle confined in a potential well. In this case the momentum assumes both positive and negative values at a given point in space. Since $p=\pm dW/dq$, where W is defined by $S=-Et\pm W(q)$, there are two classical actions which may be used to form independent solutions of Eq. (7). These solutions are easily seen to be

$$\Psi_C{}^+=R_+e^{(i/\hbar)(-Et+W_+)},\quad \Psi_C{}^-=R_-e^{(i/\hbar)(-Et+W_-)}, \tag{11}$$

where $R_+=iR_-$ and $W_+=-W_-$. The sum of these solutions is also a solution of (7),

$$\Psi_C=\tfrac{1}{2}(\Psi_C{}^+ +\Psi_C{}^-)=R_+e^{i\pi/4}\cos(W_+/\hbar-\pi/4). \tag{12}$$

Since solutions of (7) satisfy the law of continuity, (10), we find that the density of particles in our ensemble is

$$\Psi_C{}^*\Psi_C=D\cos^2(W_+/\hbar-\pi/4). \tag{13}$$

This is a curious classical ensemble since the density distribution arises from the superposition of classical amplitudes. In the WKB theory, the density in Eq. (13) is preferred to the classical density D, a preference which could never be justified from purely classical arguments.

Other interesting solutions to Eq. (7) have been studied by Dirac,[6] Feynman,[7] and Pauli[3] in their investigations of the so-called "sum over paths" formulation of the quantum theory. They have found solutions of the classical equation, (7), describing ensembles in which all of the particles are located at the point $q_0{}^i$ at the time t_0. These wave functions are constructed from the complete integrals of the Hamilton-Jacobi equation for which the constants α^i are the initial coordinates $q_0{}^i$. We call these special ensembles point source ensembles and specify them by means of the letter K, i.e., $\Psi_C(q,t;q_0,t_0)\equiv K$. The q^i and the $q_0{}^i$ are assumed to be Cartesian coordinates.

If one calculates K for infinitesimal time intervals, $t-t_0=\epsilon$, one finds, for a wide range of classical forces, that K is a solution of the Schrödinger equation, as the last term on the right of Eq. (7) vanishes.[3]

All solutions of the Schrödinger equation may now be generated by the transformation

$$\Psi(q,t_0+\epsilon)=\int K(q,t_0+\epsilon;q_0,t_0)\Psi_0(q_0,t_0)dq_0, \tag{14}$$

where $\Psi_0(q_0,t_0)$ is an arbitrary function of its arguments. Of course these solutions of the Schrödinger equation satisfy the equation of continuity Eq. (10), although

[6] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Oxford University Press, New York, 1958), 4th ed., Sec. 32.

[7] R. P. Feynman, Revs. Modern Phys. **20**, 367 (1948).

they rarely have the form $\Psi=R\exp(iS/h)$. An exception occurs when K is a solution of the Schrödinger equation for finite time intervals and the arbitrary function Ψ_0 in (14) is chosen as $K_0(q_0, t_0; q_0', t_0-\epsilon)$. In this case, (14) becomes

$$\bar{K}(q, t_0+\epsilon; q_0', t_0-\epsilon) = \int K(q, t_0+\epsilon; q_0, t_0)K(q_0, t_0; q_0', t_0-\epsilon)dq_0, \quad (14')$$

and $\bar{K}$ is again of the form $\bar{R}\exp(i\bar{S}/h)$. For ensembles of particles described by Eq. (14'), the probability of finding a system of particles at the point q^i and the time t, if it was known with certainty to be at the point $q_0{}^i$ at the time t_0, is the same in both classical and quantum mechanics.

We may interpret the integral equation, (14), as a sum over classical paths.[8] We first construct an $(n+1)$-dimensional configuration space with coordinates q^i and t. We assign amplitude values on a spatial hypersurface, Σ_0, at the time t_0, by prescribing the function $\Psi_0(q_0,t_0)$. From each point of our hypersurface we draw the classical paths for an ensemble of particles emanating from that point. The ensemble is constructed by assigning to the ensemble members all possible initial momentum values consistent with the classical integrals of the motion. Each trajectory leaving Σ_0 strikes a point on a neighboring spatial hypersurface, Σ, a time ϵ away. The classical action for each trajectory contributes to the integral in Eq. (14) and thus determines the state vector at the time $t_0+\epsilon$.

This procedure may be continued an arbitrary number of times until the time interval, $t-t_0$, becomes finite. There are many cases however where K is a solution of the Schrödinger equation for finite time intervals. The infinitesimal transformation law, (14), then may be replaced by a finite law of transformation with the classical action for finite paths appearing in the kernel K of (14).

Since the classical paths carry quantum states at the time t_0 into the same states at the time $t_0+\epsilon$, one wonders whether nonclassical trajectories might not perform the same function for the solutions of the quasi-classical equation, (7). This is indeed the case, as we shall now show.

The original Hamilton-Jacobi equation is

$$\partial S/\partial t+H=0, \quad (1)$$

and the solution, S, as a function of its arguments, is $S=S(q^i,\alpha^i,t)$. Given these solutions we can always construct the classical density, $D=\|\partial^2 S/\partial q\partial\alpha\|$.

We now seek a solution of the modified Hamilton-Jacobi equation,

$$\frac{\partial S'}{\partial t}+H\left(q^i,\frac{\partial S'}{\partial q^i},t\right)+\frac{\nabla^2\hbar^2}{2m}\frac{D^{\frac{1}{2}}}{D^{\frac{1}{2}}}=0, \quad (15)$$

where the final term acts as a quantum-mechanical potential energy. We are interested in point source solutions to Eq. (15), for infinitesimal time differences, $t-t_0$. For Hamiltonians quadratic in the momenta, these approximate solutions are

$$S'=\tfrac{1}{2}m\frac{(\mathbf{q}-\mathbf{q}_0)^2}{t-t_0}-V(q)-V_{\mathrm{QM}}(q) +\frac{1}{2}\frac{e}{c}[\mathbf{A}(q,t)+\mathbf{A}(q_0,t)]\cdot(\mathbf{q}-\mathbf{q}_0), \quad (16)$$

where $V_{\mathrm{QM}}=(\hbar^2/2m)(\nabla^2 D^{\frac{1}{2}}/D^{\frac{1}{2}})$. We construct the density $D'=\|\partial^2 S'/\partial q\partial q_0\|$ and form the kernel $K'(q, t_0+\epsilon; q_0, t_0)$. It is not difficult to show that Ψ_C, given by

$$\Psi_C(q, t_0+\epsilon)=\int K'(q, t_0+\epsilon; q_0, t_0)\Psi_{0C}(q_0,t_0)dq_0, \quad (17)$$

is a solution of the quasi-classical equation, (7),[9] $\Psi_{0C}(q_0,t_0)$ is an arbitrary function of its arguments.

In the classical "sum over paths" defined by Eq. (17), nonclassical trajectories carry a classical solution of (7) from one time t_0 to another time $t_0+\epsilon$.

How are we to interpret these ensemble aspects of the classical theory? In classical physics the appearance of ensembles is related to the mathematical properties of Hamiltonian systems. The existence of these families of solutions in no way restricts the classical measurement process, for we can always select from the ensemble a single trajectory, and thus determine a particular particle's simultaneous position and velocity. On the other hand, in a wave theory such as quantum mechanics, the signaling out of one trajectory from the ensemble of trajectories is strictly forbidden. The wave-like nature of matter rules out any complete analysis of the motion of an individual member of the ensemble as is permitted in the classical theory. A parallel situation exists in ray optics, where diffraction effects rule out complete knowledge of the ray trajectories. In wave-like phenomena the ensemble is irreducible.

IV. QUANTUM ASPECTS OF CLASSICAL THEORY

In this section we should like to outline some formal aspects of classical mechanics which closely parallel developments in quantum mechanics.

We shall show the existence of a classical operator formalism and develop a quasi-classical theory in

[8] We amplify the arguments of Dirac and Feynman in references 6 and 7.

[9] The proof follows the arguments of Feynman for the Schrödinger equation in reference 7.

momentum space. We give an example of a canonical transformation which transforms a quasi-classical equation into an exact equation of quantum mechanics, and at the same time find the classical analog of creation and destruction operators.

A. Classical Operator Formalism

It is clear from our earlier discussion in Sec. III B, that if energy is conserved, the following eigenvalue equation is always satisfied,

$$i\hbar\partial\Psi_C/\partial t=E\Psi_C=H_{\rm op}\Psi_C, \tag{18}$$

where $H_{\rm op}$ is given by the right-hand side of Eq. (7).

Similarly if we have radial forces derivable from a potential, the angular momentum in the z direction, α_ϕ, appears in the eigenvalue equation,

$$-i\hbar\partial\Psi_C/\partial\phi=\alpha_\phi\Psi_C. \tag{19}$$

The eigenvalue equation for the square of the total angular momentum can also be found. The calculation for the general case would take us too far afield so that we shall content ourselves with the operator equation when $\alpha_\phi=0$. We find that the classical operator equation for the square of the total angular momentum is

$$-\left[\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}-\frac{1}{4}\left(\frac{1}{\sin^2\theta}+1\right)\right]\Psi_C=\frac{\alpha_\theta^2}{\hbar^2}\Psi_C. \tag{20}$$

As one might expect, all the operators introduced commute with one another.

In the classical theory no deep significance should be attached to these operator equations since the operators are unrestricted, and the eigenvalues can assume arbitrary continuous values.

B. Quasi-Classical Theory in Momentum Space

The momentum space representation is important in quantum mechanics, and for this reason we should like to develop the corresponding representation in the quasi-classical theory.

In classical mechanics one can always perform a canonical transformation which interchanges the position coordinates and their canonically conjugate momenta. If q_i and p_i are the original phase space coordinates then the corresponding transformed coordinates are $-P_i$ and Q_i.

Under this transformation, and for a Hamiltonian quadratic in the momenta, the Hamilton-Jacobi equation is

$$\frac{\partial\bar{S}}{\partial t}+\sum_i\frac{1}{2\mu_i}\left[Q_i-\frac{e_i}{C}A_i\left(-\frac{\partial\bar{S}}{\partial Q}\right)\right]^2+V\left(-\frac{\partial\bar{S}}{\partial Q}\right)=0. \tag{21}$$

The Hamilton-Jacobi function $\bar{S}$ depends on the new coordinates Q_i (the old momenta p_i), the N constants α_i, and the time t. It is easy to show that (21) defines an equation of continuity in the new configuration space, which is in reality the old momentum space.

The equation of continuity for the determinant $\bar{D}=\|\partial^2\bar{S}/\partial Q_i\partial\alpha^k\|$ is

$$\frac{\partial\bar{D}}{\partial t}+\sum_i\frac{\partial}{\partial Q_i}\left\{\bar{D}\left[\frac{\partial V}{\partial(\partial\bar{S}/\partial Q_i)}-\sum_m\frac{\partial A_m}{\partial(\partial\bar{S}/\partial Q_i)}\left(Q_m-\frac{e_m}{C}A_m\right)\right]\right\}=0. \tag{22}$$

If we now reintroduce the original coordinates in (22), we find that $\bar{D}$ satisfies the law in momentum space

$$\frac{\partial\bar{D}}{\partial t}+\sum_i\frac{\partial}{\partial p_i}(\bar{D}\dot{p}_i)=0. \tag{23}$$

The quasi-classical equation which is equivalent to (21) and (22) is

$$i\hbar\frac{\partial\bar{\Psi}_C}{\partial t}=\sum_i\frac{1}{2\mu_i}\left(Q_i-\frac{e_i}{C}A_i\right)^2\bar{\Psi}_C+V\bar{\Psi}_C-\frac{i\hbar}{2\bar{R}^2}\left[\sum_i\frac{\partial}{\partial Q_i}\left\{\left[\frac{\partial V}{\partial(\partial\bar{S}/\partial Q_i)}-\sum_m\frac{e_m}{\mu_mC}\frac{\partial A_m}{\partial(\partial\bar{S}/\partial Q_i)}\times\left(Q_m-\frac{e_m}{C}A_m\right)\right]\bar{R}^2\right\}\right]\bar{\Psi}_C, \tag{24}$$

where $\bar{\Psi}_C=\bar{R}\exp(i\bar{S}/h)$ and $\bar{R}=\bar{D}^{\frac{1}{2}}$. The difference between the quasi-classical equation in momentum space and the Schrödinger equation in momentum space depends on the nature of the potential V and **A**, although the general form of the two equations is similar.

C. Classical Creation and Destruction Operators

We shall construct creation and destruction operators in the quasi-classical theory of the harmonic oscillator. We shall then rewrite the energy eigenvalue equation of the harmonic oscillator so that it is identical with the corresponding Schrödinger equation written in terms of the same variables. We conjecture that for an arbitrary problem it will always be possible to transform the quasi-classical equation so that it becomes identical with the corresponding Schrödinger equation, provided that the quasi-classical theory predicts the same eigenvalues as the quantum theory.

The Hamiltonian for the oscillator is

$$H=\tfrac{1}{2}(p^2+\omega^2q^2),$$

and if we transform to the new coordinates

$$Q=-i(p+i\omega q)/(2\omega)^{\frac{1}{2}},$$
$$P=(p-i\omega q)/(2\omega)^{\frac{1}{2}},$$

the transformed Hamiltonian becomes $K=iQP\omega$.

The Hamilton-Jacobi equation corresponding to this Hamiltonian is

$$\partial S/\partial t+i\omega Q\partial S/\partial Q=0,$$

and a solution is $S=-Et-i(E/\omega)\ln Q$. If we introduce the amplitude $R=(\partial^2 S/\partial E\partial Q)^{\frac{1}{2}}$ and construct the quasi-classical wave function, $\Psi_C=R\exp(iS/\hbar)$, we find with appropriate normalization that

$$\Psi_C(Z)=e^{-iEt/\hbar}Q^Z/[\Gamma(Z+1)]^{\frac{1}{2}},$$

where $Z=(E/\hbar\omega)-\frac{1}{2}$ and Γ is the gamma function.

It is readily seen that the following relations hold:

$$\frac{\partial}{\partial Q}\Psi_C(Z)=Z^{\frac{1}{2}}\Psi_C(Z-1),$$

$$Q\Psi_C(Z)=(Z+1)^{\frac{1}{2}}\Psi_C(Z+1), \tag{25}$$

and Ψ_C satisfies the transformed quasi-classical equation

$$(E-\tfrac{1}{2}\hbar\omega)\Psi_C=\hbar\omega Q\partial\Psi_C/\partial Q. \tag{26}$$

Equations (25) and (26) are identical with the corresponding equations in quantum mechanics except for the fact that in the classical theory Z is not necessarily an integer and Q and $\partial/\partial Q$ are special representations of the abstract creation and destruction operators η and $\bar{\eta}$.[10]

We must emphasize that the Eqs. (25) and (26) are classical equations since they in no way restrict the value of the energy. It is only when we insist that the operators introduced have properly defined boundary conditions that we find that $Z=n$, where n is a positive integer or zero, and the energy assumes the values $E_n=(n+\frac{1}{2})\hbar\omega$.

V. APPLICATIONS OF THE QUASI-CLASSICAL THEORY

In this section we shall show that the requirement of single-valuedness for the classical wave function yields the same energy eigenvalues for the nonrelativistic and the relativistic hydrogen atom as do the Schrödinger equation and Klein-Gordon equation, respectively.

The theory applied to Coulomb scattering proves that the quasi-classical wave functions and the solutions of Schrödinger's equation are identical at great distances from the scattering center.

A. Nonrelativistic Hydrogen Atom

The Hamilton-Jacobi equation for a particle in a spherically symmetrical potential is

$$\frac{\partial S}{\partial t}+\frac{1}{2\mu}\left[\left(\frac{\partial S}{\partial r}\right)^2+\frac{1}{r^2}\left(\frac{\partial S}{\partial\theta}\right)^2+\frac{1}{r^2\sin^2\theta}\left(\frac{\partial S}{\partial\phi}\right)^2\right]+V(r)=0. \tag{13}$$

[10] See reference 6, Sec. 34.

This equation may be reduced to quadratures by assuming a solution of the form $S=-Et+W_r(r)+W_\theta(\theta)+W_\phi(\phi)$. It is then easy to prove that

$$W_\phi=\alpha_\phi\phi,$$

$$W_\theta=\pm\int(\alpha_\theta^2-\alpha_\phi^2/\sin^2\theta)^{\frac{1}{2}}d\theta, \tag{27}$$

$$W_r=\pm\int[2\mu(E-V)-\alpha_\theta^2/r^2]^{\frac{1}{2}}dr.$$

The constants α_ϕ and α_θ are, respectively, the z component of the angular momentum and the total angular momentum of the moving charge.

The Van Vleck determinant is

$$D=\begin{Vmatrix} \frac{\partial^2 W_r}{\partial r\partial E} & \frac{\partial^2 W_r}{\partial r\partial\alpha_\theta} & \frac{\partial^2 W_r}{\partial r\partial\alpha_\phi} \\ \frac{\partial^2 W_\theta}{\partial\theta\partial E} & \frac{\partial^2 W_\theta}{\partial\theta\partial\alpha_\theta} & \frac{\partial^2 W_\theta}{\partial\theta\partial\alpha_\phi} \\ \frac{\partial^2 W_\phi}{\partial\phi\partial E} & \frac{\partial^2 W_\phi}{\partial\phi\partial\alpha_\theta} & \frac{\partial^2 W_\phi}{\partial\phi\partial\alpha_\phi} \end{Vmatrix},$$

and when evaluated has the absolute value

$$|D|=\mu\alpha_\theta/[2\mu(E-V)-\alpha_\theta^2/r^2]^{\frac{1}{2}}[\alpha_\theta^2-\alpha_\phi^2/\sin^2\theta]^{\frac{1}{2}}. \tag{28}$$

We shall now discuss quantization of the theory.

For the hydrogen atom the solution Ψ_C is separable, as (27) and (28) indicate. The radial and polar solutions are of the form $R_\pm\exp(iW_\pm/\hbar)$. These solutions have two signs associated with them because of the oscillatory character of the motion. The particle motion is bounded in the configuration space and in these two independent directions the momentum passes through zero and then changes sign on reversal of path.

In the WKB method,[11] quantization is achieved by joining the classical solutions to exponentially damped solutions in the nonclassical regions. Now the solutions of the form $R_\pm\exp(iW_\pm/\hbar)$ cannot be joined to an exponentially damped solution, but since the equations are linear we can always take some linear combination of $\pm$ solutions and this new solution can be joined to the wave functions in the nonclassical regions. Eigenvalues arise when one requires that the different classical wave functions defined for the different classical turning points be continuous in the classical regions.

However, in place of this quantization technique due to Kramers, we shall instead adopt an equivalent procedure due to Keller,[12] who showed that the same

[11] H. A. Kramers, Z. Physik **39**, 828 (1926), and L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), 2nd ed., Sec. 28.

[12] J. B. Keller, Ann. Phys. **4**, 180 (1958).

results could be obtained by simply requiring that the quasi-classical wave function be single-valued when one traverses an appropriate closed particle path in the classical part of the configuration space.

For example, in our present example we may keep r and θ fixed and let ϕ go through the angle 2π. The single-valuedness requirement on Ψ_C leads to the quantum condition $\alpha_\phi = mh$, where m is a positive or negative integer, or zero.

One may similarly evaluate the change in Ψ_C, $\Delta\Psi_C$, in a complete cycle when we keep r and ϕ fixed. The change in Ψ_C then reduces to calculating the change ΔW_θ and the change in phase of the amplitude of Ψ_C. In order to evaluate ΔW_θ it is simpler to introduce a new angle γ which measures the angular change in the actual plane of motion of the particle. The invariant $\sum_i p_i dq_i$ becomes $p_r\dot{r}+p_\theta\dot{\theta}+p_\phi\dot{\phi}=p_r\dot{r}+p_\gamma\dot{\gamma}$. From its definition, p_γ is the total angular momentum α_θ.

We find that

$$\Delta W_\theta = \oint p_\theta d\theta = \oint p_\gamma d\gamma - \oint p_\phi d\phi,$$

and since p_γ and p_ϕ are constants of the motion,

$$\Delta W_\theta = 2\pi(\alpha_\theta - \alpha_\phi).$$

We note in addition that W_θ changes sign when we traverse half the particle orbit. This reversal of sign introduces a phase change of $-\pi$ in the amplitude during the cycle,[12] so that the total change in phase of the wave function, $\Delta\sigma_\theta$, is

$$\Delta\sigma_\theta = 2\pi(\alpha_\theta - \alpha_\phi)/\hbar - \pi.$$

For the wave function to remain single-valued we must choose $\Delta\sigma_\theta = 2\pi l'$, where l' is an integer. We introduce a new integer $l = l'+m$, note that $\alpha_\phi = mh$, and derive the value of the total angular momentum

$$\alpha_\theta = \hbar(m+l'+\tfrac{1}{2}) = \hbar(l+\tfrac{1}{2}).$$

This is the value of the angular momentum assumed by Sommerfeld to fit experiment, and derived in the WKB limit of the usual quantum mechanics.[13]

The energy levels may be calculated by considering a path integral along any radius with constant angles θ and ϕ. We have to evaluate the change ΔW_r in the cycle, for the attractive Coulomb potential $V = -e^2/r$. The change is

$$\Delta W_r = -2\pi\alpha_\theta + \pi e^2(-2\mu/E)^{\frac{1}{2}}.$$

Again, there is a change in sign in W_r as we pass along the path, and this induces an additional change in phase of $-\pi$. The total change in phase $\Delta\sigma_r$ must equal $2\pi n'$, so that we find

$$\Delta\sigma_r = -2\pi\alpha_\theta/\hbar + \pi\mu e^2(-2\mu/E\hbar^2)^{\frac{1}{2}} - \pi = 2\pi n'.$$

[13] R. E. Langer, Phys. Rev. **51**, 669 (1937).

If we define $n = n'+l+1$, and substitute $\alpha_\theta = (l+\frac{1}{2})\hbar$, we secure the correct energy eigenvalues of the non-relativistic hydrogen atom,

$$E = -\mu e^4/2\hbar^2 n^2.$$

B. Rutherford Scattering

Next we shall derive the Rutherford scattering formula from our quasi-classical theory as an example of a system that is not bound.[14] We shall model our work after the usual quantum theory calculation in a parabolic coordinate system.

We introduce the following coordinates:

$$x = (\xi\eta)^{\frac{1}{2}}\cos\phi, \quad y = (\xi\eta)^{\frac{1}{2}}\sin\phi, \quad z = \tfrac{1}{2}(\xi-\eta), \quad r = \tfrac{1}{2}(\xi+\eta),$$

and the inverse relations

$$\eta = r - z, \quad \xi = r + z, \quad \phi = \tan^{-1}y/x.$$

In these coordinates the time-independent Hamilton-Jacobi equation is

$$E = \frac{1}{2\mu}\left[\frac{4\xi}{\xi+\eta}\left(\frac{\partial W}{\partial\xi}\right)^2 + \frac{4\eta}{\xi+\eta}\left(\frac{\partial W}{\partial\eta}\right)^2 + \frac{1}{\xi\eta}\left(\frac{\partial W}{\partial\phi}\right)^2\right] + \frac{2ZZ'e^2}{\xi+\eta}, \quad (29)$$

where we have assumed the repulsive potential energy $ZZ'e^2/r$.

We seek a solution of the form

$$W = W_\xi(\xi) + W_\eta(\eta) + W_\phi(\phi)$$

and immediately find $W_\phi = \alpha_\phi\phi$, where the constant α_ϕ is the component of the angular momentum in the z direction. Continued separation yields the equations

$$\begin{aligned} \xi\left(\frac{dW_\xi}{d\xi}\right)^2 + \frac{1}{4\xi}\alpha_\phi^2 - \tfrac{1}{2}\mu E\xi + \tfrac{1}{2}ZZ'e^2\mu &= -\tfrac{1}{2}\beta, \\ \eta\left(\frac{dW_\eta}{d\eta}\right)^2 + \frac{1}{4\eta}\alpha_\phi^2 - \tfrac{1}{2}\mu E\eta + \tfrac{1}{2}ZZ'e^2\mu &= \tfrac{1}{2}\beta, \end{aligned} \quad (30)$$

where $\frac{1}{2}\beta$ is a separation constant.

We now construct the classical amplitude $R = (Dg^{-\frac{1}{2}})^{\frac{1}{2}}$. The Van Vleck determinant is

$$D = \frac{\partial^2 W_\xi}{\partial\xi\partial E}\frac{\partial^2 W_\eta}{\partial\eta\partial\beta} - \frac{\partial^2 W_\eta}{\partial\eta\partial E}\frac{\partial^2 W_\xi}{\partial\xi\partial\beta},$$

and

$$g = \|g_{ik}\| = [(\xi+\eta)/4]^2.$$

In this problem we are interested only in the asymp-

[14] The Rutherford scattering cross section may be calculated in many ways. The sole virtue that we claim for the present derivation is that it exclusively uses the solutions of the classical Hamilton-Jacobi theory in constructing the quasi-classical wave function, and the derivation of the scattering law is analogous to the usual derivation in quantum mechanics.

totic solutions of the classical wave equation. As r approaches infinity and θ approaches π we have the asymptotic solution for the incoming particle, and as r approaches infinity and θ approaches the scattering angle Θ we have the asymptotic solution for the outgoing particle. In these limits both ξ and η become infinite and the amplitude reduces to

$$R=(\xi\eta)^{-\frac{1}{2}}(2\mu E)^{-\frac{1}{2}}. \tag{31}$$

For the solution of our problem we need the asymptotic form of the phase. We shall look for a characteristic function W of the form

$$W=-(\mu E/2)^{\frac{1}{2}}(\xi+\eta)+F(\xi)+G(\eta), \tag{32}$$

and assume that the component of the angular momentum in the z-direction vanishes. When (32) is substituted in Eqs. (30), we find

$$\begin{aligned}&\left(\frac{dF}{d\xi}\right)^2-(2\mu E)^{\frac{1}{2}}\frac{dF}{d\xi}+\frac{ZZ'e^2\mu}{2\xi}+\frac{\beta}{2\xi}=0,\\&\left(\frac{dG}{d\eta}\right)^2-(2\mu E)^{\frac{1}{2}}\frac{dG}{d\eta}+\frac{ZZ'e^2\mu}{2\eta}-\frac{\beta}{2\eta}=0.\end{aligned} \tag{33}$$

These quadratic equations, (33), are easily solved and integrated in the asymptotic limit as ξ and η become large. The final results are:

$$\begin{aligned}F_+&=(2\mu E)^{\frac{1}{2}}\xi-\tfrac{1}{2}(ZZ'e^2\mu+\beta)(2\mu E)^{\frac{1}{2}}\ln\xi,\\F_-&=\tfrac{1}{2}(ZZ'e^2\mu+\beta)(2\mu E)^{\frac{1}{2}}\ln\xi,\\G_+&=(2\mu E)^{\frac{1}{2}}\eta-\tfrac{1}{2}(ZZ'e^2\mu-\beta)(2\mu E)^{\frac{1}{2}}\ln\eta,\\G_-&=\tfrac{1}{2}(ZZ'e^2\mu-\beta)(2\mu E)^{\frac{1}{2}}\ln\eta.\end{aligned} \tag{34}$$

We are interested in only certain combinations of the above solutions; those for which the incoming wave is of the form e^{ikz} and the outgoing wave is of the form e^{ikr}. It is clear from our choice of W in Eq. (32), that we must choose the solutions F_++G_- for the incoming wave and the solution F_++G_+ for the outgoing wave.

The solution for the incoming wave is then of the form

$$\Psi_{\text{in}}=\left\{\exp\frac{i}{\hbar}\left[(2\mu E)^{\frac{1}{2}}z-\frac{(ZZ'e^2\mu+\beta)\ln\xi}{(8\mu E)^{\frac{1}{2}}}+\frac{(ZZ'e^2\mu-\beta)\ln\eta}{(8\mu E)^{\frac{1}{2}}}\right]\right\}\frac{1}{(2\mu E\xi\eta)^{\frac{1}{4}}}. \tag{35}$$

This solution is not yet in the proper form since it does not represent a plane wave nor is it normalized properly. The separation constant β, which has remained unspecified in our calculations, must be chosen so that the coefficient $(\xi\eta)^{-\frac{1}{4}}$ in the amplitude is cancelled. This will occur if $ZZ'e^2+\beta=i\hbar(2\mu E)^{\frac{1}{2}}$. In addition, the incoming wave may be normalized so that $(2E/\mu)^{\frac{1}{2}}=v$ particles are fired each second through a unit area. We accomplish this normalization by adding constants to the solutions F and G.

With these changes the wave function (35) becomes

$$\Psi_{\text{in}}=\exp\{i[kz-n\ln(k\eta)]\}, \tag{36}$$

with $k=(2\mu E)^{\frac{1}{2}}/\hbar$ and $n=ZZ'e^2\mu/\hbar(2\mu E)^{\frac{1}{2}}$. If we normalize the outgoing wave function so that the total number of outgoing particles is equal to the total number of incoming particles, the outgoing wave function becomes

$$\Psi_{\text{out}}=(n/i\eta k)\exp\{i[kr+n\ln(k\eta)]\}. \tag{37}$$

The asymptotic solutions, Eqs. (36) and (37), are identical, modulo phase factors, with the asymptotic solutions of the Schrödinger equation.

The scattering cross-section is defined as

$$\sigma_C(\Theta)=\Psi_{\text{out}}{}^*\Psi_{\text{out}}r^2=\left(\frac{n}{2k\sin^2(\frac{1}{2}\Theta)}\right)^2=\frac{1}{4}\left(\frac{ZZ'e^2}{2E}\right)^2\csc^4(\Theta/2). \tag{38}$$

This is the usual Rutherford scattering formula.

C. Relativistic Hydrogen Atom

The relativistic theory of the hydrogen atom is carried through in exactly the same manner as the nonrelativistic theory. Our first task is to find the relativistic quasi-classical equation.

For a charged particle is a given electromagnetic field the relativistic Hamilton-Jacobi equation is

$$\left(\frac{\partial S}{\partial t}+V\right)^2-\mu^2c^4+c^2\sum_{i,k}g^{ik}\left(\frac{\partial S}{\partial q_i}-\frac{e}{c}A_i\right)\times\left(\frac{\partial S}{\partial q^k}-\frac{e}{c}A_k\right)=0. \tag{39}$$

As in the nonrelativistic theory, this equation defines a quantity that is conserved in configuration space. If we proceed exactly as in Sec. II we find that the determinant,

$$\bar{D}=\left\|\frac{\partial^2 S}{\partial q^i\partial\alpha^k}\right\|, \tag{40}$$

satisfies the conservation law

$$\frac{\partial\bar{D}}{\partial t}+\sum_{i,k}\frac{1}{\mu}\frac{\partial}{\partial q^i}\left[g^{ik}\bar{D}\left(\frac{\partial S}{\partial q^k}-\frac{e}{c}A_k\right)\right]=0. \tag{41}$$

However $\bar{D}$ does not satisfy our requirements of Lorentz invariance. It must be replaced by the quantity,

$$D=\bar{D}\Big/\left[1+\frac{1}{\mu^2c^2}\sum_{i,k}g^{ik}\left(\frac{\partial S}{\partial q_i}-\frac{e}{c}A_i\right)\left(\frac{\partial S}{\partial q^k}-\frac{e}{c}A_k\right)\right]^{\frac{1}{2}}, \tag{42}$$

which is simply

$$D=\bar{D}\left(1-\sum_{i,k} g^{ik}\frac{v_i v_k}{c^2}\right)^{\frac{1}{2}}.$$

We now introduce the quasi-classical wave function

$$\Psi_C=Re^{iS/\hbar}, \tag{43}$$

where $R=(Dg^{-\frac{1}{2}})^{\frac{1}{2}}$.

The wave function Ψ_C satisfies the classical relativistic wave equation,

$$\frac{1}{c^2}\left(i\hbar\frac{\partial}{\partial t}-V\right)^2\Psi_C+\frac{1}{g^{\frac{1}{2}}}\left(i\hbar\frac{\partial}{\partial q^i}+\frac{e}{c}A_i\right)g^{\frac{1}{2}}g^{il}\left(i\hbar\frac{\partial}{\partial q^l}+\frac{e}{c}A_l\right)\Psi_C$$

$$-\mu^2c^2\Psi_C=-\frac{\hbar^2}{2\mu}\left[\frac{1}{Rg^{\frac{1}{2}}}\frac{\partial}{\partial q^i}\left(g^{\frac{1}{2}}g^{il}\frac{\partial R}{\partial q^l}\right)-\frac{1}{c^2R}\frac{\partial^2 R}{\partial t^2}\right]\Psi_C. \tag{44}$$

Equation (44) is just the Klein-Gordon equation in curvilinear coordinates with additional terms on the right hand side.

We are now in a position to calculate the energy levels of the relativistic hydrogen atom. The relativistic Hamilton-Jacobi equation is

$$\frac{1}{c^2}\left(\frac{\partial S}{\partial t}-\frac{e^2}{r}\right)^2-\mu^2c^2-\left(\frac{\partial S}{\partial r}\right)^2$$

$$-\frac{1}{r^2}\left[\left(\frac{\partial S}{\partial\theta}\right)^2+\frac{1}{\sin^2\theta}\left(\frac{\partial S}{\partial\phi}\right)^2\right]=0. \tag{45}$$

We reduce to quadratures by considering a solution of the form $S=-Et+W_r(r)+W_\theta(\theta)+W_\phi(\phi)$. Once again, as in the nonrelativistic theory, we find that

$$W_\phi=\alpha_\phi\phi,$$

$$W_\theta=\pm\int(\alpha_\theta^2-\alpha_\phi^2/\sin^2\theta)^{\frac{1}{2}}d\theta, \tag{46}$$

$$W_r=\pm\int\left[\frac{1}{c^2}(E+e^2/r)^2-\mu^2c^2-\alpha_\theta^2/r^2\right]^{\frac{1}{2}}dr.$$

Quantization of angular momentum and energy arise through the requirement of single-valuedness for the quasi-classical wave function. The calculation parallels that for the nonrelativistic theory so that we need only quote the results: (a) The total angular momentum, α_θ, has the values $\alpha_\theta=(l+\frac{1}{2})$. (b) The z component of the angular momentum, α_ϕ, has the values $\alpha_\phi=m\phi$. (c) The total energy, E, has the values

$$E=\mu c^2(1+\gamma^2/\lambda^2)^{-\frac{1}{2}}, \tag{47}$$

where $\gamma=e^2/\hbar c$ and $\lambda=n+\frac{1}{2}+[(l+\frac{1}{2})^2-\gamma^2]^{\frac{1}{2}}$.

These are precisely the energy levels given by the Klein-Gordon equation.

The correct Dirac energy levels were predicted by Sommerfeld because he neglected the changes in phase arising from the requirements of continuity for the quasi-classical wave function at the boundaries of the classical motion. It is hoped that the incorrect half-integral quantum numbers appearing in Eq. (47) will become the correct integral quantum numbers when we include spin in our quasi-classical theory.

V. CONCLUSION

In this paper we have attempted to show the richness of classical mechanics in precisely those aspects which have proved important in quantum mechanics.

In a future paper we shall apply the techniques outlined here to boson fields. At the present time it appears that one can similarly reconstruct classical field theory so that it differs only slightly from quantum field theory.

A more difficult problem is that of fermion fields, and specifically the field of the spinning electron. In a paper which follows the present one, the author has taken his first step in this direction.

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