Quasi-Classical Transformation Theory*

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The quasi-classical theory is the theory of the WKB approximation as defined by Van Vleck. This approximate wave theory is invariant under canonical transformations. We derive the transformation laws for wave functions and operators in this theory. The connection problem of the ordinary configuration space is discussed from the point of view of Van Vleck. The usual method of WKB quantization is then contrasted with another method of quantization in a classical configuration space of creation and destruction operators. In this new configuration space we find that, for some problems, the quasi-classical solutions are exact solutions of the Schrödinger equation. Finally, we show that the canonical transformations of the quasi-classical theory may be put into one-to-one correspondence with a group of approximate unitary transformations.

I. INTRODUCTION

In the preceding article in this journal,[1] the author has shown how purely classical methods, devised originally by Van Vleck,[2] could be used to simulate many of the formal aspects of the quantum theory.

At the same time these methods could be used to construct WKB solutions to the Schrödinger equation.[3] It is known that these are asymptotic solutions of the wave equation, and are valid approximations to the true solutions in regions of space some distance from the classical turning points.

In the WKB approximation method, as applied to the Schrödinger equation, the assumption is made that the wave function may be written as a power series in $\hbar$,

$$\Psi=\exp[i(S-i\hbar S'+\cdots)/\hbar].$$

As is well known, the first term in the expansion, S, is a solution of the classical Hamilton-Jacobi equation,

$$\partial S/\partial t+H=0, \tag{1}$$

with H the classical Hamiltonian as a function of arbitrary canonical variables. Already in this first approximation the solutions of the wave theory are linked to the classical motion of particles. Van Vleck[2] showed that the second term in the expansion could also be given a classical meaning. If one writes $\exp S'=D^{\frac{1}{2}}$, one can show[1,2] that D satisfies an equation of continuity in the classical configuration space,

$$\frac{\partial D}{\partial t}+\sum_k \frac{\partial}{\partial q_k}\left(D\frac{\partial H}{\partial(\partial S/\partial q_k)}\right)=0. \tag{2}$$

A D which always satisfies (2) is the Van Vleck determinant,

$$D=c\left|\left|\frac{\partial^2 S}{\partial q_i \partial \alpha_k}\right|\right|, \tag{3}$$

where the q_i are the particle coordinates, and the α_k the classical constants of the motion appearing in the solution S. c is an arbitrary normalization constant. The quantity D exists if S is a solution of Eq. (1). It is assumed that the q's and α's span the entire phase space available to the classical system so that D nowhere vanishes.

Thus, according to Van Vleck, an approximate solution of the Schrödinger equation, valid through the first power in $\hbar$, may always be written as

$$\psi=D^{\frac{1}{2}}e^{iS/\hbar}\equiv Re^{iS/\hbar}. \tag{4}$$

It is significant that Van Vleck's formulation of the WKB approximation holds for arbitrary canonical systems and is not restricted to its usual representation in space-time.[4] This general theory of the WKB approximation we call the quasi-classical theory, for although the methods used in the construction of the asymptotic solutions are exclusively classical, we are in main motivated by the desire to use these solutions within the framework of the wave theory.

In this note we shall discuss the transformation theory of the quasi-classical wave functions, (4), and of the operators which act on them. The transformation theory is of some interest because it permits us to find novel classical quantities which are in close analogy with similar ones in the quantum theory. In particular, we shall show that within the framework of the classical theory it is possible to introduce creation and destruction operators without in any way implying quantization of the theory. The configuration space in which these creation and destruction operators are defined is very different from the configuration space of the usual WKB theory, where the wave functions cannot be written as single continuous functions over the entire space.[5] In this new space of the creation operators the wave functions are continuous. As a consequence new boundary conditions must be imposed on the quasi-classical wave functions in order to quantize the

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[1] R. Schiller, preceding paper [Phys. Rev. 125, 1100 (1962)], hereafter referred to as I.

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

[3] See reference 1.

[4] See, for example, L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, New York, 1955), 2nd ed., Sec. 28, for the usual theory.

[5] See reference 4, Sec. 28.

classical constants of the motion, for the quantization of the old WKB theory rests squarely on the existence of different solutions in different regions of the configuration space. These new boundary conditions turn out to be identical with the boundary conditions imposed in the creation and destruction operator representation of the quantum theory. In fact, for a set of dynamical problems, the quasi-classical theory becomes identical with the quantum theory, and classical techniques may be used to find exact solutions of the Schrödinger equation.

II. CANONICAL TRANSFORMATION THEORY

It is of interest to discover how the quasi-classical wave functions of Eq. (4), and the operators associated with these solutions, transform under the group of canonical transformations.

The canonical transformations are defined by the generating function $F(q_i,Q_k)$, where the q_i are the original coordinates and the Q_k the transformed coordinates. The Hamilton-Jacobi function transforms as

$$\bar{S}(Q_i,\alpha_k)=S(q_i,\alpha_k)-F(q_i,Q_k). \tag{5}$$

The original and transformed actions, S and $\bar{S}$, are functions of the same constants of the motion, so that the transformation simply provides a new description of the identical experimental situation.

We know from the theory of canonical transformations and the Hamilton-Jacobi theory that the following relations are valid:

$$\begin{aligned} p_i&=\partial S/\partial q_i=\partial F/\partial q_i,\\ P_i&=\partial\bar{S}/\partial Q_i=-\partial F/\partial Q_i. \end{aligned} \tag{6}$$

The p_i are the old momenta and the P_i the corresponding new momenta. Equations (6) imply the following relations among determinants:

$$\begin{aligned} \left|\left|\frac{\partial^2 S}{\partial q_i\partial\alpha_k}\right|\right|&=\left|\left|\frac{\partial^2 F}{\partial q_i\partial Q_l}\right|\right|\times\left|\left|\frac{\partial Q_l}{\partial\alpha_k}\right|\right|,\\ \left|\left|\frac{\partial^2 \bar{S}}{\partial Q_i\partial\alpha_k}\right|\right|&=-\left|\left|\frac{\partial^2 F}{\partial q_l\partial Q_i}\right|\right|\times\left|\left|\frac{\partial q_l}{\partial\alpha_k}\right|\right|. \end{aligned} \tag{7}$$

In two different representations the wave functions are $\psi=R\exp(iS/h)$ and $\bar{\psi}=\bar{R}\exp(i\bar{S}/h)$, with $R=\|\partial^2S/\partial q_i\partial\alpha_k\|^{\frac{1}{2}}$ and $\bar{R}=\|\partial^2\bar{S}/\partial Q_i\partial\alpha_k\|^{\frac{1}{2}}$. Equations (5) and (7) then give us the transformation law for the wave functions,

$$\bar{\psi}=U\psi,\quad U=i\left|\left|\frac{\partial q_i}{\partial\alpha_m}\right|\right|^{\frac{1}{2}}\times\left|\left|\frac{\partial Q_k}{\partial\alpha_n}\right|\right|^{-\frac{1}{2}}e^{-iF/\hbar}. \tag{8}$$

U is a function and not an operator, since the q_i and the Q_k are classical variables. This transformation law for the wave functions is not only valid for changes in the description of the same physical situation, but holds equally well for new experimental arrangements. For if we reverse the roles of coordinates and constants in the classical action S, the canonical transformation is contained in the relations

$$\begin{aligned} \bar{S}(\beta_i,q_k)&=S(\alpha_i,q_k)-F(\alpha_i,\beta_k),\\ \partial S/\partial\alpha_i&=\partial F/\partial\alpha_i,\\ \partial\bar{S}/\partial\beta_i&=-\partial F/\partial\beta_i. \end{aligned} \tag{9}$$

The constants α_i describe the initial experimental arrangement and the constants β_i the new one. The transformation function U which generates the change in the experimental situation is

$$U=i\left|\left|\frac{\partial\alpha_i}{\partial q_m}\right|\right|^{\frac{1}{2}}\times\left|\left|\frac{\partial\beta_k}{\partial q_n}\right|\right|^{-\frac{1}{2}}e^{-iF/\hbar}. \tag{10}$$

An interesting example of a canonical transformation is provided by that change which carries the canonical variables at time t_0 into those at time t. In terms of the configuration space coordinates q and their values q_0 at the initial instant t_0, the transformation is generated by the generating function F, where

$$\bar{S}(q_i,t,\alpha_i)=S(q_{0i},t_0,\alpha_i)-F(q_i,t;q_{0i},t_0). \tag{11}$$

Since F satisfies the relations

$$\begin{aligned} p_i&=-\partial F/\partial q_i,\\ p_{0i}&=\partial F/\partial q_{0i}, \end{aligned} \tag{12}$$

F must be the negative of the classical action,

$$S(q_i,t;q_{0i},t_0)=\int_{t_0}^{t}Ldt.$$

The transformation law, (8), with $F=-\int_{t_0}{}^{t}Ldt$, is thus the canonical analog of the unitary transformation law of the quantum theory,

$$\Psi(q_i,t)=\int_{V_0}K(q_i,t;q_{0i},t_0)\Psi(q_{0i},t_0)dV_0, \tag{13}$$

where the kernel, or transformation matrix, is[6]

$$K=C(t-t_0)^{-\frac{3}{2}}\exp\left(i/\hbar\int_{t_0}^{t}Ldt\right).$$

To complete the quasi-classical transformation theory we need the transformation law of operators. Before we can find this law we must first ascertain how quantum operators behave when the wave solutions go

[6] The kernel K forms the basis of an integral equation representation of the quantum theory due to R. P. Feynman, Revs. Modern Phys. **20**, 267 (1948).

over to their asymptotic form, $\psi=R\exp(iS/\hbar)$. If we retain terms that go as the first power in $\hbar$, we find that the quantum operator acting on a true wave solution, $G_{\rm op}{}^Q(q_i,-i\hbar\partial/\partial q_i)\Psi$, becomes $G_{\rm op}R\exp(iS/\hbar)$, where $G_{\rm op}$ is

$$G_{\rm op}=G\left(q_i,\frac{\partial S}{\partial q_k}\right)-\frac{i\hbar}{R}\frac{\partial R}{\partial q_i}\frac{\partial G}{\partial(\partial S/\partial q_i)}-\frac{i\hbar}{2}\frac{\partial^2 G}{\partial q_i\partial(\partial S/\partial q_i)}. \quad (14)$$

The G appearing on the right of Eq. (14) is a classical function of the canonical coordinates. The terms on the right are to be understood as follows: The first term arises whenever the operator $-i\hbar\partial/\partial q_i$ acts on the phase of the wave function, and the second term when this operator acts on the amplitude. The final term is due to the ordering of factors in $G_{\rm op}{}^Q$. The coefficient $\frac{1}{2}$ appears in this term because we deal with quantum operators which have completely symmetrized factor sequences. In fact, for these asymptotic operators, the associative law, $H_{\rm op}G_{\rm op}=(HG)_{\rm op}$, will fail for products of operators, $H_{\rm op}G_{\rm op}$, unless these products are symmetrized to $\frac{1}{2}(HG+GH)$.[7]

The asymptotic form for the symmetrized quantum operators which act on the wave functions $\psi=R\exp(iS/h)$ is thus given by Eq. (14). The transformation theory of these operators is very simple, because under the quasi-classical transformation the wave functions always retain their form. To find the transformed quasi-classical operator, $\bar{G}_{\rm op}\bar{R}\exp(i\bar{S}/h)$, we note that the new operator, in terms of the new variables Q_i, must be of the form,

$$\bar{G}_{\rm op}=\bar{G}\left(Q_i,\frac{\partial\bar{S}}{\partial Q_i}\right)-\frac{i\hbar}{\bar{R}}\frac{\partial\bar{R}}{\partial Q_i}\frac{\partial\bar{G}}{\partial(\partial\bar{S}/\partial Q_i)}-\frac{i\hbar}{2}\frac{\partial^2\bar{G}}{\partial Q_i\partial(\partial\bar{S}/\partial Q_i)}. \quad (15)$$

From Eq. (15) we see that the law of transformation for quasi-classical operators depends on the transformation properties of the classical function, G, and the classical action, S.

III. WKB WAVE FUNCTIONS AND OPERATORS IN ORDINARY CONFIGURATION SPACE

We are interested in the precise definition of WKB wave functions over the entire configuration space, since this knowledge is critical if we are to derive quantized values for the classical constants of the motion. In this section we retrace the well-trod ground of the usual WKB theory, but by techniques which conform more to the spirit of our Sec. II. These techniques permit us to emphasize the important role of the classical boundaries in the WKB quantization procedure. At the same time our methods provide contrast with those of the following section where we discuss "WKB" quantization in the configuration space of classical creation operators.

We now examine the quasi-classical Schrödinger equation in ordinary configuration space. It is not difficult to show by use of Eq. (14), that the quasi-classical Hamiltonian operator for a particle in an electromagnetic field is

$$H_{\rm op}=\frac{1}{2m}(-i\hbar\nabla-e\mathbf{A})^2+e\phi+\frac{\hbar^2}{2m}\frac{\nabla^2 R}{R}. \quad (16)$$

The approximate Schrödinger equation is then

$$i\hbar\partial\psi/\partial t=H_{\rm op}\psi. \quad (17)$$

The quasi-classical solutions are in the form $\psi=R\exp(iS/h)$, where R is the square root of the Van Vleck determinant and S is a solution of the classical Hamilton-Jacobi equation.

We are particularly interested in bound-state operators and wave functions. For bound-state problems the Hamiltonian operator, Eq. (16), and the quasi-classical wave functions are singular at the classical turning points, since R is infinite there. These singularities in R are well known in classical theory and they appear at points in configuration space where the classical momentum vanishes. In the classical theory these singularities are of no import, but in a wave theory, where the wave functions must be bounded and continuous, these singularities are inadmissible. And since it is the wave theory that really interests us, we must define bounded WKB functions at these points. In addition we must choose the solutions of Eq. (17) in the classical and nonclassical regions of space so that they will join continuously to the solutions chosen at the classical turning points.

The research experience of the last 35 years in the analysis of WKB solutions provides us with a prescription for defining and joining the WKB functions in the various parts of the configuration space.[8] We assume that the classical problem has been reduced to quadratures by separation of variables. This means that we can write the canonical momentum as $p_\pm=\pm p(q,\alpha)$, where α is a classical constant of motion. The ambiguity in sign arises because of the two different directions the momentum can assume. In the Hamilton-Jacobi theory $p_\pm=\partial S_\pm/\partial q$, and so the two actions, $S_\pm$, can both be used in forming independent solutions of Eq. (17). These two solutions can then be added to secure another solution. The two independent solutions are

$$\psi_+=R_+e^{iS_+/\hbar},\quad \psi_-=R_-e^{iS_-/\hbar}. \quad (18)$$

[7] See reference 2, pp. 182–183.

[8] We follow the careful arguments of L. I. Schiff, reference 4, and the authors quoted there.

If we substitute for R and S we find

$$\psi_+=c\left(\frac{\partial p_+}{\partial\alpha}\right)^{\frac{1}{2}}\exp\left(i\int_{a_1}^{q}k_+dq\right), \tag{19}$$

and

$$\psi_-=ic\left(\frac{\partial p_+}{\partial\alpha}\right)^{\frac{1}{2}}\exp\left(-i\int_{a_1}^{q}k_+dq\right), \tag{20}$$

where $k_+=p_+/\hbar$ and c is a normalization constant. We have written the phase of the wave function as a definite integral. The lower limit of integration, a_1, is chosen as the classical turning point which is farthest to the left. The classical region is to the right of this point and the convention is to choose the limits of integration so that the action is always increasing as q increases. In the neighborhood of the point a_1, and in the classical region, we choose as our WKB solution $\psi_{a_{1+}}=\frac{1}{2}(\psi_++\psi_-)$. If we put in the values for ψ_+ and ψ_- we find

$$\psi_{a_{1+}}=c\left(\frac{\partial p_+}{\partial\alpha}\right)^{\frac{1}{2}}e^{i\pi/4}\cos\left[\int_{a}^{q}k_+dq-\frac{\pi}{4}\right]. \tag{21}$$

A similar argument gives us the form of the wave function in the neighborhood of the other classical turning point, a_2, to the right of a_1. If we adhere to our convention for increasing phase, we find in the classical region near the point a_2,

$$\psi_{a_{2-}}=c\left(\frac{\partial p_+}{\partial\alpha}\right)^{\frac{1}{2}}e^{i\pi/4}\cos\left[\int_{q}^{a_2}k_+dq-\frac{\pi}{4}\right]. \tag{22}$$

In the nonclassical region to the right of a_1 we find that the momentum becomes imaginary, and in this region we choose the solution that is exponentially damped,

$$\psi_{a_{2+}}=c''\left(\frac{\partial p_+}{\partial\alpha}\right)^{\frac{1}{2}}\exp\left(-\int_{a_2}^{q}\kappa_+dq\right), \tag{23}$$

where $\kappa=-ik$.

Similarly to the left of the turning point a_1, the WKB solution is of the form

$$\psi_{a_{1-}}=c'''\left(\frac{\partial p_+}{\partial\alpha}\right)^{\frac{1}{2}}\exp\left(-\int_{q}^{a_1}\kappa_+dq\right). \tag{24}$$

At the classical turning points we choose the solutions of the true Schrödinger equation.[9] It is known that these solutions can be joined continuously to the WKB solutions of Eqs. (21)–(24), provided that the constant c'' is chosen properly. In those problems where the constant α is the total energy, one finds that $c''=c'/2$, $c'''=c/2$.

The requirement that the wave function be continuous in the classical region at some arbitrary point q, i.e., $\psi_{a_{1+}}=\psi_{a_{2-}}$, immediately yields the WKB quantum condition, $\oint pdq=(n+\frac{1}{2})h$, when $c=(-1)^nc'$.

In many problems the WKB solutions yield the exact eigenvalues of the original Schrödinger theory. This is remarkable when we consider that the quasi-classical equation, (17), and the boundary conditions associated with that equation, differ significantly from the Schrödinger equation and the boundary requirements on solutions in that theory. As for the solutions themselves, the Schrödinger wave functions are continuous and bounded, while the WKB wave functions are singular at isolated points and have to be defined in different ways in the classical and nonclassical regions.

In view of the above, the question might be asked as to why we have to restrict the WKB approximation to ordinary configuration space. After all, we have at our disposal the group of canonical transformations and a different quasi-classical solution associated with each transformation. Amongst these transformations there must surely be many for which the WKB solutions are continuous and bounded everywhere. And if the eigenvalues of the WKB and Schrödinger theories agree in some representation, why cannot there be a transformed quasi-classical equation which is identical with a similarly transformed Schrödinger equation?

IV. CLASSICAL CREATION AND DESTRUCTION OPERATORS

In the following we shall show that there are quasi-classical solutions which are bounded and continuous everywhere, and these solutions satisfy equations identical with a transformed Schrödinger equation. The classical representation in which these properties are exhibited is of interest in itself because it provides us with a classical theory of creation and destruction operators.

As we have already stated, if we seek continuous WKB wave functions, then the usual configuration space is indeed badly chosen. In classical mechanics, a configuration space with more desirable characteristics is the periodic space of the so-called angle variables. If we carry out a canonical transformation to action-angle variables, or simple functions of these variables, we shall find quasi-classical wave functions which are continuous everywhere.

To illustrate our method we shall first carry out this transformation for the one-dimensional harmonic oscillator.[10] For the oscillator it is well known that the energy E is related to the action variable J

$$J=2\pi E/\omega. \tag{25}$$

ω is the angular frequency of the oscillator and the action variable J is a momentum variable conjugate to the angle variable w.

[9] In actuality the quasi-classical solutions cannot be matched to the exact Schrödinger solutions at the classical turning points. They are rather matched to other asymptotic solutions of Schrödinger's equation found by expanding $E-V$ in a power series and then solving the modified Schrödinger equation in the neighborhood of the turning points.

[10] In I we carried out a similar transformation, except that the method employed in that paper was tailor-made for the oscillator. The transformations of this note have a wide range of applicability and are not restricted to the oscillator problem.

We now carry out the following canonical transformation to the new variables Q and P:

$$Q=(J/2\pi\hbar)^{\frac{1}{2}}e^{i2\pi w},$$
$$P=-i(J\hbar/2\pi)^{\frac{1}{2}}e^{-i2\pi w}. \tag{26}$$

Under this transformation Eq. (25) becomes

$$E=iQP\omega, \tag{27}$$

and the Hamilton-Jacobi equation corresponding to (27) is

$$E=iQ(\partial S/\partial Q)\omega. \tag{28}$$

The solution of this equation is $S=-i(E/\omega)\ln Q$. The density D is

$$D\equiv\partial^2S/\partial E\partial Q=-i/\omega Q, \tag{29}$$

and the quasi-classical wave function is

$$\psi=[\Gamma(Z+1)]^{-\frac{1}{2}}Q^Z, \tag{30}$$

where $Z=(E/\hbar\omega)-\frac{1}{2}$. The Γ function is a normalization constant.

The creation and destruction operators of the theory are brought into evidence by the following relations:

$$Q\psi(Z)=(Z+1)^{\frac{1}{2}}\psi(Z+1),$$
$$\frac{\partial}{\partial Q}\psi(Z)=Z^{\frac{1}{2}}\psi(Z-1). \tag{31}$$

The quasi-classical equation is

$$(E-\hbar\omega/2)\psi=\hbar\omega Q\partial\psi/\partial Q, \tag{32}$$

which is an exact equation of quantum mechanics with Q and $\partial/\partial Q$ particular representations of the creation and destruction operators. The theory which we have presented is classical throughout since the energy E can assume continuous values.

How is this WKB theory to be quantized? We may if we wish use the arguments of the usual quantum theory.[11] The critical requirements in that theory are that the energy be positive and that

$$\langle E'|E'\rangle>0,$$
$$\langle E'|\eta\bar{\eta}|E'\rangle\geq 0. \tag{33}$$

η ane $\bar{\eta}$ are the creation and destruction operators, respectively. The corresponding conditions that have to be satisfied in our representation are

$$\int_0^{\prime}\psi^*\psi dw>0, \tag{34}$$

$$\int_0^{\prime}\psi^*Q\frac{\partial}{\partial Q}\psi dw\geq 0. \tag{35}$$

If we also require that the quasi-classical wave functions be eigenstates of the Hamilton operator in Eq. (32), we find by the usual methods that $Z=n$, and $E=(n+\frac{1}{2})\hbar\omega$.

The methods that we have employed in the WKB quantization of the oscillator may be extended to arbitrary bound state classical problems. Assume that we have solved a given bound state problem in the form

$$J_i=J_i(\alpha_k), \tag{36}$$

where the J_i are the independent action variables and the α_k are an equal number of constants of the motion of the mechanical problem. Then the creation operators may be introduced by the canonical transformations,

$$Q_i=(J_i/2\pi\hbar)^{\frac{1}{2}}e^{i2\pi w_i}, \quad \text{(no summation}$$
$$P_i=-i(J_i\hbar/2\pi)^{\frac{1}{2}}e^{i2\pi w_i}. \quad \text{convention)} \tag{37}$$

The Hamilton-Jacobi equations corresponding to the Eqs. (36), and written in terms of the variables Q_i and P_i, take the form

$$2\pi iQ_i\partial S/\partial Q_i=J_i(\alpha_k).$$
$$\text{(no summation convention).} \tag{38}$$

The solutions of (38) may be used to form quasi-classical wave functions, and in terms of these wave functions Q_i and $\partial/\partial Q_i$ act as creation and destruction operators.

An example is provided by the radial equation of the Kepler problem,

$$J_r=\pi e^2(-2\mu/E)^{\frac{1}{2}}-J_\theta-J_\phi. \tag{39}$$

We assume that we have found the values of J_θ and J_ϕ by the usual techniques of the WKB theory, $J_\theta=(l'+\frac{1}{2})h$ and $J_\phi=mh$,[12] or by the alternative method we are now prescribing. Equation (39) becomes

$$J_r=\pi e^2(-2\mu/E)^{\frac{1}{2}}-(l'+m+\tfrac{1}{2})h. \tag{40}$$

Introduce the new canonical variables,

$$Q_r=(J_r/2\pi\hbar)^{\frac{1}{2}}e^{i2\pi w_r}, \tag{41}$$
$$P_r=-i(J_r\hbar/2\pi)^{\frac{1}{2}}e^{-i2\pi w_r},$$

and we find that the quasi-classical solutions corresponding to Eqs. (40) and (41) are

$$\psi=cQ^{n'}, \tag{42}$$

with $n'\hbar=(-\mu e^2/2E)^{\frac{1}{2}}-(l'+m+1)\hbar$, and c is an arbitrary constant. The energy levels of the hydrogen atom are as expected, $E_n=-\mu e^4/2n^2\hbar^2$, with $n=n'+l'+m+1$.

There is however one caution which must be observed in deriving eigenvalues from the quasi-classical creation and destruction operator formalism. If the same method is applied to rotations, one finds that the eigenvalues derived from our scheme do not agree with the correct eigenvalues derived from the Schrödinger or WKB theories. This pecularity arises because in librational motion there is a characteristic change of phase when the particle is reflected from the classical turning point,[13]

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

[12] In the WKB approximation $J_\theta=(l'+\frac{1}{2})h$ and $J_\phi=mh$, as shown in I or in L. Landau and E. Lifshitz, *Quantum Mechanics* (Pergamon Press, Ltd., New York, 1958), Sec. 49.

[13] See the work of J. B. Keller, Ann. Phys. 4, 180 (1958).

and this phase change is incorporated into the scheme we have outlined. In a rotation, on the other hand, there is no change of phase so that we must formulate our problem somewhat differently. If the particle undergoes a rotation, then the proper choice of creation and destruction operators is given by the canonical transformations,

$$\bar{J}=J(\alpha)+\tfrac{1}{2}h,\qquad \bar{w}=w, \tag{43}$$

and

$$\bar{Q}=(\bar{J}/2\pi\hbar)^{\frac{1}{2}}\exp(i2\pi\bar{w}),\qquad \bar{P}=-i(\bar{J}\hbar/2\pi)^{\frac{1}{2}}\exp(-i2\pi\bar{w}). \tag{44}$$

A simple example of a rotation is provided by the azimuthal angular motion of a particle in a radial potential. In that case $J_\phi=2\pi\alpha_\phi$, and in order to quantize the theory we must first carry out the canonical transformation $\bar{J}_\phi=J_\phi+\frac{1}{2}h$. We then introduce the creation and destruction operators in terms of the new action variable $\bar{J}_\phi$. Quantization yields the true value $\alpha_\phi=m\hbar$.

In more-complex problems, the proper definition of creation and destruction operators depends in large measure on the result of quantizing the same problems in the usual configuration space of the WKB theory. The connection formulas will then determine the WKB eigenvalues. These eigenvalues govern the choice of the proper operators and boundary conditions in other spaces such as the configuration space of the creation and destruction operators.

V. APPROXIMATE UNITARY TRANSFORMATIONS

Before discussing the unitary transformations,[14] we note that the quasi-classical wave function ψ of Eq. (4), and the canonical transformation functions U of Eq. (8), have the form $Ae^{-iB/\hbar}$. We now inquire if there is a unitary transformation matrix of the same form. We assume a representation diagonal in the original and transformed coordinates q and Q, respectively. For the transformation matrix $T(q_i,Q_i)$ to be unitary, the following condition must hold:

$$\int T^*(Q_i',q_k)T(Q_i,q_k)dq_1dq_2\cdots dq_n=\delta(Q_i-Q_i'). \tag{45}$$

Since we insist that T have the form $Ae^{-iB/\hbar}$, we cannot require the equality in Eq. (45), but only that

$$\int A^*(Q',q)A(Q,q)\exp\{(i/\hbar)[-B(Q,q)+B(Q',q)]\}\times dq_1dq_2\cdots dq_n\sim\delta(Q-Q'). \tag{46}$$

[14] Most of the results appearing in this section are due to V. A. Fock, Vestnick Leningrad Univ., Ser. Fiz. i Khim. No. 16(3), 67 (1959). I am indebted to Professor P. G. Bergmann for calling to my attention a translation of this work prepared for the Air Force Cambridge Research Center. I have incorporated Fock's results in this paper so that the approximate unitary transformations may readily be compared with the canonical transformations of the quasi-classical theory.

The exponential in the integrand is a rapidly varying function so that the integral has nonzero values only when Q is close to Q'. We expand B in a Taylor series and obtain for the left-hand side of Eq. (46)

$$\int|A(Q,q)|^2\exp\left[(i/\hbar)\frac{\partial B}{\partial Q_i}(-Q_i+Q_i')\right]\times dq_1dq_2\cdots dq_n. \tag{47}$$

If we call $\partial B/\partial Q_i=-P_i$ and let A be proportional to the square root of the absolute value of the determinant $\|\partial P_i/\partial q_k\|$, we find that

$$(2\pi\hbar)^{-n}\int\left\|\frac{\partial P_i}{\partial q_k}\right\|\exp[(i/\hbar)P_i(Q_i-Q_i')]\times dq_1dq_2\cdots dq_n\sim\delta(Q-Q'), \tag{48}$$

when we note that

$$\|\partial P_i/\partial q_k\|dq_1dq_2\cdots dq_n=dP_1dP_2\cdots dP_n.$$

Thus T is a unitary matrix. If we identify B with the canonical generating function F, and define the new and old momenta by the canonical transformation,

$$p_i=\partial F/\partial q_i,\qquad P_i=-\partial F/\partial Q_i, \tag{49}$$

we find that the unitary matrix T is given by

$$T=(2\pi\hbar)^{-n/2}\|\partial^2F/\partial Q_i\partial q_k\|^{\frac{1}{2}}e^{iF/\hbar}. \tag{50}$$

How do quantum mechanical operators transform under the unitary transformations generated by F? For an arbitrary operator the law of transformation is

$$\bar{G}_{\text{op}}(Q,P_{\text{op}})\psi(Q)=\int\int T^*(Q',q)G_{\text{op}}(q,p_{\text{op}})T(Q,q)\psi(Q')dqdQ'. \tag{51}$$

When the transformation matrix T is given by Eq. (50), the right-hand side of Eq. (51) becomes

$$X=(2\pi\hbar)^{-n}\int\int\left\|\frac{\partial^2F}{\partial Q'\partial q}\right\|e^{-iF'/\hbar}G_{\text{op}}(q,p_{\text{op}})\left\|\frac{\partial^2F}{\partial Q\partial q}\right\|\times e^{iF/\hbar}\psi(Q')dqdQ'. \tag{52}$$

We shall find that X equals $\bar{G}_{\text{op}}(Q,P_{\text{op}})\psi(Q)$ only in the limit as h vanishes. This limit is to be understood as follows: p_{op} can only act on the phase of the matrix T. Any other operation will give a null contribution when h goes to zero. In effect we may replace G_{op} by the function $G(q,p)$, and this function by the transformed function $\bar{G}(Q,P)$. With these substitutes Eq. (52) becomes

$$X=(2\pi\hbar)^{-n}\int\int\bar{G}(Q,P)e^{iP\cdot(Q'-Q)/\hbar}dP\,\psi(Q')dQ'. \tag{53}$$

In Eq. (53) we have again expanded the phase of the integrand in a power series about the point Q. In our approximation we may replace the function P appearing in $\bar{G}$ by the operator $-i\hbar\partial/\partial Q'$, and we finally have

$$X=\int \bar{G}\left(Q, -i\hbar\frac{\partial}{\partial Q'}\right)\delta(Q-Q')\psi(Q')dQ'$$

$$=\bar{G}\left(Q, -i\hbar\frac{\partial}{\partial Q}\right)\psi(Q). \quad (54)$$

We see that the approximate unitary transformations generated by F in Eq. (50) transform quantum mechanical operators into quantum mechanical operators, but only in the limit as h vanishes. On the other hand, the canonical transformations of the quasi-classical theory are a superior approximation to the original wave theory than the approximate unitary transformations, since the quasi-classical operators of Eq. (14) do depend on h. There is a one-to-one correspondence between the two transformations, since the same function of the canonical variables, F, generates both transformations.