

THE WKB APPROXIMATION FOR GENERAL MATRIX HAMILTONIANS *

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ABSTRACT

We present a method of obtaining WKB type solutions for generalized Schroedinger equations for which the Hamiltonian is an arbitrary matrix function of any number of pairs of canonical operators.

Our solution reduces the problem to that of finding the matrix which diagonalizes the classical Hamiltonian and determining the scalar WKB wave functions for the diagonalized Hamiltonian's entries (presented explicitly in terms of classical quantities). If the classical Hamiltonian has degenerate eigenvalues, the solution contains a vector in the classically degenerate subspace. This vector satisfies a classical equation and is given explicitly in terms of the classical Hamiltonian as a Dyson series.

As an example, we obtain, from the Dirac equation for an electron with anomalous magnetic moment, the relativistic spin-precession equation.

Submitted to Physical Review D

* Work supported by the Department of Energy, contract DE-AC03-76SF00515.

I. INTRODUCTION

The WKB approximation¹ forms a bridge between classical mechanics and quantum mechanics. Classical features of the system are clearly displayed, and the quantum features are introduced in a simple way, with only minimal appearances of \hbar . And while quantum mechanics, at best, is no easier a problem than classical mechanics, a virtue of the WKB approximation is that it makes it not much harder.

The WKB approximation is usually presented in the context of a non-relativistic Schroedinger equation for a scalar wave function of a single spatial variable. It has been extended to general Hamiltonians²⁻⁵ and several²⁻⁷ (or even an infinite number⁸ of) co-ordinate variables. The WKB method has also been applied to particular systems with internal degrees of freedom, e.g., the Dirac equation.^{2,4,9} Our purpose is to present a straightforward extension of the WKB approximation for a more general case which will include each of the above, and combinations thereof, as special cases. In such a case, the Hamiltonian is an $L \times L$ matrix, \underline{H} with respect to some internal space (a tilde under a quantity denotes a matrix or vector with respect to internal co-ordinates), as well as being a function of some number of pairs of canonical operators x_1, \dots, x_n and P_1, \dots, P_n . [Here the operator $P_i \equiv -i\hbar(\partial/\partial x_i)$. We will frequently make use of the corresponding classical Hamiltonian, $\underline{H}(\vec{p}, \vec{x})$.]

The mathematics of the WKB approximation may be approached from various points of view.^{1-7,10-17} The same approximation may be derived in many ways, e.g., as the first term of an asymptotic, or even a convergent,^{11,12,17} series. Many of these methods do not seem to afford

an easy generalization to the case of interest.^{18,19} The method we do use is not an especially novel one, and the idea does occur in the mathematical literature on the subject. However, we have not succeeded in finding a general discussion with direct applicability to the quantum-mechanics problem we address. In treating our general case, we take a simple approach, and work from a case which can be solved exactly, namely $\underline{H}(\vec{p}, \vec{x}) = \underline{H}(\vec{p}, \vec{x}_0)$, independent of \vec{x} . In such a case, the solution will be a linear combination of plane wave solutions

$$\underline{\Psi}(\vec{x}) = \underline{R}(\vec{p}^{(N)}(\vec{x}_0), \vec{x}_0) e^{\frac{i}{\hbar} \vec{p}^{(N)}(\vec{x}_0) \cdot \vec{x}} \underline{\lambda}^{(N)} \quad (1.1)$$

$$\underline{\lambda}^{(N)} \equiv \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \text{ Nth place}$$

In this expression, $\underline{R}(\vec{p}, \vec{x})$ is the matrix which diagonalizes $\underline{H}(\vec{p}, \vec{x})$, while $\vec{p}^{(N)}$ and $\vec{p}^{(N)} \cdot \vec{x} \equiv U^{(N)}$ are the classical momentum and action associated with $H_D^{(N)}(\vec{p}, \vec{x})$, the Nth entry of the diagonalized Hamiltonian. By no considerable feat of imagination, we might conjecture that gentle modulation of \underline{H} with respect to \vec{x} might be closely fitted by an approximation of the form

$$\underline{\Psi}^{(N)}(\vec{x}) = \underline{R}(\vec{p}^{(N)}(\vec{x}), \vec{x}) \underline{L}^{(N)}(\vec{x}) e^{\frac{i}{\hbar} U^{(N)}(\vec{x})} \quad (1.2)$$

Modulo a normalization factor (analogous to the $1/\sqrt{v}$ factor in the usual WKB approximation), we would expect $\underline{L}^{(N)}(\vec{x}) = \underline{\lambda}^{(N)} + O(\hbar)$.

Our treatment, following through on this motivation, leads to a quite straightforward generalization of the single channel (i.e., $L=1$)

problem, provided that no two of classical functions $H_D^{(N)}(\vec{p}, \vec{x})$ are identical. If some M dimensional subset of the $H_D^{(N)}$'s is degenerate, it is necessary to go further — to do an analogue of degenerate perturbation theory. $\underline{L}^{(N)}(\vec{x})$ (modulo the "1/ v" factor) now has an O(1) subvector $\underline{c}^{(N)}(\vec{x})$. We will determine an equation for $\underline{c}^{(N)}(\vec{x}(t))$ over all configuration space (t being a parameter which is a solution of the corresponding classical mechanical equations for time). This equation has the Schroedinger-like appearance:

$$\frac{d\underline{c}(t)}{dt} = \underline{M}(t) \underline{c}(t) \quad (1.3)$$

where the matrix $\underline{M}(t)$ is determined in terms of the original Hamiltonian. The closed expression, Eq. (2.39), for $\underline{M}(t)$ is a principal result of this paper.

As an application for this formalism, we may consider the motion of a Dirac electron in an arbitrary static external electromagnetic field which varies slowly in space. The local diagonalizing matrix is then just the Foldy-Wouthuysen transformation, and the diagonalized Hamiltonian is pairwise degenerate, corresponding to the twofold spin degeneracy. Thus our equation for the evolution of the internal state vector can be directly applied in order to obtain the relativistic equation of motion for the spin-precession of the classical particle. We have checked that the method works; it is in fact a quite straightforward calculation to obtain the spin motion.

This paper is organized as follows: in Section II we develop the matrix WKB formalism in detail. Section III is devoted to a discussion of the example of the Dirac electron. In Section IV we conclude with a summary and cautionary remarks regarding unanswered questions.

II. THE GENERALIZED MATRIX WKB METHOD

We begin with a brief sketch of how we use our method to obtain the usual WKB approximation. The Schroedinger equation is

$$\left\{ \frac{P^2}{2m} + V(x) - E \right\} \Psi(x) = 0 \quad , \quad \left(P \equiv \frac{\hbar}{i} \frac{d}{dx} \right) \quad (2.1)$$

We choose, as an ansatz, $\Psi(x) = X(x)e^{\frac{i}{\hbar}U(x)}$ where $X(x)$ and $U(x)$ will be chosen later. We find that

$$\begin{aligned} \left(\frac{P^2}{2m} + V(x) - E \right) X(x)e^{\frac{i}{\hbar}U(x)} &= \left\{ \left[\frac{1}{2m} \left(\frac{dU}{dx} \right)^2 + V(x) - E \right] X \right. \\ &\quad + \frac{\hbar}{i} \left[\frac{1}{2m} \frac{d^2U}{dx^2} X + \frac{1}{m} \left(\frac{dU}{dx} \right) \frac{dX}{dx} \right] \\ &\quad \left. + O(\hbar^2) \right\} e^{\frac{i}{\hbar}U} \end{aligned} \quad (2.2)$$

To set this expression equal to zero, within corrections of $O(\hbar^2)$, we simply choose U and X such that

$$\begin{aligned} \frac{P^2}{2m} + V(x) - E &= 0 \quad , \quad \left(P \equiv \frac{dU}{dx} \right) \\ \frac{1}{2m} \frac{dp}{dx} X + \frac{p}{m} \frac{dX}{dx} &= 0 \end{aligned} \quad (2.3)$$

These are two equations involving only classical quantities. Solution of the second equation gives

$$\Psi_{\text{WKB}}(x) \sim \frac{1}{\sqrt{p(x)}} e^{\frac{i}{\hbar} \int^x p(x') dx'} \quad (2.4a)$$

Solution of the first equation gives

$$p(x) = \sqrt{2m(E - V(x))} \quad (2.4b)$$

We will follow the same line of argument in the general case, which is defined to be a system with N spacial and L internal degrees of freedom, characterized by the matrix Schroedinger equation:

$$\underline{H}(\vec{P}, \vec{x}) \underline{\psi}(\vec{x}) = E \underline{\psi}(\vec{x}) \quad (2.5)$$

Here $\vec{x} = (x_1, \dots, x_N)$ represents the spacial coordinates of the system, and

$$\vec{P} = (P_1, \dots, P_N) = \frac{\hbar}{i} \frac{\partial}{\partial x_1}, \dots, \frac{\hbar}{i} \frac{\partial}{\partial x_N} \quad (2.6)$$

is the spacial momentum operator. The wavefunction $\underline{\psi}$ is now an L-component vector and the Hamiltonian is an L x L Hermitian matrix

$$\underline{\psi}(\vec{x}) = \begin{pmatrix} \psi_1(\vec{x}) \\ \vdots \\ \psi_L(\vec{x}) \end{pmatrix} \quad \underline{H}(\vec{P}, \vec{x}) = \begin{pmatrix} H_{11}(\vec{P}, \vec{x}) & \dots & H_{1L}(\vec{P}, \vec{x}) \\ \vdots & & \vdots \\ H_{L1}(\vec{P}, \vec{x}) & \dots & H_{LL}(\vec{P}, \vec{x}) \end{pmatrix} \quad (2.7)$$

We shall assume that all \hbar dependence of \underline{H} is contained in the \hbar dependence of the spatial momentum operator. (However, at the end of this section we will consider Hamiltonians with explicit \hbar dependence.) We assume $\underline{H}(\vec{P}, \vec{x})$ may be expanded as a power series of the form

$$\underline{H}(\vec{P}, \vec{x}) = \sum_{k=0}^{\infty} \sum_{\vec{m}^{(1)}, \vec{r}^{(1)}; \dots; \vec{m}^{(k)}, \vec{r}^{(k)}=0} \frac{d(\vec{m}^{(1)}, \vec{r}^{(1)}; \dots; \vec{m}^{(k)}, \vec{r}^{(k)})}{2} \quad (2.8)$$

$$\otimes \left[\begin{array}{cccccccc} m_1^{(1)} & m_N^{(1)} & r_1^{(1)} & r_N^{(1)} & m_1^{(2)} & m_N^{(2)} & r_1^{(k)} & r_N^{(k)} \\ P_1 & \dots P_N & x_1 & \dots x_N & P_1 & \dots P_N & \dots x_1 & \dots x_N \end{array} + \text{h.c.} \right]$$

(The Hermitian conjugate (h.c.) is simply the factors written in reverse order) where the \underline{d} 's are Hermitian matrices. It is not hard to show, by using the canonical commutation relations, that terms of the form

$$\left(\begin{array}{c} \text{Monomial in} \\ P\text{'s and } x\text{'s} \end{array} \right) + \text{h.c.}$$

are equal, independent of the ordering of the P's and x's through $O(\hbar)$. Since we will be neglecting $O(\hbar^2)$ terms, for the remainder of the paper we may take

$$\underline{H}(\vec{P}, \vec{x}) = \sum_{\vec{M}} \frac{1}{2} \left[\underline{a}_{\vec{M}}(\vec{x}) P_1^{M_1} \dots P_N^{M_N} + P_1^{M_1} \dots P_N^{M_N} \underline{a}_{\vec{M}}(\vec{x}) \right] \quad (2.9)$$

Now, in analogy to the simple WKB treatment, we shall take for the matrix problem a similar exponential ansatz for the wave function. We again introduce what will turn out to be an action-function $U(\vec{x})$, to be determined later, and define the classical momentum $\vec{p}(\vec{x})$:

$$p_i = \frac{\partial U}{\partial x_i} \quad \text{or} \quad \vec{p} = \vec{\nabla}_x U \quad (2.10)$$

The ansatz for the wave function is again

$$\underline{\psi}(\vec{x}) = \underline{\chi}(\vec{x}) e^{\frac{i}{\hbar} U(\vec{x})} \quad (2.11)$$

We shall need the effect of the momentum operators on this wave function. We note that

$$e^{-\frac{i}{\hbar} U} P_1^{M_1} \dots P_N^{M_N} \left(\underline{\chi} e^{\frac{i}{\hbar} U} \right) = P_1^{M_1} \dots P_N^{M_N} \underline{\chi} + \frac{\hbar}{i} \left[\frac{1}{2} \sum_{r,s=1}^N \frac{\partial^2 U}{\partial x_r \partial x_s} \frac{\partial^2}{\partial p_r \partial p_s} \right. \\ \left. \left[P_1^{M_1} \dots P_N^{M_N} \right] \underline{\chi} + \sum_{r=1}^N \frac{\partial}{\partial p_r} \left[P_1^{M_1} \dots P_N^{M_N} \right] \frac{\partial \underline{\chi}}{\partial x_r} \right] + O(\hbar^2) \quad (2.12)$$

We may now see how a general Hermitian operator, \underline{F} , of the form

$$\underline{F}(\vec{P}, \vec{x}) = \frac{1}{2} \sum_{\{\vec{M}\}} \left[b_{\{\vec{M}\}}(\vec{x}) P_1^{M_1} \dots P_N^{M_N} + P_1^{M_1} \dots P_N^{M_N} b_{\{\vec{M}\}}(\vec{x}) \right] \quad (2.13)$$

(where the expansion coefficients $b_{\vec{M}}(\vec{x})$ are Hermitian matrices) acts on such a wave function. Using Eq. (2.12) we find

$$\begin{aligned} e^{-\frac{i}{\hbar} U} \underline{F}(\vec{P}, \vec{x}) \left(\underline{X} e^{\frac{i}{\hbar} U} \right) &= \underline{F}(\vec{P}, \vec{x}) \underline{X} + \frac{\hbar}{i} \left[\frac{1}{2} \sum_{r,s=1}^N \frac{\partial^2 U}{\partial x_r \partial x_s} \frac{\partial^2 \underline{F}(\vec{P}, \vec{x})}{\partial p_r \partial p_s} \underline{X} \right. \\ &\quad \left. + \sum_{r=1}^N \frac{\partial \underline{F}(\vec{P}, \vec{x})}{\partial p_r} \frac{\partial \underline{X}}{\partial x_r} + \frac{1}{2} \sum_{r=1}^N \frac{\partial^2 \underline{F}(\vec{P}, \vec{x})}{\partial p_r \partial x_r} \underline{X} \right] + o(\hbar^2) . \end{aligned} \quad (2.14)$$

In particular, the above expression is valid for the matrix Hamiltonian, $\underline{H}(\vec{P}, \vec{x})$. It may be simplified by using gradient notation and introducing the derivative operator Df/Dx_i as follows: for a function $f(\vec{p}(\vec{x}); \vec{x})$, define

$$\left(\frac{D}{Dx} f \right)_i \equiv \frac{Df}{Dx_i} = \sum_j \frac{\partial f}{\partial p_j} \frac{\partial p_j}{\partial x_i} + \frac{\partial f}{\partial x_i} .$$

Then

$$\begin{aligned} e^{-\frac{i}{\hbar} U} \underline{H}(\vec{P}, \vec{x}) e^{\frac{i}{\hbar} U} \underline{X} &= \underline{H}(\vec{P}, \vec{x}) \underline{X} + \frac{\hbar}{i} \left[\frac{1}{2} \left(\frac{D}{Dx} \cdot \vec{\nabla}_p \underline{H}(\vec{P}, \vec{x}) \right) \underline{X} \right. \\ &\quad \left. + \left(\vec{\nabla}_p \underline{H}(\vec{P}, \vec{x}) \right) \cdot \left(\vec{\nabla}_x \underline{X} \right) \right] + o(\hbar^2) \end{aligned} \quad (2.15)$$

We have now obtained the equivalent of Eq. (2.2):

$$\begin{aligned}
 & e^{-\frac{i}{\hbar} U(\vec{x})} \left(\tilde{H}(\vec{p}, \vec{x}) - E \right) e^{\frac{i}{\hbar} U(\vec{x})} \tilde{X}(\vec{x}) \\
 & = \left(\tilde{H}(\vec{p}, \vec{x}) - E \right) \tilde{X} + \frac{\hbar}{i} \left[\left(\frac{1}{2} \vec{D}_x \cdot \vec{\nabla}_p \tilde{H} \right) \tilde{X} + (\vec{\nabla}_p \tilde{H}) \cdot (\vec{\nabla}_x \tilde{X}) \right] + o(\hbar^2) = 0 .
 \end{aligned} \tag{2.16}$$

Because \tilde{H} is a matrix and \tilde{X} a vector, this equation cannot be solved by inspection as Eq. (2.2) was. If $\tilde{H}(\vec{p}, \vec{x})$ could be diagonalized by a constant matrix, \tilde{R} , the solution would be straightforward. However, \tilde{R} is a slowly varying function of \vec{p} and \vec{x} because \tilde{H} is. Therefore, we will follow the method used for a constant \tilde{R} , keeping track of extra terms.

We write

$$\begin{aligned}
 \tilde{H}(\vec{p}, \vec{x}) & = \tilde{R}(\vec{p}, \vec{x}) \tilde{H}_D(\vec{p}, \vec{x}) \tilde{R}^{-1}(\vec{p}, \vec{x}) \\
 \tilde{H}_D(\vec{p}, \vec{x}) & = \begin{pmatrix} H_D^{(1)}(\vec{p}, \vec{x}) & \dots & 0 \\ \vdots & H_D^{(2)}(\vec{p}, \vec{x}) & \vdots \\ \vdots & \vdots & \vdots \\ 0 & \dots & H_D^{(L)}(\vec{p}, \vec{x}) \end{pmatrix}
 \end{aligned} \tag{2.17}$$

where, by convention,

$$H_D^{(1)} \leq H_D^{(2)} \leq \dots \leq H_D^{(L)} \tag{2.18}$$

in the neighborhood of the region of interest. Because \tilde{H} is Hermitian, \tilde{R} can be taken to be unitary. Defining $\tilde{L}(\vec{p}, \vec{x})$ by $\tilde{X}(\vec{p}, \vec{x}) = \tilde{R}(\vec{p}, \vec{x}) \tilde{L}(\vec{p}, \vec{x})$,

we obtain

$$\begin{aligned} (\underline{H}_{\underline{D}} - E)\underline{L} + \frac{\hbar}{i} \left\{ \frac{1}{2} \left[\underline{D}_{\underline{x}} \cdot \underline{\nabla}_{\underline{p}} \underline{H}_{\underline{D}} + \underline{R}^{-1} \underline{A} \underline{R} \right] \underline{L} + (\underline{\nabla}_{\underline{p}} \underline{H}_{\underline{D}} + \underline{R}^{-1} \underline{\nabla}_{\underline{x}} \underline{B} \underline{R}) \cdot \underline{D}_{\underline{x}} \underline{L} \right. \\ \left. + (\underline{\nabla}_{\underline{p}} \underline{H}_{\underline{D}} + \underline{R}^{-1} \underline{\nabla}_{\underline{x}} \underline{B} \underline{R}) \cdot (\underline{R}^{-1} \underline{D}_{\underline{x}} \underline{R}) \underline{L} \right\} = o(\hbar^2) \end{aligned} \quad (2.19)$$

where

$$\begin{aligned} \underline{A} = (\underline{D}_{\underline{x}} \cdot \underline{\nabla}_{\underline{p}} \underline{R}) \underline{H}_{\underline{D}} \underline{R}^{-1} + (\underline{\nabla}_{\underline{p}} \underline{R}) \cdot (\underline{D}_{\underline{x}} \underline{H}_{\underline{D}}) \underline{R}^{-1} + (\underline{\nabla}_{\underline{p}} \underline{R}) \cdot \underline{H}_{\underline{D}} (\underline{D}_{\underline{x}} \underline{R}^{-1}) \\ + (\underline{D}_{\underline{x}} \underline{R}) \cdot (\underline{\nabla}_{\underline{p}} \underline{H}_{\underline{D}}) \underline{R}^{-1} + \underline{R} (\underline{\nabla}_{\underline{p}} \underline{H}_{\underline{D}}) \cdot (\underline{D}_{\underline{x}} \underline{R}^{-1}) + (\underline{D}_{\underline{x}} \underline{R}) \cdot \underline{H}_{\underline{D}} (\underline{\nabla}_{\underline{p}} \underline{R}^{-1}) \\ + \underline{R} (\underline{D}_{\underline{x}} \underline{H}_{\underline{D}}) \cdot (\underline{\nabla}_{\underline{p}} \underline{R}^{-1}) + \underline{R} \underline{H}_{\underline{D}} (\underline{D}_{\underline{x}} \cdot \underline{\nabla}_{\underline{p}} \underline{R}^{-1}) \end{aligned} \quad (2.20)$$

$$\underline{B} = (\underline{\nabla}_{\underline{p}} \underline{R}) \underline{H}_{\underline{D}} \underline{R}^{-1} + \underline{R} \underline{H}_{\underline{D}} (\underline{\nabla}_{\underline{p}} \underline{R}^{-1})$$

Were $\underline{R}(\underline{p}, \underline{x})$ independent of \underline{p} and \underline{x} , then \underline{A} and \underline{B} would vanish and we would have

$$(\underline{H}_{\underline{D}} - E)\underline{L} + \frac{\hbar}{i} \left[\frac{1}{2} (\underline{D}_{\underline{x}} \cdot \underline{\nabla}_{\underline{p}} \underline{H}_{\underline{D}}) \underline{L} + (\underline{\nabla}_{\underline{p}} \underline{H}_{\underline{D}}) \cdot (\underline{D}_{\underline{x}} \underline{L}) \right] = o(\hbar^2) \quad (2.21)$$

This is a diagonal matrix equation, which may be solved in the same way we solved Eq. (2.2). Let us for the moment assume no classical degeneracy, i.e., all eigenvalues of $\underline{H}(\underline{p}, \underline{x})$ distinct; then our solutions will take the form

$$\underline{L}^{(N)} = \omega^{(N)}(\underline{x}) \underline{\lambda}^{(N)} \quad (2.22)$$

where $\tilde{\lambda}^{(N)}$ is a unit eigenvector, i.e.,

$$\tilde{\lambda}^{(1)} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \tilde{\lambda}^{(2)} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \dots \quad (2.23)$$

and $\omega^{(N)}$ satisfies

$$\left(H_D^{(N)} - E \right) \omega^{(N)} + \frac{\hbar}{i} \left[\frac{1}{2} \left(\vec{D}_x \cdot \vec{\nabla}_p H_D^{(N)} \right) \omega^{(N)} + \left(\vec{\nabla}_p H_D^{(N)} \right) \cdot \left(\vec{D}_x \omega^{(N)} \right) \right] = 0 \quad (\hbar^2). \quad (2.24)$$

To make the leading term vanish, we choose $U(\vec{x}) = U^{(N)}(\vec{x})$, that function satisfying

$$H_D^{(N)} \left(\vec{\nabla}_x U^{(N)}(\vec{x}); \vec{x} \right) - E = 0 \quad (2.25)$$

So, to no one's surprise, $U^{(N)}$ is Hamilton's characteristic function for the Nth eigenvalue of $H(\vec{p}, \vec{x})$.

To make the next term of order \hbar vanish, we must have

$$\frac{1}{2} \left(\vec{D}_x \cdot \vec{\nabla}_p H_D^{(N)} \right) \omega^{(N)} + \left(\vec{\nabla}_p H_D^{(N)} \right) \cdot \left(\vec{D}_x \omega^{(N)} \right) = 0 \quad (2.26)$$

Define the classical velocity

$$\vec{v}^{(N)}(\vec{x}) \equiv \vec{\nabla}_p H_D^{(N)}(\vec{p}, \vec{x}) \Big|_{\vec{p} = \vec{p}^{(N)}(\vec{x})} \quad (2.27)$$

and the probability density $\rho^{(N)}$ by

$$\omega^{(N)} = \left[\rho^{(N)} \right]^{\frac{1}{2}} \quad (2.28)$$

Then Eq. 2.26 transforms into the continuity equation

$$\vec{\nabla}_x \cdot \left(\vec{v}^{(N)} \rho^{(N)} \right) = 0 \quad (2.29)$$

In one space dimension, this equation is easy, and we get the usual WKB amplitude,

$$\omega(\mathbf{x}) = \frac{\text{const.}}{\sqrt{v(\mathbf{x})}} \quad (2.30)$$

In more than one dimension ρ is a conserved density in configuration space, found by Van Vleck⁵ to be a determinant formed of partial derivatives of Hamilton's principal function S with respect to coordinates and initial-condition parameters. In any case, $\omega^{(N)}$ may be calculated in the context of classical mechanics, in the same way $U^{(N)}$ may.

We have just found that our "unperturbed" equation (2.21) has solutions

$$\underline{L}_0^{(N)}(\vec{\mathbf{x}}) = \omega^{(N)}(\vec{\mathbf{x}}) \underline{\lambda}^{(N)} \quad (2.31)$$

However, we must now investigate the effect of the $\vec{\mathbf{x}}$ and $\vec{\mathbf{p}}$ dependence of the diagonalizing matrix \underline{R} . We go back to Eq. (2.19), letting

$$\underline{L}^{(N)}(\vec{\mathbf{x}}) \equiv \omega^{(N)}(\vec{\mathbf{x}}) \underline{\phi}^{(N)}(\vec{\mathbf{x}}) \quad (2.32)$$

with $\omega^{(N)}(\vec{\mathbf{x}})$ given above.

We obtain

$$\begin{aligned} & \left(\underline{H}_D - E \right) \underline{\phi}^{(N)} + \frac{\hbar}{i} \left[\frac{1}{2} \left(\underline{D}_x \cdot \underline{\nabla}_p \underline{H}_D + \underline{R}^{-1} \underline{A} \underline{R} \right) \underline{\phi}^{(N)} + \left(\underline{\nabla}_p \underline{H}_D + \underline{R}^{-1} \underline{B} \underline{R} \right) \cdot \left(\frac{1}{\omega^{(N)}} \underline{\nabla}_x \omega^{(N)} \right) \underline{\phi}^{(N)} \right. \\ & \left. + \underline{\nabla}_x \underline{\phi}^{(N)} + \left(\underline{\nabla}_p \underline{H}_D + \underline{R}^{-1} \underline{B} \underline{R} \right) \cdot \underline{R}^{-1} \left(\underline{D}_x \underline{R} \right) \underline{\phi}^{(N)} \right] = O(\hbar^2) \end{aligned} \quad (2.33)$$

If we set $\vec{\mathbf{p}}(\vec{\mathbf{x}}) = \vec{\mathbf{p}}^{(N)}(\vec{\mathbf{x}})$ defined above and let $\underline{\phi}^{(N)}(\vec{\mathbf{x}}) \equiv \sum_{i=1}^L c_i^{(N)}(\vec{\mathbf{x}}) \underline{\lambda}^{(i)}$, we obtain the following equations for the expansion

coefficients $c_i^{(N)}$:

$$\begin{aligned}
 & \left[\underline{H}_D^{(m)}(\vec{p}^{(N)}, \vec{x}) - E \right] c_m^{(N)} + \frac{\hbar}{i} \left[\frac{1}{2} \sum_i \left\{ \vec{D}_x \cdot \vec{\nabla}_p H_D^{(i)} \delta_{mi} + \left(\underline{R}^{-1} \underline{A} \underline{R} \right)_{mi} \right\} c_i^{(N)} \right. \\
 & + \sum_i \left\{ \left(\vec{\nabla}_p H_D^{(i)} \right) \delta_{mi} + \left(\underline{R}^{-1} \underline{B} \underline{R} \right)_{mi} \right\} \cdot \left\{ \frac{1}{\omega^{(N)}} \vec{\nabla}_x \omega^{(N)} c_i^{(N)} + \vec{\nabla}_x c_i^{(N)} \right\} \\
 & \left. + \sum_{i,j} \left\{ \left(\vec{\nabla}_p H_D^{(i)} \right) \delta_{mi} + \left(\underline{R}^{-1} \underline{B} \underline{R} \right)_{mi} \right\} \cdot \left\{ \left(\underline{R}^{-1} \left(\vec{D}_x \underline{R} \right) \right)_{ij} c_j^{(N)} \right\} \right] = O(\hbar^2) . \quad (2.34)
 \end{aligned}$$

At this point, we also generalize back to the case in which there may be degenerate eigenvalues of \underline{H} . We may then divide the L-dimensional internal space into degenerate subspaces; i.e., $\lambda^{(i)}$ and $\lambda^{(j)}$ are in the same subspace if $H_D^{(i)}(\vec{p}, \vec{x}) = H_D^{(j)}(\vec{p}, \vec{x})$. In the case $\underline{R}(\vec{p}, \vec{x}) = \text{const.}$, all coefficients $c_i^{(N)}$ for which $\lambda^{(i)}$ is in a degenerate subspace containing $\lambda^{(N)}$ must be expected to be of order unity with those $c_i^{(N)}$, s outside the subspace remaining zero.

In considering the general case, we take the hint from the constant \underline{R} case to estimate the magnitude of the $c_i^{(N)}$, s outside and inside the classically degenerate subspace. We will then be able to obtain simplified expressions involving these. Because the extra terms in Eq. (2.34) for the $c_i^{(N)}$, s are of $O(\hbar)$, we are led to suspect that in the case of non-constant \underline{R} , the $c_i^{(N)}$, s outside the degenerate subspace will be of $O(\hbar)$, while those in the subspace remain of $O(1)$.

In that case we can rewrite Eq. (2.34) using this assumption to drop terms of $O(\hbar^2)$. For $\lambda^{(m)}$ not in the degenerate subspace

containing $\lambda^{(N)}$, we obtain the expression

$$c_m^{(N)} = \frac{i\hbar \mathcal{N}_m^{(N)}}{H_D^{(m)}(\vec{p}^{(N)}, \vec{x}) - E} \quad (2.35)$$

with

$$\begin{aligned} \mathcal{N}_m^{(N)} = & \sum_{\substack{i \text{ in} \\ \text{degenerate} \\ \text{subspace}}} \left\{ \left(\vec{\nabla}_{\vec{p}} H_D^{(m)} \right) \cdot \left(\tilde{R}^{-1} \vec{\nabla}_{\vec{x}} \tilde{R} \right)_{mi} + \frac{1}{2} \left(\tilde{R}^{-1} \tilde{A} \tilde{R} \right)_{mi} \right. \\ & \left. + \left(\tilde{R}^{-1} \vec{\nabla}_{\vec{x}} \tilde{B} \tilde{R} \right)_{mi} \cdot \left[\frac{1}{\omega^{(N)}} \left(\vec{\nabla}_{\vec{x}} \omega^{(N)} \right) + \vec{\nabla}_{\vec{x}} \right] + \left(\tilde{R}^{-1} \vec{\nabla}_{\vec{x}} \tilde{D} \tilde{R} \right)_{mi} \right\} c_i^{(N)} \quad (2.36) \end{aligned}$$

We note that all quantities in this expression for $c_m^{(N)}$ are classical except for the overall factor of \hbar ; thus, as anticipated, it is indeed $O(\hbar)$.

We also note that for the special case $\tilde{H} = T(\vec{p})\tilde{I} + \tilde{V}(\vec{x})$, only the first term in \mathcal{N} survives.

Now we turn to the $O(1)$ components $c_n^{(N)}$ in the classically degenerate subspace; i.e. the subspace spanned by those $\lambda^{(n)}$ for which $H_D^{(n)}(\vec{p}, \vec{x}) = H_D^{(N)}(\vec{p}, \vec{x})$. We will not be able to explicitly solve for these, but we will be able to derive a purely classical differential equation for them which may be formally solved.

Let us concatenate the subspace coefficients $c_n^{(N)}$ into a vector $\overline{c}^{(N)}$ in the degenerate subspace. We will also consider matrices projected onto the degenerate subspace; thus an $L \times L$ matrix \tilde{A} will have a projection $\tilde{\overline{A}} = \tilde{P}^{(N)} \tilde{A} \tilde{P}^{(N)}$, with $\tilde{P}^{(N)}$ a diagonal projection

such that

$$\left(P^{(N)} \right)_{ii} = \begin{cases} 1 & \text{if } i \text{ is degenerate with } N \\ 0 & \text{if } i \text{ is not degenerate with } N \end{cases} \quad (2.37)$$

We note that $\overline{AB} \neq \overline{A} \overline{B}$. After considerable manipulation, and remembering $\vec{v}^{(N)} \equiv \vec{v}_p H_D^{(N)}$, we obtain

$$\begin{aligned} -\vec{v}^{(N)} \cdot \vec{v}_{x\tilde{c}}^{(N)} &= \left[\vec{v}^{(N)} \cdot \overline{\tilde{R}_D^{-1} \tilde{D}_{x\tilde{c}} \tilde{R}} + \frac{1}{2} \overline{\tilde{R}^{-1} (\vec{v}_p \tilde{R}) (\tilde{H}_D - H_D^{(N)} \tilde{I}) \cdot \tilde{R}^{-1} (\tilde{D}_{x\tilde{c}} \tilde{R})} \right. \\ &\quad \left. - \frac{1}{2} \overline{\tilde{R}^{-1} (\tilde{D}_{x\tilde{c}} \tilde{R}) (\tilde{H}_D - H_D^{(N)} \tilde{I}) \cdot \tilde{R}^{-1} (\vec{v}_p \tilde{R})} \right] \tilde{c}^{(N)} \end{aligned} \quad (2.38)$$

Taking a cue from hydrodynamics, we may interpret $\vec{v} \cdot \vec{v}_x$ and $\vec{v} \cdot \vec{D}_x$ as the flow derivative d/dt ; i.e., given a time independent field $f(\vec{x})$, $(\vec{v} \cdot \vec{v}_x) f$ would be the observed rate of change of f observed because of the motion of an observer moving with velocity, \vec{v} .

Thus, if we switch to a time parametrization, where \vec{x} and $\vec{p}^{(N)}$ are assumed to have been found by classical mechanics in terms of t (which here is taken to be just a convenient parametrization), we obtain:

$$\begin{aligned} \frac{d}{dt} \tilde{c}^{(N)}(t) &= \overline{\tilde{M}^{(N)}}(t) \tilde{c}^{(N)}(t) \\ -\overline{\tilde{M}^{(N)}}(t) &= + \overline{\tilde{R}^{-1} \frac{d\tilde{R}}{dt}} + \frac{1}{2} \overline{\tilde{R}^{-1} (\vec{v}_p \tilde{R}) (\tilde{H}_D - H_D^{(N)} \tilde{I}) \cdot \tilde{R}^{-1} (\tilde{D}_{x\tilde{c}} \tilde{R})} \\ &\quad - \frac{1}{2} \overline{\tilde{R}^{-1} (\tilde{D}_{x\tilde{c}} \tilde{R}) (\tilde{H}_D - H_D^{(N)} \tilde{I}) \cdot (\tilde{R}^{-1} \vec{v}_p \tilde{R})} \\ &= + \overline{\tilde{R}^{-1} \frac{d\tilde{R}}{dt}} + \frac{1}{2} \overline{\tilde{R}^{-1} \vec{v}_p \tilde{R} (\tilde{H}_D - H_D^{(N)} \tilde{I}) \cdot \tilde{R}^{-1} (\tilde{D}_{x\tilde{c}} \tilde{R})} \\ &\quad - \frac{1}{2} \overline{\tilde{R}^{-1} (\tilde{D}_{x\tilde{c}} \tilde{R}) (\tilde{H}_D - H_D^{(N)} \tilde{I}) \cdot (\tilde{R}^{-1} \vec{v}_p \tilde{R})} \end{aligned} \quad (2.39)$$

This equation may be solved as a convergent Dyson series:

$$\begin{aligned} \bar{\zeta}^{(N)}(t) = & \left\{ \bar{\zeta} + \int_0^t dt_1 \bar{M}^{(N)}(t_1) \right. \\ & \left. + \int_0^t dt_1 \bar{M}^{(N)}(t_1) \int_0^{t_1} dt_2 \bar{M}^{(N)}(t_2) + \dots \right\} \bar{\zeta}^{(N)}(0). \end{aligned} \quad (2.40)$$

Thus, we have found here an expression for the evolution of the large components of the wave function in terms of purely classical quantities. Notice that, because \bar{R} is unitary, the submatrix $i\bar{M}^{(N)}(t)$ is Hermitian. This implies that the norm of $\bar{\zeta}^{(N)}(t)$ is preserved along classical trajectories; all normalization changes in the wave function have been taken into account in the WKB amplitude factor $\omega^{(N)}(\vec{x})$.

Notice also that in the nondegenerate case

$$\bar{M}^{(N)}(t) = - \left(\bar{R}^{-1} \frac{d\bar{R}}{dt} \right)_{NN} \quad (2.41)$$

Thus an additional phase of order 1 is accumulated (in addition to the WKB phase):

$$c_N^{(N)}(t) = \exp \left[- \int_0^t \left(\bar{R}^{-1} \frac{d\bar{R}}{dt'} \right)_{NN} dt' \right] c_N^{(N)}(0) \quad (2.42)$$

If R is not only unitary, but also orthogonal, then

$$\left(\bar{R}^{-1} \frac{d\bar{R}}{dt} \right)_{NN} = 0 \quad (2.43)$$

then this extra phase vanishes.

Before closing this section, we consider what modifications must be made if there exists an explicit term in the Hamiltonian of order \hbar ; as in the example of the Dirac equation for an electron with anomalous magnetic moment, considered in the next section. If

$$\mathcal{H}(\vec{P}, \vec{x}) = \underline{H}(\vec{P}, \vec{x}) + \hbar \underline{H}^{(1)}(\vec{P}, \vec{x}) + \hbar^2 \underline{H}^{(2)}(\vec{P}, \vec{x}) + \dots \quad (2.44)$$

where all the $\underline{H}^{(i)}$'s are assumed to only depend implicitly on \hbar via the momentum operator \vec{P} , and where the ordering of operators of $\underline{H}^{(i)}$ is chosen as in Eq. (2.9), then all of our results of this section hold, except that one must make the replacement

$$\underline{A} \rightarrow \underline{A} + 2i\hbar \underline{H}^{(1)} \quad (2.45)$$

in Eq. (2.19) and those following. This implies, in particular, that Eq. (2.39) must be modified by the replacement

$$\overline{\underline{M}}^{(N)} \rightarrow \overline{\underline{M}}^{(N)} - i \overline{\underline{R}^{-1} \underline{H}^{(1)} \underline{R}} \quad (2.46)$$

III. EXAMPLE - THE DIRAC EQUATION

The results of the preceding section may be applied directly to the single particle Dirac equation for a particle with an anomalous magnetic moment in an external electromagnetic field. The equation we will derive will give us the correct classical precession equation, obtained by many methods in the past.^{2,9,20-22}

The Dirac equation is:²³

$$\mathcal{H}(\vec{P}, \vec{x}) \underline{\Psi}(\vec{x}) = E \underline{\Psi}(\vec{x}) \quad (3.1)$$

where

$$\begin{aligned} \mathcal{H}(\vec{p}, \vec{x}) &= \vec{\alpha} \cdot (c\vec{p} - e\vec{A}(\vec{x})) + \beta mc^2 + e\phi(\vec{x}) - \frac{\kappa \hbar e}{4mc} \beta \underline{g}_{\mu\nu} F^{\mu\nu}(\vec{x}) \\ &\left(\kappa = \frac{g-2}{2} \right) \end{aligned} \quad (3.2)$$

As mentioned in Section II, this Hamiltonian has an explicit \hbar term, and the modifications, such as in Eq. (2.46), must be kept in mind in what follows. The matrices, $\mathcal{R}(\vec{p}, \vec{x})$ [which diagonalized $\mathcal{H}(\vec{p}, \vec{x})$] and $\mathcal{H}_D(\vec{p}, \vec{x})$, are easily obtained from those used in the Foldy-Wouthouysen transformation for the free Dirac theory:²⁴

$$\begin{aligned} \mathcal{R}(\vec{p}, \vec{x}) &= \cos \left[|\vec{c}\vec{p} - e\vec{A}| \theta \right] - \frac{\beta \vec{\alpha} \cdot (\vec{c}\vec{p} - e\vec{A})}{|\vec{c}\vec{p} - e\vec{A}|} \sin \left[|\vec{c}\vec{p} - e\vec{A}| \theta \right] \\ 2\theta &= \frac{\tan^{-1} \left[\frac{|\vec{c}\vec{p} - e\vec{A}|}{mc^2} \right]}{|\vec{c}\vec{p} - e\vec{A}|} \end{aligned} \quad (3.3)$$

$$\mathcal{H}_D = \begin{pmatrix} \sqrt{m^2 c^4 + (c\vec{p} - e\vec{A})^2} + e\phi & & & 0 \\ & \sqrt{m^2 c^4 + (c\vec{p} - e\vec{A})^2} + e\phi & & \\ & & -\sqrt{m^2 c^4 + (c\vec{p} - e\vec{A})^2} + e\phi & \\ 0 & & & -\sqrt{m^2 c^4 + (c\vec{p} - e\vec{A})^2} + e\phi \end{pmatrix} \quad (3.4)$$

We see that there are two classically degenerate, two component subspaces.

We can simply insert Eqs. (3.3) and (3.4) into Eq. (2.39) with modifications from Eq. (2.46) and obtain the equation of motion for the positive-energy subspace components $\bar{\zeta}$.

We find, after considerable algebra,

$$\frac{d\vec{\zeta}}{dt} = i \vec{\zeta} \cdot \frac{\vec{Q}}{2\zeta} \vec{\zeta} \quad (3.5)$$

with

$$\vec{Q} = \frac{e}{m\gamma} \left[(1 + \gamma\kappa) \frac{\vec{B}}{c} + (1 - \gamma)\kappa \frac{\vec{v}(\vec{v} \cdot \vec{B})}{v^2 c} + \gamma \left(\kappa + \frac{1}{\gamma + 1} \right) \frac{\vec{E} \times \vec{v}}{c^2} \right] \quad (3.6)$$

$$\gamma = \left(1 - \frac{v^2}{c^2} \right)^{-\frac{1}{2}}$$

The classical polarization vector, \vec{P} , is defined by

$$\vec{P}(t) \equiv \vec{\zeta}^\dagger(t) \vec{\sigma} \vec{\zeta}(t) \quad (3.7)$$

From Eq. (3.5) it follows that

$$\frac{d\vec{P}}{dt} = -(\vec{Q} \times \vec{P}) \quad (3.8)$$

which is the correct classical precession equation.²⁰

IV. DISCUSSION

We have found approximate WKB solutions of the matrix Schroedinger equation, $\mathbb{H}\Psi = E\Psi$, of the form

$$\Psi^{(N)}(\vec{x}) = \mathbb{R} \left(\vec{p}^{(N)}(\vec{x}, \vec{x}) \right) \sqrt{\rho^{(N)}(\vec{x})} e^{\frac{i}{\hbar} U^{(N)}(\vec{x})} \vec{\zeta}^{(N)}(\vec{x}) \otimes [1 + O(\hbar)] \quad (4.1)$$

This factors the problem into (1) an overall rotation \mathbb{R} in internal coordinate space which locally diagonalizes the Hamiltonian matrix, \mathbb{H} (in phase space), (2) a problem of the dynamics of a scalar particle (i.e., one with no internal degrees of freedom) with a WKB wave

function $\sqrt{\rho} e^{(i/\hbar)U}$, and (3) a problem of the dynamics of the vector $\bar{\xi}$ which lies in the subspace spanned by all eigenvectors of the classical Hamiltonian with degenerate eigenvalues equal to $H_D^{(N)}$.²⁵ We note that, for bound-state problems, the derivatives of $\bar{\xi}$ appearing in the equation of motion, Eq. (2.39), for $\bar{\xi}(t)$, in general breaks the degeneracy of energy levels in the classically degenerate subspace.

The general solution for Ψ would then be linear combinations of the $\Psi^{(N)}(\vec{x})$ for all N . We set our problem in a region where all $U^{(N)}$'s were real so that there were "plane waves" in all L channels. Were some $U^{(N)}$ imaginary throughout the region, we would obtain the usual type of increasing or decreasing exponentials, replacing $iU^{(N)}(\vec{x})$ in the exponent by $V^{(N)}(\vec{x})$, where

$$H_D^{(N)} \left(-i \vec{\nabla} V^{(N)}(\vec{x}), \vec{x} \right) = E \quad (4.2)$$

However, we have not studied the question of turning-points in detail. Nevertheless, we believe there is cause for optimism that the problem is no worse than for a single-channel WKB problem. In a companion paper,²⁶ we will discuss one dimensional bound state problems with two turning points and present analogues of the Bohr-Sommerfeld conditions for the energy levels, as well as the wave functions. In the general bound-state problem, we could also obtain Bohr-Sommerfeld rules by the Einstein prescription.^{3,27} Quantize the classical actions $U^{(N)}$.

Because our method can accommodate any number of spatial coordinates, it should be possible to go to the continuum limit and construct semiclassical limits of field theories within a canonical Hamiltonian formalism.

Our method might also be applied to classical wave equations in slowly varying media.^{12,17,28}

Keller and Keller have shown¹¹ that the WKB approximation is a special case of an approximate solution of the first order, single variable, matrix equation $(dy(x)/dx) = \underline{M}(x) y(x)$. In an analogous way, our result may be applied^{19,25} for approximate solutions to equations of the form

$$\underline{L} \left(\frac{\partial}{\partial x_1}, x_1 \right) \underline{y}(x_1) = 0$$

when the equations

$$\underline{L}_D^{(N)}(v_1, x_1) = 0$$

have solutions for v_1 .

Finally, there is the question of how good our approximation is. We simply don't know. We could obtain some hints if we could find a reliable way to iterate our method and get higher order terms. Short of that, we can only be guided by the results for single-channel WKB problems¹⁰ and matrix WKB problems of the simpler form

$\underline{H} = (p^2/2m)\underline{I} + \underline{V}(x)$.^{11,17} Without going into detail, we are led to expect that higher order terms would involve integrals of rapidly oscillating exponentials of the form $\exp(i/\hbar) (U^{(N)} - U^{(M)})$. This would make these terms small, certainly no larger than $\hbar/(U^{(N)} - U^{(M)})$.

Basically, the problem is one of estimating the probability of a transition from the Nth channel where the classical particle would have momentum $p^{(N)}$ to a distinct Mth channel where the classical particle would have momentum $p^{(M)}$. This is not too different from

the usual WKB problem of a calculation of the reflection coefficient from a smoothly varying potential, away from a turning point (i.e., spontaneous transition from rightward (+p) motion of a wave packet to leftward (-p) motion). This is a subtle calculation, even for a single-channel one-dimensional WKB problem,²⁹ but the answer is indubitably small—typically²⁹ of order $e^{-\text{const.}/\hbar}$. Thus it is quite plausible that amplitudes of inter-orbit transitions are of similar magnitude. Even transitions at a turning point, from the channel undergoing reflection to another which is not undergoing reflection appear to have rapidly oscillating phases, hence are comparably small. However, a detailed analysis of all these issues is well beyond the scope of this paper.

ACKNOWLEDGMENTS

We gratefully acknowledge all the help and time given us including that of Thomas L. Savarino, Leonid A. Turkevich, Joseph B. Keller, and our colleagues at the Stanford Linear Accelerator Center. We would also like to thank the Stanford University Physics Department and SLAC for their support.

This work was supported by the Department of Energy under contract DE-AC03-76SF00515.

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