Geometric phases in the asymptotic theory of coupled wave equations

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Traditional approaches to the asymptotic behavior of coupled wave equations have difficulties in the formulation of a consistent version of the Bohr-Sommerfeld quantization conditions. These difficulties can be circumvented by using the Weyl calculus to diagonalize the matrix of wave operators. In analyzing the diagonalized wave equations, geometric phases enter in an important way, especially in the development of Bohr-Sommerfeld quantization rules. It turns out that a version of Berry's phase is incorporated into the symplectic structure in the ray phase space, influencing the classical Hamiltonian orbits, the construction of solutions to the Hamiltonian-Jacobi equation, and the computation of action integrals. Noncanonical coordinates in the ray phase space are useful in carrying out these calculations and in making the construction of eigenvalues and wave functions manifestly gauge invariant.

I. INTRODUCTION

This paper concerns the application of WKB theory to systems of coupled, linear wave equations. The wave fields that are coupled together are usually the components of some vector or tensor of physical significance; thus the wave equations we will consider govern multicomponent wave fields. Examples include electromagnetic waves in plasmas, elastic waves in solids, light waves in anisotropic and inhomogeneous media, gravitational waves in general relativity, Pauli or Dirac spinors in quantum mechanics, and nuclear wave functions in the Born-Oppenheimer approximation. In this paper we will deal especially with the problem of Bohr-Sommerfeld quantization of multicomponent wave fields, and more generally with the role of geometric phases in their WKB analysis.

A complete set of WKB equations for multicomponent wave fields has been worked out by Bernstein [1], who had in mind applications to the propagation of electromagnetic waves in plasmas. The subject was later reviewed by Bernstein and Friedland [2]. The equations presented by these authors are complete in the sense that they apply in any number of spatial dimensions, they make no assumptions about the form of the dispersion matrix, and they give all the information needed to transport amplitudes and phases of a wave along the rays of the wave system. These works did not, however, deal with the Bohr-Sommerfeld quantization problem for multicomponent wave fields, by which we mean the multicomponent generalization of Bohr-Sommerfeld quantization of scalar fields (in its modern form sometimes also called Einstein-Brillouin-Keller [3] or torus quantization [4]). Neither did these works recognize that one of the phases occurring in the WKB problem is anholonomic, although a contemporary paper by Budden and Smith [5], working with a slab model and some special cases of dispersion matrices, did make such a recognition.

The anholonomic, geometric phase occurring in the multicomponent WKB problem is an example of Berry's phase [6], as has been pointed out by Yabana and Horiu-

chi [7]. Given the current understanding of geometric phases [8–11], it comes as no surprise that something like them should appear in the asymptotic behavior of multicomponent wave fields, for as one moves along a ray of the wave field, the local dispersion matrix, describing the properties of the medium in the various directions and the coupling among the components of the wave field, changes adiabatically. Thus one must expect the dispersion matrix, regarded as a function of time (or other parameter) along the ray, to play the same role as the Hamiltonian matrix in Berry's original analysis [6] of adiabatic processes in quantum mechanics. This indeed is precisely how things work out.

The Bohr-Sommerfeld quantization problem for multicomponent wave fields has been considered by Berk and Pfirsch [12] and Yabana and Horiuchi [7] with success primarily in the case of one spatial dimension. Of the two references, it seems that Yabana and Horiuchi made the clearer statement of the one-dimensional quantization condition, which turns out to be like the scalar case except for two additional phases. One of these is Berry's phase, and the other is an additional phase which cannot be represented by a differential form (as can Berry's phase). Yabana and Horiuchi also attempted to state a multidimensional quantization condition, but were able to do so only for special dispersion matrices. Their results are not obvious generalizations of torus quantization as it is known for scalar wave fields, nor are they as geometrically compelling. In Sec. II of this paper we provide a critique of this existing theory of multicomponent wave fields, and provide our interpretation of the difficulty in formulating a consistent quantization condition.

We break the impasse in the formulation of a quantization condition by diagonalizing the matrix of wave operators [13], which we discuss in Sec. III. Our diagonalization of the matrix of wave operators is equivalent, through lowest order in the WKB ordering parameter, to diagonalizing the dispersion matrix (a matrix of numbers), which is done in all treatments of this subject. Nevertheless, the general analyses of Bernstein and Fried-

land [1,2] and others do not actually diagonalize the matrix of wave operators beyond lowest order, and in this respect their work differs from ours. This distinction may seem small, but the diagonalization of the matrix of wave operators, in principle to all orders, has the definite advantage that it reduces the multicomponent WKB problem to a set of uncoupled scalar problems. Thus all known results of scalar theory can be immediately transcribed to the multicomponent case.

This is not to say that all the analysis subsequent to the diagonalization of the matrix of wave operators is completely standard, for it turns out that the diagonalization leads to gauge-dependent ray Hamiltonians (in the sense of the gauge transformations of Berry's [14] adiabatic theory). This leads to the discussion of Sec. IV, which has much to do with the proper interpretation of these gauge-dependent ray Hamiltonians, and how to extract gauge-invariant wave functions and quantization rules from them. It turns out to be helpful in this process to introduce certain noncanonical but gauge-invariant coordinates on the classical ray phase space, because in terms of these coordinates, both the ray Hamiltonian and the equations of motion are gauge invariant, as are the Lagrangian manifolds representing physical, gauge-invariant wave functions.

In our formulation of the quantization conditions, Berry's phase plays a fundamental role by being incorporated into the symplectic structure on the classical ray phase space. From this position, Berry's phase influences the classical equations of motion, the very meaning of the Lagrangian condition entering into solutions of the Hamilton-Jacobi equation, and in the computation of actions and symplectic areas in phase space. When all is said and done, our quantization condition is exactly the same as in the scalar case, but with a different symplectic structure on phase space from the usual one, and with a different ray Hamiltonian from that used in the theory of Bernstein and Friedland [1,2].

A definite limitation of this paper is our restriction to Hermitian dispersion matrices. These are decidedly unrealistic in many applications in optics, plasma physics, and other areas, but are mathematically simpler than general dispersion matrices. Our reasons for making this restriction are partly that we are not completely satisfied with existing treatments of non-Hermitian dispersion matrices, and partly that the simpler case we consider is sufficient to make our points about geometric phases and quantization. In any case, Hermitian dispersion matrices do occur in many applications, notably quantum-mechanical ones, but others as well.

Another limitation is the fact that we have ignored the problem of mode conversion, i.e., the coupling between polarizations that occurs when there is a near degeneracy in the dispersion matrix. This problem has been dealt with from a rather general standpoint by Friedland and Kaufman [15], from whom we have borrowed some techniques important to our method, especially the use of the Weyl calculus for diagonalizing the matrix of wave operators.

The problem of multidimensional Bohr-Sommerfeld (or Einstein-Brillouin-Keller) quantization for one-

component wave fields is well known in some fields and not in others. Since this paper is intended to appeal to an interdisciplinary audience, it is perhaps appropriate to provide some comments on this subject here. More details may be found in reviews such as those by Berry and Mount [16] and Berry [17].

The standard quantization condition in one dimension is that the integral $\oint k\,dx$, taken around a closed orbit, should be either an integer or a half-integer. Textbook discussions of higher-dimensional quantization are often limited to the case in which the Hamilton-Jacobi equation is separable, for which the quantization condition assigns $\oint k_i dq_i$ (no sum on i) to an integer n_i or a half-integer $n_i + \frac{1}{2}$, giving one quantum number n_i for each degree of freedom. It is now recognized, however, that separability is not a fundamental issue; rather, the fundamental issue is whether the classical motion is integrable. For if the motion is integrable, then the orbits are quasi-periodic and lie on tori in phase space, and solutions of the Hamilton-Jacobi equation exist. The solutions that are allowed for WKB purposes are those that give a single-valued wave function. These are supported by tori for which $\sum_i \oint k_i dq_i$ is quantized, where now the integral is taken around a complete set of independent closed contours on the torus, giving again one quantum number for each degree of freedom. This is Einstein-Brillouin-Keller quantization, which is described again in Sec. II. Since the classical ray motion is not always integrable, this paper also deals briefly with the nonintegrable case in Sec. V.

II. REVIEW AND CRITIQUE OF EXISTING THEORY

In this section we establish notation, review parts of existing theory which will be of use to us later, and provide a critique of this theory, especially in regard to the problem of Bohr-Sommerfeld quantization. We also provide a discussion of such issues as monopole strings, which seems to be new in the context of multicomponent WKB theory. We begin with the case of a scalar wave equation.

Let the scalar wave field be $\psi(x)$, where $x = (x_1, \ldots, x_N)$. Usually we will not attempt to distinguish notationally between the one-dimensional case ($N = 1$) and that of higher dimensions, since usually the required placement of indices will be obvious. We let the wave equation be $\hat{D}\psi = 0$, where $\hat{D}$ is the wave operator, regarded as being composed of the operators $\hat{x} = $ (multiplication by x) and $\hat{k} = -i\epsilon\partial/\partial x$. We assume that $\hat{D}$ is Hermitian. The formal ordering parameter ϵ is the expansion parameter of the WKB expansion. We use carets to denote operators, and especially to distinguish them from their classical counterparts or "symbols" (see Appendix A). We denote the x-space kernel of the operator $\hat{D}$ by $K_D(x,y)$, so that the wave equation can be written

$$\int dy\, K_D(x,y)\psi(y) = 0 , \qquad (2.1)$$

and so that in Dirac bra-ket notation,

$$K_D(x,y) = \langle x | \hat{D} | y \rangle . \qquad (2.2)$$

The wave equation may be either a differential or integral equation; if it is a differential equation, then K_D contains derivatives of $\delta(x - y)$. If the wave equation contains the time or derivatives with respect to time, then we simply treat t as one of the x's. In quantum-mechanical applications, we obtain the usual formulas by replacing ϵ by $\hbar$, and k by the momentum p. In applications to classical wave fields, it is easiest to regard ϵ as a dimensionless parameter, giving physical results when $\epsilon = 1$, so that k is the usual wave vector. In quantization or normal mode problems, the operator $\hat{D}$ and its Weyl symbol $D(x,k)$ (see Appendix A) will contain a parameter such as energy or frequency; for example, in the ordinary Schrödinger equation, $D(x,p) = p^2/2m + V(x) - E$; and in application to plasma physics, $D(x,k)$ is often parametrized by ω, so that when $D(x,k;\omega) = 0$ is solved for ω, we obtain the local dispersion relation $\omega = \omega(x,k)$.

The WKB ansatz is $\psi(x) = A(x)e^{iS(x)/\epsilon}$, where $A(x)$ is the real and positive amplitude and $S(x)$ is the action. (The total WKB wave function is a sum of such terms, properly matched and phased.) The equations for the unknowns A and S are obtained by substituting this ansatz into the wave equation $\hat{D}\psi = 0$ and expanding in powers of ϵ. The lowest two orders of the expansion are the most interesting and analytically tractable, so most WKB treatments stop with these; we shall follow this custom in this paper, and always neglect terms of relative order ϵ^2 and higher. If the wave equation is a differential equation, then the expansion can be carried out directly; but for general wave equations, an approach based on the Weyl transform is convenient (see Appendix A). In terms of the Weyl symbol $D(x,k)$ of the wave operator $\hat{D}$, the equation for $S(x)$ is the Hamilton-Jacobi equation, $D(x,k) = 0$, where we set $k = k(x) = \partial S(x)/\partial x$ in the argument of D. The equation for $A(x)$ is the amplitude transport equation,

$$\frac{\partial}{\partial x_i} \left[[A(x)]^2 \frac{\partial D(x,k)}{\partial k_i} \right] = 0 , \qquad (2.3)$$

where we use Latin indices $i,j,\ldots$ to run over $1,\ldots,N$ and where again $k = \partial S/\partial x$ in D. We sum over repeated indices, with an important exception to be noted later.

There are three methods of solving the Hamilton-Jacobi equation for the action $S(x)$ that will be of concern to us. One of these is separation of variables; the second is integrating along characteristics; and the third method obtains the action $S(x)$ from the knowledge of a complete set of conserved quantities $A_1(x,k),\ldots,A_N(x,k)$ in involution, i.e., functions that commute with one another and with $D(x,k)$ under the (x,k) Poisson bracket. We will call the third method the "Liouville method," since it is based on one of the theorems of Liouville [18]. The second and third methods will be of special interest to us because they are easily generalized to noncanonical coordinates in phase space.

The solutions $S(x)$ of the Hamilton-Jacobi equation are best viewed geometrically in terms of Lagrangian manifolds [19,20] in phase space. A Lagrangian manifold is an N-dimensional surface in the $2N$-dimensional phase space which, when written in the form $k = k(x)$, is expressed in terms of a curl-free wave vector, i.e., a vector field $k(x)$ satisfying $\partial k_i/\partial x_j = \partial k_j/\partial x_i$; equivalently, it is a surface upon which the canonical symplectic 2-form $dk \wedge dx$ vanishes. Given a Lagrangian manifold, we can construct a corresponding action function by integrating $S(x) = \int k(x)dx$. In view of the curl-free condition on $k(x)$, the value of the action is independent of the path of integration, which need not be a ray, i.e, an orbit of the Hamiltonian $D(x,k)$. If, furthermore, the Lagrangian manifold is a subset of the $(2N-1)$-dimensional surface $D(x,k) = 0$, which we will call the "dispersion surface," then the function $S(x)$ satisfies the Hamilton-Jacobi equation. Conversely, every solution of the Hamilton-Jacobi equation is associated with a Lagrangian manifold imbedded in the dispersion surface. In the Liouville method for solving the Hamilton-Jacobi equation, the simultaneous contour surface or level set of the A's is automatically a Lagrangian manifold, as a consequence of the A's being in involution; and by varying the contour values, the Lagrangian manifold can be made to lie within the dispersion surface, thereby giving a solution of the Hamilton-Jacobi equation.

If the Lagrangian manifold is topologically nontrivial (typically a cylinder or a torus), then single valuedness of the wave function requires that the actions be quantized, i.e., that

$$J_i = \frac{1}{2\pi} \oint_{\Gamma_i} k \, dx = n_i + m_i/4 , \qquad (2.4)$$

where Γ_i is a closed contour on the Lagrangian manifold, n_i is the corresponding quantum number, and m_i is the Maslov index [20,21], an even integer. A Lagrangian manifold satisfying this condition will be referred to as a quantized Lagrangian manifold. When the Lagrangian manifolds lying in the dispersion surface are topologically nontrivial, then the only ones that are acceptable for solutions of the Hamilton-Jacobi equation are those that are quantized; but unless the parameter (energy or frequency) of $D(x,k)$ is appropriately chosen, such quantized Lagrangian manifolds lying in the dispersion surface generally will not exist. By varying the parameter, however, the dispersion surface itself is varied, and solutions can be found. The values of the parameter for which this occurs are the eigenenergies or eigenfrequencies. This is the modern form of the Bohr-Sommerfeld quantization rule for scalar wave fields, otherwise known as Einstein-Brillouin-Keller or torus quantization; it can be stated somewhat more simply for the Schrödinger equation, for which the parameter E enters into $D(x,p)$ in a sample way, due to the fact that the time-dependent version of the Schrödinger equation is first order in time.

Consider now a multicomponent wave field $\psi_\alpha(x)$, satisfying the wave equation

$$\hat{D}_{\alpha\beta}\psi_\beta = 0 . \qquad (2.5)$$

We use Greek indices $\alpha,\beta = 1,\ldots,M$, which we call "spinor indices," to index the components of the wave field; $\hat{D}_{\alpha\beta}$ represents a component of the $M \times M$ matrix $\hat{D}$

of "orbital" operators, i.e., functions of $\hat{x}$ and $\hat{k}$. We assume $\hat{D}$ is Hermitian, $(\hat{D}_{\alpha\beta})^\dagger = \hat{D}_{\beta\alpha}$. The multicomponent WKB ansatz is

$$\psi_\alpha(x) = A_\alpha(x)e^{iS(x)/\epsilon} , \qquad (2.6)$$

where the amplitude $A_\alpha(x)$ is now a spinor with generally complex components. The derivation of the WKB equations is now more difficult than in the scalar case, but can be worked out with the help of the Weyl correspondence and variational principles [1,2,12,22].

The results are the following. At lowest order in ϵ we have

$$D_{\alpha\beta}(x,k)A_\beta(x) = 0 , \qquad (2.7)$$

where $D_{\alpha\beta}(x,k)$ is a component of the $M \times M$ matrix $\mathbf{D}(x,k)$ of Weyl symbols of the operator matrix $\hat{D}$. The symbol matrix $D_{\alpha\beta}(x,k)$, which we call the "dispersion matrix," is itself Hermitian, $D_{\alpha\beta}(x,k)^* = D_{\beta\alpha}(x,k)$. As in the scalar case, k is to be replaced by $\partial S/\partial x$ inside $D_{\alpha\beta}$, so Eq. (2.7) is a simultaneous equation for $S(x)$ and $A_\alpha(x)$.

We denote the eigenvalues of $D_{\alpha\beta}(x,k)$ by $\lambda_0^{(\mu)}(x,k)$, where $\mu = 1, \ldots, M$ is a "polarization index," and where the subscript 0 will be explained later. We place polarization indices in parentheses to distinguish them from component indices of spinors. The dispersion matrix may have degeneracies at some points of phase space; we will refer to these as "mode-conversion points" (not exactly the same terminology used by other authors). The set of mode-conversion points forms a surface in phase space whose dimensionality follows definite rules, depending on the symmetry properties of the dispersion matrix. For example, if the dispersion matrix is a general complex Hermitian matrix with no particular symmetries, then the mode-conversion points typically form a surface of codimension 3 in phase space. We will assume that the eigenvalues $\lambda_0^{(\mu)}(x,k)$ are distinct and sufficiently well separated (in a sense to be made more precise later) over some region of interest in the (x,k) phase space, i.e., that our region of interest is sufficiently far away from any mode-conversion point. This is a major simplifying assumption of this paper. Typically, a "region of interest" is a Lagrangian manifold or a family of Lagrangian manifolds, representing physical solutions of the wave equation.

Equation (2.7) can be converted into an equation purely in S by noting that it can be satisfied for nonzero $A_\alpha(x)$ only if at least one of the eigenvalues of D vanishes. By our assumptions, at most one eigenvalue can vanish at a time within the region of interest in phase space; choosing one of these, we have a Hamiltonian Jacobi equation for S.

$$\lambda_0^{(\mu)}(x,k) = 0 , \qquad (2.8)$$

where again we set $k = \partial S(x)/\partial x$. Thus there is a different Hamilton-Jacobi equation for each polarization, as well as a different dispersion surface and a different action $S(x)$, which might with greater clarity be written $S^{(\mu)}(x)$. The eigenvalue $\lambda_0^{(\mu)}(x,k)$ serves as the ray Hamiltonian for polarization μ.

We denote the eigenvectors of $D_{\alpha\beta}(x,k)$ by $\tau_\alpha^{(\mu)}(x,k)$, so that

$$D_{\alpha\beta}(x,k)\tau_\beta^{(\mu)}(x,k) = \lambda_0^{(\mu)}(x,k)\tau_\alpha^{(\mu)}(x,k) . \qquad (2.9)$$

This equation illustrates a convenient rule, which we follow throughout this paper, of *not* assuming an implicit summation on any index (such as μ above) that appears anywhere in an equation as a polarization index. Equation (2.9) defines a field of eigenvectors over all of phase space, although the major subset of phase space of physical importance is the dispersion surface, upon which the right-hand side vanishes. The eigenvectors $\tau^{(\mu)}$ are assumed to be orthonormal and complete,

$$\tau_\alpha^{(\mu)*}\tau_\alpha^{(\nu)} = \delta_{\mu\nu}, \quad \sum_\mu \tau_\alpha^{(\mu)}\tau_\beta^{(\mu)*} = \delta_{\alpha\beta} . \qquad (2.10)$$

The phase conventions for the eigenvectors are chosen in an arbitrary but smooth manner, insofar as possible, over phase space. A change in the phase convention is given by a scalar field $\theta(x,k)$, specifying the new eigenvectors in terms of the old,

$$\tau(x,k) \rightarrow e^{i\theta(x,k)}\tau(x,k) . \qquad (2.11)$$

Here and frequently below, we drop the polarization index (μ) in an equation referring to a single polarization; note, however, that both θ and τ depend on (μ). Equation (2.11) is a gauge transformation in the sense of Berry's theory [6] of adiabatic processes in quantum mechanics, in which the eigenvector τ plays the role of the adiabatically transported quantum state, $D_{\alpha\beta}$ plays the role of the Hamiltonian with slowly varying parameters, and the (x,k) phase space plays the role of the parameter space. We will refer to various quantities as being gauge invariant or gauge dependent, depending on their transformation properties under Eq. (2.11); for example, the eigenvector τ itself is gauge dependent.

For topological reasons, it is in general not possible to find a phase convention for $\tau(x,k)$ that is smooth over all of phase space. For example, if $D_{\alpha\beta}$ is a complex Hermitian matrix with no particular symmetry, then one may expect to find a surface of codimension 2 in phase space upon which τ becomes discontinuous, due to its overall phase. This surface typically also of codimension 2 within a particular dispersion surface, and joins up somewhere with the codimension 3 surface of mode conversion points. The surface upon which τ becomes singular has the same mathematical structure as the string of a monopole, so we will call this surface the "monopole string." Facts like these are widely appreciated in the literature on Berry's phase [8–11] but seem not to have been applied to the asymptotic behavior of multicomponent wave fields. Strings are important in the construction of electron wave functions in the presence of a magnetic monopole [23], for which the gauge transformations are ordinary gauge transformations on the magnetic vector potential. The monopole string forces one to use at least two different gauges in constructing the wave function; as we will show in Sec. IV, completely analogous situations arise in the multicomponent WKB problem.

If S satisfies the Hamilton-Jacobi equation (2.8), then the amplitude that satisfies Eq. (2.7) must be proportional to the eigenvector τ (all referring to a particular polarization μ). Thus we can write

$$A_\alpha(x) = B(x)e^{i\gamma(x)}\tau_\alpha(x,k) , \qquad (2.12)$$

where again $k = \partial S/\partial x$, and where the proportionality factor is decomposed into its real and positive amplitude $B(x)$ and its phase $\gamma(x)$. The phase $\gamma(x)$ has no analog in scalar WKB theory, for which, effectively, $\gamma = 0$. The equations for B and γ can be obtained from the $O(\epsilon)$ terms in the WKB expansion; that for B is the amplitude transport equation with λ_0 as Hamiltonian,

$$\frac{\partial}{\partial x_i}\left[B(x)^2\frac{\partial\lambda_0(x,k)}{\partial k_i}\right] = 0 , \qquad (2.13)$$

with $k = \partial S/\partial x$ in λ_0. Thus finding $S(x)$ and $B(x)$ given $\lambda_0(x,k)$ is exactly the same problem as finding the action and amplitude in scalar WKB theory.

As equation for the phase γ was derived by Bernstein and Friedland [1,2]. Their result was later expressed in terms of Poisson brackets by Kaufman, Ye, and Hui [22], who wrote it in the form

$$\frac{d\gamma}{dt} = i\tau_\alpha^*\{\tau_\alpha,\lambda_0\} + (i/2)D_{\alpha\beta}\{\tau_\alpha^*,\tau_\beta\} , \qquad (2.14)$$

where t is the parameter of the rays of λ_0 (t is not necessarily time), and where the curly bracket is the x-k Poisson bracket. This equation gives the rate of change of γ along a ray of the Hamiltonian λ_0, i.e., along the orbits given by Hamilton's equations,

$$\frac{dx}{dt} = \{x,\lambda_0\} = \frac{\partial\lambda_0}{\partial k} ,$$
$$\frac{dk}{dt} = \{k,\lambda_0\} = -\frac{\partial\lambda_0}{\partial x} . \qquad (2.15)$$

The rays of interest lie in the dispersion surface $\lambda_0(x,k) = 0$, and sweep out a Lagrangian manifold in that surface.

The first term in Eq. (2.14) can be written $\dot{\gamma}_B = i\tau_\alpha^*\dot{\tau}_\alpha = i\tau^\dagger\dot{\tau}$, so the contribution of this term to γ is

$$\gamma_B = i\int\tau^\dagger d\tau , \qquad (2.16)$$

where the B stands for "Berry." This term is an example of Berry's phase, as first noted by Yabana and Horiuchi [7]. The properties of γ_B are just as in the standard theory of Berry's phase, with phase space identified as the parameter space. For example, the integrand of Eq. (2.16) can be regarded as a differential 1-form in phase space,

$$i\tau^\dagger d\tau = i\tau^\dagger\left[\frac{\partial\tau}{\partial x_j}dx_j + \frac{\partial\tau}{\partial k_j}dk_j\right] = i\tau^\dagger\frac{\partial\tau}{\partial z_a}dz_a , \qquad (2.17)$$

where $z = (x,k)$ and where Latin indices $a,b,\ldots$ are reserved for phase-space coordinates and run over $1,\ldots,2N$. An interesting feature of this manifestation of Berry's phase is that the path through parameter space along which the adiabatic transport takes place is actual-

ly an orbit of the Hamiltonian λ_0. As expected, Berry's phase is not gauge invariant, but rather transforms according to

$$\gamma_B \rightarrow \gamma_B - \theta , \qquad (2.18)$$

so that the product $\tau e^{i\gamma_B}$ is overall gauge invariant.

The second term of Eq. (2.14) has no name, so we write $\dot{\gamma}_2$ for it. This term can be integrated along orbits just as well as the Berry's-phase term, but the result cannot be represented as a line integral of a differential form. Thus the phase γ_2 is not "geometrical" in the same sense as Berry's phase; for example, it depends not only on the path through phase space, but also on the rate at which the path is traversed. The second term is, however, gauge invariant, in spite of the fact that it is represented in terms of the gauge-dependent eigenvector τ; for under the gauge transformation (2.11), the second term transforms according to

$$\dot{\gamma}_2 \rightarrow \dot{\gamma}_2 + \tfrac{1}{2}D_{\alpha\beta}(\tau_\alpha^*\{\theta,\tau_\beta\} - \tau_\beta\{\tau_\alpha^*,\theta\})$$
$$= \dot{\gamma}_2 + \tfrac{1}{2}\lambda_0(\tau_\alpha^*\{\theta,\tau_\alpha\} - \tau_\alpha\{\tau_\alpha^*,\theta\})$$
$$= \dot{\gamma}_2 - \tfrac{1}{2}\lambda_0\{\tau^\dagger,\tau,\theta\} = \dot{\gamma}_2 \qquad (2.19)$$

since τ is normalized. (Here we use the algebra of Poisson brackets, e.g., $\{fg,h\} = f\{g,h\} + \{f,h\}g$, etc.) Thus, in Eq. (2.12), all the gauge dependence on the right-hand side cancels out, and $A_\alpha(x)$ is gauge invariant, as it should be.

The development of the multicomponent WKB problem up to this point is complete in the sense that the amplitude and total phase of the wave $\psi_\alpha(x)$ can be determined by integrating along rays, assuming suitable initial conditions have been given. Nevertheless, it presents certain difficulties when the Bohr-Sommerfeld quantization problem is considered. These are least severe in the one-dimensional case, which we consider first.

Suppose the dispersion surface $\lambda_0(x,k) = 0$ is a closed curve in the two-dimensional (x,k) phase plane, which can be varied by varying the parameter (energy or frequency) of λ_0. The dispersion surface coincides with an orbit of λ_0, and is also a Lagrangian manifold. Therefore we have $S(x) = \int k(x)dx$ along the orbit in the usual way for one-dimensional WKB problems. The wave function will be single valued on going around the orbit if the total phase, including S, γ, and the Maslov phase is is an integer multiple of 2π. The phase S is the x-k area of the orbit, and the Maslov phase is (usually) π. The phase $\gamma = \gamma_B + \gamma_2$ is of the same order as the Maslov phase and presumably will affect the quantization condition in the same way as the Maslov phase, i.e., by a shift in the quantized value of the action by a fraction of an integer. (This presumption is verified in a numerical study by Yabana and Horiuchi [7].) The Berry's-phase contribution to γ is the net accumulated phase due to parallel transport of the polarization vector τ around the orbit, and can be interpreted as the net "angle flux" intercepted by the orbit. The sum of S and γ_B can be regarded as the total area of the orbit, if we use a modified rule for computing the area. That is, if we write $\Omega_c = dk\wedge dx$ for the usual,

canonical symplectic 2-form on phase space, and $\Omega_B = id\tau_\alpha^* \wedge d\tau_\alpha$ for Berry's 2-form, then we have

$$S + \epsilon\gamma_B = \int_{\text{orbit}} \Omega_c + \epsilon\Omega_B , \qquad (2.20)$$

representing the area of the orbit with respect to the modified 2-form $\Omega_c + \epsilon\Omega_B$.

The idea of including Berry's 2-form in the symplectic form on phase space is an appealing one, but it is applied only selectively. That is, although the area of the orbit is computed in Eq. (2.20) by using the total 2-form, equations of motion of the orbit itself, Eqs. (2.15), use only the standard canonical structure. Furthermore, in the case of higher dimensions, we must find Lagrangian manifolds in order to solve the Hamilton-Jacobi equation, Eq. (2.8). A Lagrangian manifold is one upon which the symplectic form vanishes, but in Eq. (2.8), it will be only the canonical form which vanishes, not the total 2-form of Eq. (2.20). (This is not an issue in the one-dimensional problem, for which all curves in the phase space are Lagrangian manifolds.) Therefore one must say that the idea of using the total 2-form of Eq. (2.20) is not one that seems to lead to particular elegance or symmetry. In any case, there is still the phase γ_2, which cannot be interpreted in terms of a modified rule for computing the symplectic area.

This is not to say that one cannot select out the quantized orbits in a one-dimensional problem by demanding single valuedness of the wave function; indeed, this has been done by Yabana and Horiuchi. It is merely to say that the quantization rule is less appealing and less tractable than in the case of scalar WKB theory.

Things get worse for the higher-dimensional case, however. To be specific, suppose we find that the solutions of the Hamilton-Jacobi equation (2.8) in a multidimensional problem are tori. What then are the conditions to be imposed to qualify certain of these tori as "quantized?" Of all the contributions to the total phase of the wave function, the action S and the Maslov phases are exactly as in scalar WKB theory. In particular, S is given by the integral $\int k\, dx$ along a contour on the torus; although S might be constructed initially by integrating $k\, dx$ along the rays of the Hamiltonian λ_0, nevertheless the contour can actually be taken along any path on the torus since the torus is a Lagrangian manifold. This fact is important when the Hamilton-Jacobi equation is solved by separation of variables or by the Liouville method because the Hamiltonian flows generated by the conserved quantities give rise to contours on the torus that are independent of the orbits of the Hamiltonian in the Hamilton-Jacobi equation. It is often desirable to integrate $k\, dx$ along these alternative contours. Furthermore, the Lagrangian property of the torus implies that the action integrals of Eq. (2.4) are invariant with respect to continuous deformations of the contours Γ_i, so that the net phase shift due to S on going around the torus does not depend on where on the torus the contour is located (see Fig. 1). This is an important consistency relation in scalar WKB theory, guaranteeing that a torus will satisfy the quantization condition as a whole, and not just at one location on the torus.
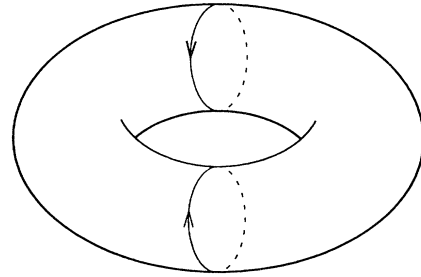

FIG. 1. The phase increment due to the action S on going around a Lagrangian torus is invariant when the path is continuously deformed. Thus the two closed paths in the figure give the same phase increment. This fact is important in establishing the consistency of torus quantization for scalar wave fields.

In multicomponent WKB theory, however, we also have to include the phase $\gamma = \gamma_B + \gamma_2$. Although the Berry's phase γ_B can be represented in terms of a line integral, we cannot expect the result to be independent of path on the torus, since the torus is a Lagrangian manifold only with respect to the canonical symplectic form Ω_c, not with respect to Berry's 2-form Ω_B. The situation in regard to γ_2 is even worse, since it cannot even be represented as a line integral. Thinking along these lines, we begin to doubt whether it is even possible to make a consistent definition of a quantized torus when the phase γ is included, in spite of the obvious fact that the original wave equation does possess eigenfunctions and eigenvalues. It seems that problems of this sort prevented Berk and Pfirsch [12] and Yabana and Horiuchi [7] from formulating a satisfactory quantization condition in the multidimensional case.

We turn now to a reformulation of the multicomponent WKB problem, which circumvents these difficulties, and allows us to formulate the desired quantization condition in a clear and general manner. As we will show, it also has several other advantages.

III. DIAGONALIZING THE MATRIX OF WAVE OPERATORS

In this section we pursue an idea going back at least to Clemmow and Heading [13] of diagonalizing the matrix $\hat{D}$ of orbital wave operators. The techniques we use for this procedure, such as introducing a linear transformation on the wave field and using the Weyl calculus for the analysis, are closely patterned on the work of Friedland and Kaufman [15]. Indeed, the work of Friedland and Kaufman is more general than our analysis here, in that they considered the problem of mode conversion. The main difference between their approach and the one we take here is that they did not quite diagonalize the matrix of wave operators; instead, they diagonalized only the dispersion matrix, recovering the formulas discussed in Sec. II.

We begin by introducing a new matrix $\hat{U}$ of orbital operators, and a new wave field $\phi_\mu(x)$ defined by

$$\psi_\alpha = \hat{U}_{\alpha\mu}\phi_\mu . \qquad (3.1)$$

We require that $\hat{\mathbf{U}}$ be unitary and therefore invertible, so that

$$\hat{U}_{\alpha\mu}(\hat{U}_{\beta\mu})^{\dagger}=\delta_{\alpha\beta}, \quad (\hat{U}_{\alpha\mu})^{\dagger}\hat{U}_{\alpha\nu}=\delta_{\mu\nu} . \tag{3.2}$$

We also require that $\hat{\mathbf{U}}$ diagonalize $\hat{\mathbf{D}}$, i.e., that

$$\hat{\mathbf{U}}^{\dagger}\hat{\mathbf{D}}\hat{\mathbf{U}}=\hat{\mathbf{\Lambda}}=(\text{a diagonal matrix}) , \tag{3.3}$$

where $(\hat{\mathbf{U}}^{\dagger})_{\alpha\beta}=(\hat{U}_{\beta\alpha})^{\dagger}$. We write

$$\hat{\Lambda}_{\mu\nu}=\hat{\lambda}^{(\mu)}\delta_{\mu\nu} , \tag{3.4}$$

so that $\hat{\lambda}^{(\mu)}$ represents the orbital operators on the diagonal of $\hat{\Lambda}$. We also set $\phi^{(\mu)}=\phi_{\mu}$, so that the wave equation in diagonalized form is

$$\hat{\lambda}^{(\mu)}\phi^{(\mu)}=0 . \tag{3.5}$$

The diagonalization decouples the polarizations, and each individual polarization is described by a scalar wave equation. Thus the multicomponent problem is reduced to the scalar problem.

If such a $\hat{\mathbf{U}}$ can be found, then many advantages follow. First, since each polarization satisfies a scalar wave equation, all the results of scalar WKB theory follow immediately. This includes the standard scalar theory of Bohr-Sommerfeld quantization, so that all the difficulties discussed in Sec. II concerning multicomponent Bohr-Sommerfeld quantization are at once circumvented. Other important results of scalar theory can now be transcribed to the multicomponent case, such as Van Vleck formulas for Green's functions [24], periodic-orbit representations for densities of states [25], and wave-packet techniques [26]. It seems that periodic-orbit expansions have not previously been considered for multicomponent wave fields; we will comment on them further in Sec. V. Furthermore, the diagonalized operators $\hat{\lambda}^{(\mu)}$ need not necessarily be treated by WKB theory; for example, if caustics or wave chaos makes the WKB analysis of Eq. (3.5) difficult, it may be possible to solve the wave equation directly. This is the approach commonly taken in the Born-Oppenheimer approximation, which is closely related to the methods described here, and which we will say more about in Sec. V.

We find the desired matrix of operators $\hat{\mathbf{U}}$ by finding its corresponding matrix $\mathbf{U}(x,k)$ of Weyl symbols. We begin by deriving the condition on the symbol matrix that the corresponding operator matrix should be unitary. We do this by applying the Moyal formula, Eq. (A3), to the second of Eqs. (3.2). We assume that the symbol matrix $\mathbf{U}$ can be expanded in powers of ϵ,

$$\mathbf{U}(x,k)=\mathbf{U}_0(x,k)+\epsilon\mathbf{U}_1(x,k)+\cdots , \tag{3.6}$$

and we also expand the Moyal formula, as in Eq. (A4). This allows us to solve for $\mathbf{U}$ order by order.

The representation of $\mathbf{U}$ as a power series in ϵ, as shown in Eq. (3.6), is definitely an assumption, to be tested by the success or failure of the program. Actually, unitary operators often have symbols which are not slowly varying in phase space; this is the case for the time evolution operator in quantum mechanics. However, as shown by Friedland and Kaufman [15], it turns out that the expansion of Eq. (3.6) is justified if we stay away from

mode-conversion points.

At zeroth order in ϵ, the expansion gives simply

$$\mathbf{U}_0^{\dagger}\mathbf{U}_0=\mathbf{I} , \tag{3.7}$$

so that $\mathbf{U}_0(x,k)$ is a unitary matrix (or a field of unitary matrices over phase space). At first order, we find

$$\mathbf{U}_0^{\dagger}\mathbf{U}_1+\mathbf{U}_1^{\dagger}\mathbf{U}_0+(i/2)\{\mathbf{U}_0^{\dagger},\mathbf{U}_0\}=0 , \tag{3.8}$$

where, when we write $\{\mathbf{A},\mathbf{B}\}$, we mean the matrix whose $\alpha\beta$ component is given by $\{A_{\alpha\nu},B_{\nu\beta}\}$. Thus the rule is that the positioning of the matrices determines the distribution of indices, exactly as in matrix multiplication. For matrices, it is not true that $\{\mathbf{A},\mathbf{B}\}=-\{\mathbf{B},\mathbf{A}\}$. We now solve Eq. (3.8) for $\mathbf{U}_1$, by first writing

$$\mathbf{U}_1=-i\mathbf{U}_0(\mathbf{G}+i\,\mathbf{A}) , \tag{3.9}$$

where both $\mathbf{G}$ and $\mathbf{A}$ are Hermitian, so that we have decomposed $i\mathbf{U}_0^{\dagger}\mathbf{U}_1$ into its Hermitian and anti-Hermitian parts. Substituting this into Eq. (3.8) and projecting out the Hermitian and anti-Hermitian parts, we find

$$\mathbf{A}=-(i/4)\{\mathbf{U}_0^{\dagger},\mathbf{U}_0\} , \tag{3.10}$$

but we find no condition at all on $\mathbf{G}$.

Altogether, the result is that if $\hat{\mathbf{U}}$ is a unitary matrix of orbital operators, then its symbol matrix, if it can be represented as a power series in ϵ, has the form

$$\mathbf{U}=\mathbf{U}_0[\mathbf{I}-i\epsilon(\mathbf{G}+\tfrac{1}{4}\{\mathbf{U}_0^{\dagger},\mathbf{U}_0\})+O(\epsilon^2)] , \tag{3.11}$$

where $\mathbf{U}_0$ is unitary and $\mathbf{G}$ is Hermitian. Neither $\mathbf{U}_0$ nor $\mathbf{G}$ is further determined by the requirement that $\hat{\mathbf{U}}$ be unitary. No new information is obtained by the unitarity condition on $\hat{\mathbf{U}}$ in the reverse order [the first of Eqs. (3.2)]. We find that the symbol matrix of a unitary matrix of operators is not itself unitary; it is unitary at lowest order, but the term represented by Eq. (3.10) spoils the unitarity of the symbol matrix at next order.

Next we require that $\hat{\mathbf{U}}$ diagonalize $\hat{\mathbf{D}}$, as in Eq. (3.3). This will determine both $\mathbf{U}_0$ and, in principle, $\mathbf{G}$. We assume that the symbol matrix $\mathbf{D}$ is not ordered in ϵ, but we still find it necessary to order the symbol matrix $\mathbf{\Lambda}$, which is diagonal like the operator matrix $\hat{\mathbf{\Lambda}}$ it represents. We write $\lambda^{(\mu)}(x,k)$ for the diagonal elements of $\mathbf{\Lambda}$, and order these according to $\mathbf{\Lambda}=\mathbf{\Lambda}_0+\epsilon\mathbf{\Lambda}_1+\cdots$, or

$$\lambda^{(\mu)}(x,k)=\lambda_0^{(\mu)}(x,k)+\epsilon\lambda_1^{(\mu)}(x,k)+\cdots . \tag{3.12}$$

The Moyal formula must be applied twice in transcribing Eq. (3.3) to symbols. At lowest order, we find

$$\mathbf{U}_0^{\dagger}\mathbf{D}\mathbf{U}_0=\mathbf{\Lambda}_0 , \tag{3.13}$$

so that $\mathbf{U}_0$ is a unitary matrix which diagonalizes $\mathbf{D}$, and so that the eigenvalues of $\mathbf{D}$ are $\lambda_0^{(\mu)}$. Thus the notation $\lambda_0^{(\mu)}$ has the same meaning here as in Sec. II. As for the eigenvectors $\tau_{\alpha}^{(\mu)}$ of $\mathbf{D}$, these are the columns of $\mathbf{U}_0$,

$$\tau_{\alpha}^{(\mu)}(x,k)=U_{0\alpha\mu}(x,k) . \tag{3.14}$$

At next order, we have

$$U_0^\dagger DU_1 + U_1^\dagger DU_0 + (i/2)\{U_0^\dagger, D\}U_0$$

$$+ (i/2)\{U_0^\dagger D, U_0\} = \Lambda_1 \ . \tag{3.15}$$

For subsequent steps we introduce some useful notation by placing presuperscripts before matrices when matrix multiplication does not take place from left to right. For example, if **A**, **B**, and **C** are matrices, we write $AB = {}^2B\,{}^1A$, $(ABC)^\dagger = {}^3A^\dagger\,{}^2B^\dagger\,{}^1C^\dagger$, etc. When matrices are used in Poisson brackets, we use the sequencing numbers to indicate the distribution of indices when an expression is transcribed to index notation. For example, $\{{}^1A, {}^3B\}{}^2C$ is the matrix whose $\alpha\beta$ component is $\{A_{\alpha\nu}, B_{\sigma\beta}\}C_{\nu\sigma}$; and $\{A, B\} = -\{{}^2B, {}^1A\}$. When sequencing numbers are not given, it is assumed that the sequence is left to right.

Using these rules, we transform the fourth term on the left-hand side of Eq. (3.15) as follows:

$$\{U_0^\dagger D, U_0\} = \{A_0 U_0^\dagger, U_0\} = A_0\{U_0^\dagger, U_0\} + {}^2U_0^\dagger\{{}^1A_0, {}^3U_0\} \ . \tag{3.16}$$

Similarly, the third term on the left-hand side of Eq. (3.15) can be rewritten

$$\{U_0^\dagger, D\}U_0 = \{U_0^\dagger, DU_0\} - {}^2D\{{}^1U_0^\dagger, {}^3U_0\}$$

$$= \{U_0^\dagger, U_0\}A_0 + \{{}^1U_0^\dagger, {}^3A_0\}{}^2U_0 - {}^2D\{{}^1U_0^\dagger, {}^3U_0\} \ . \tag{3.17}$$

The middle term on the right-hand side of this equation can also be written as $-U_0^\dagger\{U_0, A_0\}$, since $U_0^\dagger U_0 = I = \text{const}$. Finally, the first two terms in Eq. (3.15) are Hermitian conjugates; the first, for example, can be rewritten with the help of Eqs. (3.9) and (3.10):

$$U_0^\dagger DU_1 = -iA_0(G + \tfrac{1}{4}\{U_0^\dagger, U_0\}) \ . \tag{3.18}$$

Altogether, we have transformed Eq. (3.15) into

$$\left[\frac{i}{4}A_0\{U_0^\dagger, U_0\} - \frac{i}{2}U_0^\dagger\{U_0, A_0\} + \text{H.c.}\right]$$

$$-i[A_0, G] - \frac{i}{2}{}^2D\{{}^1U_0^\dagger, {}^3U_0\} = \Lambda_1 \ , \tag{3.19}$$

where the square brackets are the matrix commutator.

Next we demand that both sides of this equation be diagonal. The commutator vanishes on the diagonal,

$$-i[A_0, G]_{\mu\nu} = iG_{\mu\nu}(\lambda_0^{(\mu)} - \lambda_0^{(\nu)}) \ . \tag{3.20}$$

We see that Eq. (3.19) will only determine the off-diagonal elements of **G**. This makes sense, because the diagonal elements of **G** do nothing except to bring about an $O(\epsilon)$ gauge transformation on the eigenvectors. That is, if we replace U_0 by $U_0(I - i\epsilon G_{\text{diag}})$, then the effect is a rephasing of the μth column of U_0, i.e., the eigenvector $\tau^{(\mu)}$, by the phase factor $e^{-i\epsilon G_{\mu\mu}} \approx 1 - i\epsilon G_{\mu\mu}$ (no sum on μ). Therefore, without loss of generality, we can take the diagonal elements of **G** to be zero.

The corrections $\lambda_1^{(\mu)}$ to the symbols of the operators

$\hat{\lambda}^{(\mu)}$ are obtained from the diagonal elements of Eq. (3.19). Working out each of the terms, we find

$$\lambda_1 = -i\tau_\alpha^*\{\tau_\alpha, \lambda_0\} - (i/2)(D_{\alpha\beta} - \lambda_0\delta_{\alpha\beta})\{\tau_\alpha^*, \tau_\beta\} \ , \tag{3.21}$$

where λ_0, λ_1, and τ all refer to a single polarization μ. This equation is very similar to Eq. (2.14), the main difference being that here we have a correction to the Hamiltonian, whereas there we had a correction to the phase of the wave function. The analogy between the two equations would be even stronger if a term involving $\lambda_0\delta_{\alpha\beta}$ were inserted into Eq. (2.14); there would be no harm in doing this, since this term would vanish on the dispersion surface $\lambda_0 = 0$. We cannot, however, drop this term here, because it contributes to the equations of motion.

We find it convenient to split λ_1 into its two major terms, by writing $\lambda_1 = \lambda_{1B} + \lambda_{12}$. The first term is

$$\lambda_{1B} = -i\tau^\dagger\{\tau, \lambda_0\} \ , \tag{3.22}$$

where the B stands for "Berry"; this term is gauge dependent, transforming according to $\lambda_{1B} \to \lambda_{1B} + \{\theta, \lambda_0\}$. The second term is

$$\lambda_{12} = -(i/2)(D_{\alpha\beta} - \lambda_0\delta_{\alpha\beta})\{\tau_\alpha^*, \tau_\beta\} \ ; \tag{3.23}$$

it has no name and is gauge invariant. The gauge invariance of the part of λ_{12} involving $D_{\alpha\beta}$ was proven in Eq. (2.19), and the proof for the part involving $\lambda_0\delta_{\alpha\beta}$ is similar.

The off-diagonal elements of **G** are chosen so that the off-diagonal elements of Λ_1 in Eq. (3.19) will vanish. Thus our ability to diagonalize the wave operator at first order depends on our ability to solve for the off-diagonal elements of **G**. From Eq. (3.20), it is obvious that this cannot be done if **D** is degenerate, i.e., if $\lambda_0^{(\mu)} = \lambda_0^{(\nu)}$ for some $\mu \neq \nu$. The same is true if **D** is nearly degenerate, in the sense that two of its distinct eigenvalues should differ by an amount that is $O(\epsilon)$, for in that case the ordering scheme of Eq. (3.6) is invalidated. One can see that the situation here is closely reflected in degenerate perturbation theory in quantum mechanics. These points have been discussed more fully by Friedland and Kaufman [15]. In any case, we will always assume that **D** is far from degenerate. As for the matrix **G**, it turns out that we never need it at the order to which we are working; this is in accordance with usual ideas of WKB theory, for the correction terms U_1 can be thought of as $O(\epsilon)$ corrections to the amplitude, which are usually ignored in the simplest treatments.

We have therefore succeeded in diagonalizing the matrix of wave operators to the order to which we are working, in which Eq. (3.21) is a principal result. We now turn to WKB treatment of the diagonalized wave equations.

IV. WKB THEORY AND BOHR-SOMMERFELD QUANTIZATION

As mentioned earlier, it is not strictly necessary to use WKB theory to treat the diagonalized wave equations. That is, we have computed the symbol $\lambda = \lambda_0 + \epsilon\lambda_1$ of the

wave operator $\hat{\lambda}$; by using the Weyl calculus to turn the symbol back into its operator, we might consider solving the diagonalized wave equation (3.5) directly. Of course, there is still an approximation involved in this because we have truncated the expansion of the symbol; but a direct solution of the wave equation might be useful in order to avoid difficulties of WKB theory, such as caustics or chaotic rays.

Nevertheless, we will proceed in this section to use WKB theory to solve the diagonalized wave equation (3.5) and to convert the result back into an expression for the original wave field $\psi_\alpha(x)$. We will pay special attention to the Bohr-Sommerfeld quantization problem.

In principle, the approach is simple. The wave equation is $\hat{\lambda}\phi = 0$ (we drop the polarization indices as much as possible for the time being, it being understood that we are working with a definite polarization μ); to analyze this by WKB theory, we posit the usual scalar WKB ansatz

$$\phi(x) = B(x)e^{iS(x)/\epsilon} . \quad \text{(4.1)}$$

The symbol $\lambda(x,k) = \lambda_0(x,k) + \epsilon\lambda_1(x,k)$ is the ray Hamiltonian for the field $\phi(x)$; thus $S(x)$ satisfies the Hamilton-Jacobi equation

$$\lambda(x,k) = 0 , \quad \text{(4.2)}$$

and $B(x)$ satisfies the amplitude transport equation

$$\frac{\partial}{\partial x_i}\left[B(x)^2\frac{\partial\lambda(x,k)}{\partial k_i}\right] = 0 , \quad \text{(4.3)}$$

where in both equations k in λ is replaced by $k(x) = \partial S(x)/\partial x$. Note that $S(x)$ and $B(x)$ here differ from their counterparts in Sec. II in that the Hamilton-Jacobi and amplitude transport equations involve the full ray Hamiltonian $\lambda(x,k)$ and not just its lowest-order part $\lambda_0(x,k)$. For the same reason, the dispersion surface $\lambda(x,k) = 0$ in phase space is different, as are the Lagrangian manifolds imbedded in it.

Having found a solution $\phi(x)$ by these means, we must transform it back to the original physical wave field $\psi_\alpha(x)$, using Eq. (3.1). Since the components of $\hat{U}$ are orbital operators, we write Eq. (3.12) in the form

$$\psi_\alpha(x) = \int dy \langle x|\hat{U}_{\alpha\mu}|y\rangle\phi(y) . \quad \text{(4.4)}$$

Here we are assuming that only one polarization $\phi \equiv \phi^{(\mu)}$ is nonzero. We know the symbol of $\hat{U}_{\alpha\mu}$ to lowest order in ϵ; by Eqs. (3.6) and (3.14), it is simply $\tau_\alpha^{(\mu)}(x,k) \equiv \tau_\alpha(x,k)$. Using Eq. (A2) to express the x-space kernel of an operator in terms of its Weyl symbol, we have

$$\psi_\alpha(x) = \frac{1}{(2\pi\epsilon)^N}\int dy\, dk\, e^{ik(x-y)/\epsilon}$$

$$\times\tau_\alpha\left[\frac{x+y}{2},k\right]B(y)e^{iS(y)/\epsilon} . \quad \text{(4.5)}$$

Evaluating this by the stationary-phase approximation to lowest order, at which the correction terms to $U_{\alpha\mu} = \tau_\alpha$ are not needed, we find

$$\psi_\alpha(x) = \tau_\alpha(x,k)B(x)e^{iS(x)/\epsilon} + O(\epsilon) , \quad \text{(4.6)}$$

in which $k = \partial S/\partial x$ in τ. This is a simple result, which reproduces the multicomponent WKB ansatz of Sec. II and Eq. (2.12), but without the extra phase γ. One might say that γ has been absorbed into S by the change in the ray Hamiltonian and the consequent change in the equation which S must satisfy.

Let us now question how Eq. (4.6) changes under a gauge transformation. Certainly we demand $\psi_\alpha(x)$ to be gauge invariant, and we know how τ transforms [Eq. (2.11)]. Therefore if the right-hand side is to be gauge invariant overall, then the change in τ must be compensated by a change in S, i.e., S must transform according to $S(x) \rightarrow S(x) - \epsilon\theta(x,k)$, where $k = \partial S/\partial x$. We will give an explicit proof of this transformation law below. The gauge dependence of S is consistent with the fact that the ray Hamiltonian contains the gauge-dependent term λ_{1B}. In geometrical terms, the Lagrangian manifold that supports the solution $S(x)$ to the Hamilton-Jacobi equation will change when we do a gauge transformation, because the Hamiltonian itself and therefore the dispersion surface defined by it change. Since these objects are all gauge dependent, it is important to understand what the truly gauge-invariant geometrical constructions are in the classical phase space because only these can represent physical reality.

Similar considerations arise when we consider Bohr-Sommerfeld quantization. In a sense, Bohr-Sommerfeld quantization is straightforward; we simply look for the invariant tori of the total ray Hamiltonian $\lambda = \lambda_0 + \epsilon\lambda_1$, and then quantize the actions according to Eq. (2.4). But if the tori are not gauge invariant, then it is not clear how we can get a gauge-invariant quantization rule, as we expect.

In our analysis of this problem, we have gradually come to understand that the phase-space coordinates (x,k) themselves are, in a sense, gauge dependent, at least when they are used to describe the dynamics of a single polarization which has been decoupled from the others. These coordinates are not gauge dependent when used to describe the original wave field $\psi_\alpha(x)$ because in the original description, no gauge-dependent eigenvectors have been introduced yet. An example of what we mean by these statements is seen when we transform a physical wave operator such as $\hat{D}$ from the original matrix form to its diagonalized form, and express the latter in terms of symbols. In the original form, the wave operator $\hat{D}$ and its symbol matrix D are gauge invariant; but when $\hat{D}$ is diagonalized, the symbol λ of a diagonal element turns out to contain the gauge-dependent term λ_{1B}. We now understand this term to be, in a sense, a compensation for the intrinsic gauge dependence of the coordinates (x,k), when they are used to describe a single polarization. We have found a similar phenomenon when the original wave equation possesses conserved quantities, such as the angular momentum in certain quantum-mechanical applications. We will report on these calculations in detail in the future; for now we simply remark that a gauge-invariant conserved quantity such as angular momentum, represented by a wave operator, ends up having a symbol

whose expression in the (x,k) coordinates is gauge dependent, after the operator has been diagonalized like $\mathbf{D}$ in order to represent its effect within a single polarization.

We develop this point further by arguing for the concept of a covariant derivative. In order to simplify the following discussion, we assume for the time being that the eigenvectors τ depend only on the configuration space variables x (a common case in practice). The phase-space variable k is the symbol of the operator $-i\epsilon\partial/\partial x$, but $\partial/\partial x$ has different implications when acting on $\psi_\alpha(x)$ than when acting on $\phi(x)$. In the former case, there are no issues of gauge dependence; but in the latter there are. To see this, we write $\phi(x)=\tau_\alpha^*(x)\psi_\alpha(x)$, as follows from Eqs. (4.1) and (4.6), and we consider a small increment Δx. We have

$$\frac{\partial\phi}{\partial x}\Delta x=\tau_\alpha^*(x+\Delta x)\psi_\alpha(x+\Delta x)-\tau_\alpha^*(x)\psi_\alpha(x) . \quad (4.7)$$

This equation involves a comparison of τ at two neighboring spatial points x and $x+\Delta x$ at which differing phase conventions can be applied. Thus the operator $\partial/\partial x$ itself, when applied to ϕ, should be thought of as gauge dependent.

On the other hand, the theory of Berry's phase [14] gives rise to a concept of parallel transport of polarization vectors, which allows one to make an intrinsic comparison between polarization vectors at two neighboring spatial points. We let $\bar{\tau}(x+\Delta x)$ be the vector which is the parallel transport of τ from x to $x+\Delta x$; it can differ from $\tau(x+\Delta x)$ only by an infinitesimal phase factor

$$\bar{\tau}(x+\Delta x)=(1+i\Delta\gamma)\tau(x+\Delta x) . \quad (4.8)$$

Since the rule of parallel transport is $\tau^\dagger(x)\bar{\tau}(x+\Delta x)=1$, we have

$$\Delta\gamma=i\tau^\dagger\frac{\partial\tau}{\partial x}\Delta x . \quad (4.9)$$

In terms of the parallel transported vector, we define a covariant derivative operator D_x, whose action on $\phi=\tau_\alpha^*\psi_\alpha$ is given by

$$(D_x\phi)\Delta x=\bar{\tau}_\alpha^*(x+\Delta x)\psi_\alpha(x+\Delta x)-\tau_\alpha^*(x)\psi_\alpha(x) , \quad (4.10)$$

in analogy with Eq. (4.7). In contrast to $\partial/\partial x$, the operator D_x can be thought of as gauge invariant. By combining these results, we relate D_x to $\partial/\partial x$, finding

$$D_x=\frac{\partial}{\partial x}+\tau^\dagger\frac{\partial\tau}{\partial x} . \quad (4.11)$$

Now we multiply by $-i\epsilon$ and transcribe operators to symbols. This gives

$$k'=k-i\epsilon\tau^\dagger\frac{\partial\tau}{\partial x} , \quad (4.12)$$

where k' is the symbol for $-i\epsilon D_x$. Therefore the variable k', unlike k, may be thought of as gauge invariant.

Next we consider vectors τ, which depend on k as well as x, and repeat the analysis above. We find a new covariant derivative operator

$$D_k=\frac{\partial}{\partial k}+\tau^\dagger\frac{\partial\tau}{\partial k} , \quad (4.13)$$

and a new, gauge-invariant phase-space variable x',

$$x'=x+i\epsilon\tau^\dagger\frac{\partial\tau}{\partial k} , \quad (4.14)$$

which is the symbol of $+i\epsilon D_k$.

Combining Eqs. (4.12) and (4.14), we write

$$z_a'=z_a-i\epsilon\tau^\dagger\{\tau,z_a\} , \quad (4.15)$$

where $z=(x,k)$ and $z'=(x',k')$. We regard the primed variables z' as representing a new coordinate system in phase space; as we will show in several ways, these coordinates are to be thought of as intrinsically gauge invariant when describing the dynamics of a single polarization.

For example, let us express the ray Hamiltonian λ in terms of the primed coordinates. We transform the Hamiltonian as a scalar, writing $\lambda'(x',k')=\lambda(x,k)$. A correction term arises in the transformation of λ_0, for we have

$$\lambda_0(z)=\lambda_0(z'+i\epsilon\tau^\dagger\{\tau,z'\})$$

$$=\lambda_0(z')+i\epsilon\tau^\dagger\{\tau,\lambda_0\}$$

$$=\lambda_0(z')-\epsilon\lambda_{1B}(z') . \quad (4.16)$$

In the $O(\epsilon)$ term, we are of course free to replace z by z'. We see that the correction term from λ_0 exactly cancels the Berry's-phase term λ_{1B}, so that overall we have

$$\lambda'(z')=\lambda_0(z')+\epsilon\lambda_{12}(z') . \quad (4.17)$$

This is a pleasing result, for it shows that the ray Hamiltonian, properly expressed in terms of the gauge-invariant, primed coordinates, is given by a gauge-invariant expression. It was by looking for a transformation which would do this that we originally discovered the primed coordinates.

Similarly, when conserved quantities such as angular momentum, represented by symbols of operators acting on a single polarization, are expressed in terms of the primed coordinates, the resulting expressions become manifestly gauge invariant. The details of this will be presented in the future.

Gauge-dependent ray Hamiltonians much like λ arise in an important physical context, namely in the WKB treatment of the (scalar) Schrödinger equation for a charged particle in a magnetic field. Here the gauge transformations are the usual transformations $\mathbf{A}\rightarrow\mathbf{A}+\nabla g$ on the vector potential (we use bold face symbols for 3-vectors), and the Hamiltonian is just $(1/2m)(\mathbf{p}-e\mathbf{A}/c)^2$. We also know how the wave function must transform, namely $\psi(\mathbf{x})\rightarrow e^{ieg(\mathbf{x})/\hbar c}\psi(\mathbf{x})$, in order to represent a definite physical state. In WKB theory, we find a Lagrangian manifold imbedded in the energy shell (dispersion surface) $H=E$, and compute an action $S(\mathbf{x})=\int\mathbf{p}\cdot d\mathbf{x}$ in the usual way. If we now do a gauge transformation, then the Hamiltonian and the energy shell defined by it change accordingly. Therefore the Lagrangian manifold imbedded in it must change as well. More precisely, if the Lagrangian manifold is expressed in terms of the coordinates $(\mathbf{x},\mathbf{p})$ say by functions

$\mathbf{p} = \mathbf{p}(\mathbf{x})$, then this functional form must change under the gauge transformation, for the old Lagrangian manifold will in general not even be embedded in the new energy shell. [Equivalently, the old momentum field $\mathbf{p} = \mathbf{p}(\mathbf{x})$ will not satisfy the new Hamilton-Jacobi equation $H(\mathbf{x}, \mathbf{p}) = E$.]

The question therefore arises, how do we know when the new Lagrangian manifold in the new gauge represents the same physical state as the old Lagrangian manifold in the old gauge? The answer may be expressed in terms of the kinetic momentum $\mathbf{p}' = m\mathbf{v} = \mathbf{p} - e\mathbf{A}/c$, which is gauge invariant and directly measurable in a physical sense, unlike the canonical momentum $\mathbf{p}$. The variables $(\mathbf{x}, \mathbf{p}')$ are perfectly good coordinates in phase space, and a given Lagrangian manifold can be expressed in terms of them, say, by functions $\mathbf{p}' = \mathbf{p}'(\mathbf{x})$, even though these coordinates are noncanonical. Let us now suppose we have found a Lagrangian manifold by solving the Hamilton-Jacobi equation in some gauge, and let us express it in terms of the coordinates $(\mathbf{x}, \mathbf{p}')$ by functions $\mathbf{p}' = \mathbf{p}'(\mathbf{x})$. One can show, then, that if this expression is held fixed but the gauge is changed, then in the new canonical coordinates $(\mathbf{x}, \mathbf{p})$ the manifold is still Lagrangian and in fact satisfies the new Hamilton-Jacobi equation in the new gauge. Because of this property, it is reasonable to assume that any two Lagrangian manifolds in any two gauges will represent the same physical state if their expressions in the noncanonical but gauge-invariant coordinates $(\mathbf{x}, \mathbf{p}')$ are the same. In fact, one can show that if the expression for a Lagrangian manifold in the coordinates $(\mathbf{x}, \mathbf{p}')$ is held fixed, then under a gauge transformation the action $S(\mathbf{x})$ changes precisely in such a manner as to cause the WKB wave function to transform according to $\psi(\mathbf{x}) \to e^{ieg(\mathbf{x})/\hbar c}\psi(\mathbf{x})$ as required. We will not prove these statements because a closely related proof will be given below for the ray Hamiltonian λ and because they are physically reasonable anyway.

The coordinates $(\mathbf{x}, \mathbf{p}')$ constitute a prime example for the theory of noncanonical coordinates outlined in Appendix B. The Hamiltonian in these coordinates is $|\mathbf{p}'|^2/2m$ and is manifestly gauge invariant, and the variational form of the equations of motion is

$$\delta \int \left[\mathbf{p}' + \frac{e}{c}\mathbf{A}(\mathbf{x}) \right] \cdot d\mathbf{x} - \frac{|\mathbf{p}'|^2}{2m} dt = 0 . \tag{4.18}$$

The fundamental Poisson brackets are $\{x_i, x_j\} = 0$, $\{x_i, p_j'\} = \delta_{ij}$, and $\{p_i', p_j'\} = (e/c)\epsilon_{ijk} B_k$ where $\mathbf{B}$ is the magnetic field. Action integrals are computed by

$$J = \frac{1}{2\pi} \oint \left[\mathbf{p}' \cdot d\mathbf{x} + \frac{e}{c}\mathbf{A} \cdot d\mathbf{x} \right] , \tag{4.19}$$

involving the gauge-invariant magnetic flux in the second term.

Returning now to our multicomponent WKB problem, we will show that our coordinates $z' = (x', k')$ in Eq. (4.15) are noncanonical, very much like the coordinates $(\mathbf{x}, \mathbf{p}')$ above. We have already transformed the ray Hamiltonian to the primed coordinates and obtained Eq. (4.17); we will now transform the symplectic 1-form, as in Eq. (B4), and extract an exact differential, as in Eq. (B6).

If we write $\xi(z) = (k, 0)$ for the components of the symplectic 1-form in the canonical coordinates $z = (x, k)$, then we find

$$k\,dx = \xi_a(z)dz_a = \xi_a(z' + i\epsilon\tau^\dagger\{\tau, z'\})$$
$$\times [dz_a' + i\epsilon d(\tau^\dagger\{\tau, z_a'\})]$$
$$= \xi_a(z')dz_a' + i\epsilon\tau^\dagger\{\tau, z_b'\}\Omega_{ba}dz_a' + \epsilon\,dg , \tag{4.20}$$

where Ω is defined by Eq. (B8) and where

$$g(z) = i\tau^\dagger\{\tau, z_a\}\xi_a(z) = i\tau^\dagger\{\tau, x_j\}k_j = -i\tau^\dagger\frac{\partial\tau}{\partial k_j}k_j . \tag{4.21}$$

(In Appendix B we used contravariant and covariant indices to emphasize the tensorial character of various quantities under phase-space transformations; here for simplicity we use uniformly lower indices.) In Eq. (4.20), we can set $\Omega_{ab} = -\Gamma_{ab}$ [defined in Eq. (B13)], since the coordinates z are canonical. Again, we are free to write either z or z' in the $O(\epsilon)$ terms.

The middle term on the right-hand side of Eq. (4.20) can be simplified by writing

$$i\tau^\dagger\{\tau, z_b\}\Omega_{ba}dz_a = -i\tau^\dagger\frac{\partial\tau}{\partial z_c}\Gamma_{cb}\Gamma_{ba}dz_a$$
$$= i\tau^\dagger\frac{\partial\tau}{\partial z_a}dz_a = i\tau^\dagger d\tau ; \tag{4.22}$$

we see that it is Berry's differential 1-form. Therefore we can write $\xi_a(z)dz_a = \xi_a'(z')dz_a' + \epsilon\,dg$, where

$$\xi_a'(z') = \xi_a(z') + i\epsilon\tau^\dagger\frac{\partial\tau}{\partial z_a'} , \tag{4.23}$$

or, equivalently,

$$\xi_a'dz_a' = k'dx' + i\epsilon\tau^\dagger d\tau . \tag{4.24}$$

In the primed coordinates, the total symplectic 1-form contains the canonical expression $k'dx'$, plus Berry's 1-form as a correction. Thus action integrals can be computed in the primed coordinates according to

$$J = \frac{1}{2\pi} \oint (k'dx' + i\epsilon\tau^\dagger d\tau)$$
$$= \frac{1}{2\pi} \int_{\text{area}} (dk' \wedge dx' + i\epsilon d\tau^\dagger \wedge d\tau) ; \tag{4.25}$$

this gives a modified but gauge-invariant rule for computing areas in phase space, as suggested already in Eq. (2.20).

The exact differential $\epsilon\,dg$ does not affect the equations of motion, so we can write the variational principles for the equations of motion in the two coordinate systems z and z' as follows:

$$\delta \int k\,dx - [\lambda_0(z) - i\epsilon\tau^\dagger\{\tau, \lambda_0\} + \epsilon\lambda_{12}(z)]dt$$
$$= \delta \int (k'dx' + i\epsilon\tau^\dagger d\tau)$$
$$- [\lambda_0(z') + \epsilon\lambda_{12}(z')]dt = 0 . \tag{4.26}$$

Thus the effect of the coordinate transformation $z \rightarrow z'$ has been to shift the Berry's-phase term from the Hamiltonian into the symplectic 1-form. We feel that this is where it belongs, for with Berry's phase in this location, all physical computations involving the rays are manifestly gauge invariant. For example, the components of the symplectic 2-form are

$$\Omega'_{ab} = -\Gamma_{ab} + i\epsilon \left[\frac{\partial \tau^{\dagger}}{\partial z'_a} \frac{\partial \tau}{\partial z'_b} - \frac{\partial \tau^{\dagger}}{\partial z'_b} \frac{\partial \tau}{\partial z'_a} \right] ; \qquad (4.27)$$

the second term represents Berry's 2-form and is gauge invariant. By inverting the matrix Ω'_{ab} we obtain the fundamental Poisson brackets $J'_{ab} = \{z'_a, z'_b\}$, which are gauge invariant like Ω'_{ab}. Since both the fundamental Poisson brackets and the ray Hamiltonian $\lambda' = \lambda_0 + \epsilon \lambda_{12}$ are gauge invariant, so are the equations of motion $\dot{z}'_a = \{z'_a, \lambda'\}$. So also are the Poisson brackets of observables whose expressions in the primed coordinates are gauge invariant; as mentioned earlier, physically meaningful quantities such as angular momentum have such gauge-invariant expressions in the primed coordinates (but not in the unprimed ones). Incidentally, we recommend that when inverting Ω'_{ab} to get the fundamental Poisson brackets J'_{ab}, the inversion be carried out exactly, without truncating at $O(\epsilon)$; in this manner, important identities such as the Jacobi identity and various conservation laws will have an exact representation.

A word of warning is in order in Eq. (4.26), for there is apparently a shortcut in transferring the Berry's-phase term from the Hamiltonian to the symplectic 1-form, which, however, is incorrect. That is, if we write,

$$-\lambda_{1B} dt = i\epsilon \tau^{\dagger} \{\tau, \lambda_0\} dt = i\epsilon \tau^{\dagger} \frac{d\tau}{dt} dt = i\epsilon \tau^{\dagger} d\tau , \qquad (4.28)$$

then it appears that we have accomplished the transferral. The reason this is incorrect is that we have effectively used $\dot{z} = \{z, \lambda_0\}$ in the second equality; while these are the correct equations of motion (to lowest order), nevertheless it is not legitimate to use the result of a variational principle before the variation is carried out. In fact, in actually deriving Eq. (4.26), we have used only coordinate transformations and the addition of exact differentials to the phase-space Lagrangian, both of which are legitimate operations. Actually, it is a good thing that Eq. (4.28) is not correct, for it is a different result from that shown in Eq. (4.26). For, although Eq. (4.28) seems to cause the form of the phase-space Lagrangian to change into the desired form, it does not change the coordinates. When carried out to higher order in ϵ, a trick such as Eq. (4.28) does not even agree in form with the correct result.

Having established the importance of the noncanonical coordinates z', we now consider noncanonical methods for solving the Hamilton-Jacobi equation. We do not propose to transform the Hamilton-Jacobi equation or the action function $S(x)$ to noncanonical coordinates; while it seems that such a transformation could be defined, the result would be somewhat nonstandard, and for the most part does not seem to be needed anyway. Of course, for some purposes, such as the determination of

Bohr-Sommerfeld eigenvalues, we do not need $S(x)$, but only invariant Lagrangian tori which are imbedded in the dispersion surface. The actions of these tori must be quantized as in Eq. (2.4).

The Liouville method can be an effective way of finding invariant Lagrangian manifolds and is easily transcribed to noncanonical coordinates. Suppose, for example, we have found N conserved quantities $A_1, \ldots, A_N$ in involution, expressed as functions of z'. If A represents physically meaningful quantities, such as angular momentum, then the expressions of the A in terms of z' will be gauge invariant. The involution condition $\{A_i, A_j\} = 0$ is also gauge invariant in the coordinates z', as is the condition that they be conserved, $\{A_i, \lambda'\} = 0$. The level sets of A are the N-dimensional surfaces $A_i(z') = a_i$, where a are the contour values; these level sets are Lagrangian manifolds, and can be represented analytically by solving the equations $A_i(x', k') = a_i$ for k', giving $k' = k'(x', a)$. By varying a and possibly the parameter (such as frequency or energy) of the ray Hamiltonian $\lambda'(z')$, we can find Lagrangian manifolds lying within the dispersion surface. If these Lagrangian manifolds are topologically nontrivial, they must be quantized by computing the actions; by Eq. (4.25), the action integrals are gauge invariant and can be computed entirely within the coordinates z'. We have actually used this method in applications to particles with spin in quantum mechanics, as we shall explain in the future.

The Liouville method need not be used only for quantization, i.e., bound state, problems, but is also useful for unbound systems. For example, Green's functions are important in calculations involving antennas in the radiation of electromagnetic waves in plasmas, and their asymptotic behavior can be described in terms of Lagrangian manifolds in phase space, just like any other WKB wave function [24]. The Liouville method can be applied to Green's functions because the complete set of commuting observables whose level sets are the relevant Lagrangian manifolds is the set of the components of the initial position of a family of rays. Similar considerations apply in scattering problems, for which the complete set of commuting observables are the components of the initial momentum or wave vector, far from the scattering region.

Lagrangian manifolds can also be determined by integrating along orbits of the ray Hamiltonian. If this is done in the coordinates z', in which the equations of motion are gauge invariant, then a representation for the Lagrangian manifold in the primed coordinates, specifying a definite physical state, emerges automatically. In bound problems, the orbits are typically dense on their tori, and serve to define them; in unbound problems such as scattering problems, the integration of rays often begins from an initial surface, so that the rays sweep out the desired Lagrangian manifold inside the dispersion surface.

As for bound problems, the fact that tori can be found and represented by purely gauge-invariant means and the fact that the action integrals are also gauge invariant give us a Bohr-Sommerfeld quantization rule for multicomponent wave fields which applies in any number of spatial

dimensions, which is manifestly gauge invariant, and which has the same geometrical clarity as in the scalar case. The formulation of such a quantization rule was one of the major goals of this paper. Notice that, unlike the superficial incorporation of Berry's phase in the computation of areas in Eq. (2.20), here Berry's phase enters at a fundamental level. Not only are action integrals and symplectic areas computed with the inclusion of Berry's phase, but so are the equations of motion, through the extra terms in the symplectic 2-form and in the fundamental Poisson brackets. Furthermore, Lagrangian manifolds are manifolds upon which the total symplectic 2-form, shown in the second integral in Eq. (4.25) and including Berry's 2-form, vanishes. Therefore open integrals of the symplectic 1-form on the Lagrangian manifolds are invariant with respect to continuous deformations of path; one encounters none of the awkwardness discussed in Sec. II when attempting to construct a consistent quantization condition. Notice also that in order to compute the eigenvalues, it is never actually necessary to commit oneself to a particular gauge for $\tau(x,k)$. This is true even in the computation of action integrals, if Stoke's theorem is used as in Eq. (4.25).

For unbound problems where quantization is not an issue, especially when one wishes to integrate along rays, one might argue that all the present preoccupation with Berry's phase and noncanonical coordinates is unnecessary, and that it would be simpler just to use the ray and transport equations presented in Sec. II. Nevertheless, because unbound systems are often described by complete sets of commuting observables, and because physical observables are represented by gauge-dependent quantities in the canonical z coordinates, we feel that the considerations raised here are important not only for quantization problems, but also for unbound problems. A detailed development of these subjects is too substantial to go into here; we hope to deal with them more explicitly in the future.

Let us now consider the determination of wave functions, which requires the knowledge of the action $S(x)$. The action is intrinsically gauge dependent, so the calculation cannot be carried out exclusively in the coordinates z'. It is possible, however, to treat the calculation of $S(x)$ as a final, gauge-dependent step, superimposed on otherwise gauge-invariant procedures. For example, in the Liouville method, once the functions $k'=k'(x')$ are determined, they may be transformed by Eq. (4.15) into the functions $k=k(x)$, which will automatically represent a curl-free wave-vector field. One can then integrate immediately, obtaining $S(x)=\int k(x)dx$. Alternatively, when integrating along orbits in the z' coordinates, one can compute $S(x)$ by accumulating an integral

$$S(x)=\int_{z_0'}^{z'}(k'dx'+i\epsilon\tau^\dagger d\tau)+\epsilon[g(z')-g(z)], \qquad (4.29)$$

where z_0' and z' are, respectively, the initial and final points on the orbit.

In the computation of $S(x)$, by whatever means, it is necessary to choose a gauge for $\tau(x,k)$. This is a step that inevitably contains an arbitrary element, and which will therefore make all explicit formulas more obscure

and difficult to interpret. This is partly why we have developed the theory as far as possible with gauge-invariant constructions.

Furthermore, one may well encounter monopole strings when choosing a gauge. For example, if the wave field $\psi_\alpha(x)$ has two components, then the vectors $\tau_\alpha(x,k)$ can be modeled as two-component Pauli spinors. Quantum-mechanical rotation operators can be applied to these, showing that two-component, normalized eigenvectors τ, to within an overall phase, are represented by points on a sphere. This sphere is essentially the same as the Poincaré sphere, which is used for describing polarization states of light in optics. Of course, the original wave field need have nothing to do with spinors or quantum mechanics for this formalism to be useful. Spinor formalism of this kind is widely discussed in the literature on Berry's phase [8–11], but seems not to have been used much in applications in plasma physics. In any case, monopole strings arise because it is impossible to define a smooth phase convention for τ over the sphere; instead, there must be a singularity at at least one point on the sphere. This point can be thought of as the point where the monopole string, emanating from the center of the sphere, crosses the surface. The location of the string can be moved to any place on the sphere by a gauge transformation, but the string cannot be transformed away. Often when working in the northern hemisphere, it is convenient to choose a gauge which places the string at the south pole, and vice versa. One then has two gauges which overlap by extending each a small amount across the equator.

In the WKB treatment of the multicomponent wave field, a definite physical state will correspond to a definite Lagrangian manifold in the phase space. In N spatial dimensions, the Lagrangian manifold will be N dimensional, so that when computing the action $S(x)$, it will be necessary to choose phase conventions for $\tau(x,k)$ over the N-dimensional Lagrangian manifold. At each point of the Lagrangian manifold, the eigenvector τ will correspond to some point on the sphere discussed in the preceding paragraph, so that the WKB problem gives us a mapping from the N-dimensional Lagrangian manifold to the two-dimensional sphere. If this mapping should cover the entire sphere, which it is likely to do for large enough N, then the monopole string will be unavoidable in any gauge. It will then be necessary to use two or more choices of gauge, with overlap regions, to cover the Lagrangian manifold. The different actions $S(x)$ in the different gauges will have to agree in the overlap region, in the sense that if one action $S(x)$ in one gauge is properly transformed to the other gauge, then it will give the same action function $S(x)$ as already computed in the other gauge. The necessity of dealing with monopole strings is not limited to the formalism of this paper, but would also arise in the traditional formalism discussed in Sec. II.

Let us now give an explicit proof that the action $S(x)$ transforms according to $S \rightarrow S - \epsilon\theta$ under a gauge transformation, if the representation of the Lagrangian manifold in the coordinates z' is held fixed. This will also verify the claim made earlier, that a Lagrangian manifold

whose representation is fixed in the z' coordinates represents a definite physical state.

Let the Lagrangian manifold be represented by $k = k(x)$ in some gauge, and let this relation be $k' = k'(x')$ when transformed to the primed coordinates. The functional form of $k'(x')$ is held fixed during the gauge transformation, which means that the functional form of $k(x)$ must change. By Eqs. (4.12) and (4.14), we express $k(x)$ in terms of $k'(x')$, finding

$$k(x) = k'(x') + i\epsilon\tau^\dagger \left[\frac{\partial\tau}{\partial x} + \frac{\partial\tau}{\partial k}\frac{\partial k}{\partial x} \right] ; \qquad (4.30)$$

the term in the large parentheses can be thought of as the total derivative of τ with respect to x. From this it follows that $k(x)$ transforms according to

$$k(x) \rightarrow k(x) - \epsilon \left[\frac{\partial\theta}{\partial x} + \frac{\partial\theta}{\partial k}\frac{\partial k}{\partial x} \right], \qquad (4.31)$$

so that $S(x) = \int k(x)dx$ transforms according to

$$S(x) \rightarrow S(x) - \epsilon\theta(x, k(x)), \qquad (4.32)$$

as claimed.

Finally, we comment briefly on the amplitude transport equation, Eq. (4.3). Since the $O(\epsilon)$ corrections to the amplitude $B(x)$ are not needed at the order to which we are working, we are free to exchange primed and unprimed coordinates at will in Eq. (4.3). But if the gauge-invariant equations of motion in the primed coordinates have been used to find Lagrangian manifolds, then these coordinates may be preferable. For example, we can replace Eq. (4.3) by

$$\frac{\partial}{\partial x_i'}[B(x')^2\dot{x}_i'] = 0 , \qquad (4.33)$$

where $\dot{x}_i' = \{x_i', \lambda'\}$, so that the amplitude transport equation is manifestly gauge invariant and yet still has the form of a continuity equation for a conserved current. Thus all the standard techniques for solving for $B(x)$ can be applied.

When the Liouville method is used to find Lagrangian manifolds, another approach is possible. If the conserved quantities are $A_1, \ldots, A_N$, then it can be shown [24] that the amplitude $B(x)$ for the wave field $\phi(x)$ has the form

$$B(x) = |\det\{x_i, A_j\}|^{-1/2} . \qquad (4.34)$$

The point of this is that the amplitude is expressed in terms of Poisson brackets, so that if x is replaced by x', and if the A's are represented by gauge-invariant expressions in the primed coordinates (as they should be), then the entire expression for the amplitude is manifestly gauge invariant.

V. CONCLUDING REMARKS

One of the original motivations for this paper was to generalize the Gutzwiller trace formula [25] which seems to be understood at present only for scalar (spinless) particles, to the case of particles with spin. The Gutzwiller

trace formula expresses the density of states of a quantum-mechanical system as a sum over the periodic orbits of the corresponding classical system. Explicitly, it is

$$\rho(E) = \rho_0(E) + \frac{1}{\pi\hbar}\sum_j \frac{T_j\cos(S_j/\hbar - \mu_j\pi/2)}{|\det(\mathbf{M}_j - \mathbf{I})|^{1/2}} , \qquad (5.1)$$

where $\rho(E)$ is the density of states, $\rho_0(E)$ is the Fermi-Thomas approximation to the density of states, where j labels the classical periodic orbits, T_j is the period of the first repetition of the periodic orbit, $S = \oint p\,dx$ is the action of the periodic orbit, μ_j is its Maslov index [27], and $\mathbf{M}_j$ is the monodromy matrix in the surface of section. Periodic orbits for densities of states have proven useful in understanding shell structure in nuclear physics [28–31] but, without generalization to the case of spinning particles, have been unable to take into account the important spin-orbit effects in the dynamics of individual nucleons. Therefore we sought to generalize Eq. (5.1) to include spin-orbit effects.

In the course of doing this, we found the role of geometric phases in the asymptotic analysis of multicomponent wave fields to be a more compelling subject than our original goal. Indeed, once the other issues discussed in this paper are understood, the generalization of Eq. (5.1) to multicomponent wave fields becomes almost immediate. The total density of states is a sum over polarizations; and within each polarization, all computations can be carried out in the gauge-invariant coordinates z'. For example, the periodic orbits themselves are gauge-invariant because the equations of motion are; the actions S_j can be computed by Eq. (4.25); and the quantities $\det(\mathbf{M}_j - \mathbf{I})$ can be computed in any coordinates, canonical or otherwise. Therefore the entire trace formula for a single polarization is manifestly gauge invariant.

We have explored several examples of multicomponent wave fields and studied their quantization, as illustrations of the calculations of this paper. A simple case that occurs commonly in practice is one in which the eigenvectors τ depend only on x and are independent of k. Then the eigenvectors can be thought of as defined over configuration space, not phase space, as can also Berry's 1- and 2-forms. Also, the correction λ_{12} to the Hamiltonian vanishes, and x and x' are identical; the primed and unprimed coordinates differ only because k and k' are different. In this case, Berry's 2-form behaves mathematically exactly like a magnetic field, affecting the classical ray equations accordingly, and k and k' appear exactly like the canonical and kinetic momenta, respectively, in charged-particle motion in a magnetic field.

An example of this, which is useful for purposes of illustration, is the case of a spinning neutral particle, such as a neutron or sodium atom, in an inhomogeneous magnetic field. The quantum Hamiltonian is

$$H = \frac{\mathbf{p}^2}{2m} - \boldsymbol{\mu}\cdot\mathbf{B}(\mathbf{x}) , \qquad (5.2)$$

in which we assume the particle has spin $\frac{1}{2}$. Writing $\lambda'(\mathbf{x}, \mathbf{p}') = h(\mathbf{x}, \mathbf{p}') - E$ for the classical ray Hamiltonian in the gauge-invariant $(\mathbf{x}, \mathbf{p}')$ coordinates, we have

$$h(\mathbf{x},\mathbf{p}')=\frac{\mathbf{p}'^2}{2m}\mp\mu B(\mathbf{x}) \ , \tag{5.3}$$

where the $\mp$ sign indicates the choice of polarization. The correction to the Poisson bracket coming from Berry's phase is expressible in terms of a pseudo-magnetic-field $\mathbf{F}(x)$, defined by

$$\mathbf{F}(\mathbf{x})=\mp\hbar\left[\frac{1}{2}\mathbf{b}\left[\frac{\partial b_i}{\partial x_j}\frac{\partial b_j}{\partial x_i}-(\mathbf{\nabla}\cdot\mathbf{b})^2\right]\right.$$

$$\left.-\mathbf{b}\cdot\mathbf{\nabla}\mathbf{b}\cdot\mathbf{\nabla}\mathbf{b}+(\mathbf{\nabla}\cdot\mathbf{b})\mathbf{b}\cdot\mathbf{\nabla}\mathbf{b}\right] \ , \tag{5.4}$$

where $\mathbf{b}=\mathbf{B}/B$. This vector, when integrated over an area, is proportional to the solid angel swept out by $\mathbf{b}$ on going around the boundary of the area; its properties have previously been explored in connection with classical charged-particle motion in magnetic fields [32].

In terms of $\mathbf{F}$, the gauge-invariant Poisson bracket is

$$\{f,g\}=\frac{\partial f}{\partial\mathbf{x}}\cdot\frac{\partial g}{\partial\mathbf{p}'}-\frac{\partial f}{\partial\mathbf{p}'}\cdot\frac{\partial g}{\partial\mathbf{x}}+\mathbf{F}\cdot\left[\frac{\partial f}{\partial\mathbf{p}'}\times\frac{\partial g}{\partial\mathbf{p}'}\right] \ , \tag{5.5}$$

and the gauge-invariant equations of motion are

$$\dot{\mathbf{x}}=\mathbf{p}'/m, \quad \dot{\mathbf{p}}'=\pm\mu\nabla B+\mathbf{p}'\times\mathbf{F} \ . \tag{5.6}$$

The general problem of spinning particles in magnetic fields has been extensively studied as a paradigm of Berry's phase, and the results reported here will contain few surprises. However, as far as we know, the effect of the pseudo-magnetic-field $\mathbf{F}$ on the classical equations of motion has not been pointed out. The term involving $\mathbf{F}$ in the equations of motion is small, but it would have an effect on the semiclassical energy eigenvalues of the same order as the Maslov index. This term might be observable in the quantized behavior of particle motion in traps, if the magnetic field were sufficiently inhomogeneous.

Another example where the eigenvectors τ depend only on x is the Born-Oppenheimer approximation. Here the "spinor" indices refer to electronic quantum numbers, and the wave function $\psi_\alpha(x)$ is a nuclear wave function, with x being the nuclear coordinates. Actually, it is possible to distinguish two different approximation schemes which are given the Born-Oppenheimer label. In one of these (the original approximation of Born and Oppenheimer), both the vibrational and electronic quantum numbers are held at $O(1)$, while the small mass ratio m/M is scaled to zero (conveniently by holding the electron mass m fixed, while letting the nuclear mass M go to infinity). This version of the Born-Oppenheimer approximation does not precisely fit the analysis of this paper, for the nuclear wave functions do not have WKB form as $\epsilon\rightarrow0$, but rather have the form of a function of x/ϵ, where $\epsilon=(m/M)^{1/4}$. Nevertheless, the use of symbol calculus as in Sec. III to diagonalize the operator matrix is still applicable, and shows, for example, how the Born-Oppenheimer approximation could be generalized to include mass polarization terms, which would cause the eigenvector τ (the electronic eigenstate) to depend on both the nuclear coordinates and momenta. Another ver-

sion of the Born-Oppenheimer approximation is useful in scattering problems, or for dealing with highly excited vibrational states. In this case, one can treat the nuclear kinetic energy and the electronic quantum number as $O(1)$, and take $m/M\rightarrow0$. Now the nuclear wave function does behave as $e^{iS(x)/\epsilon}$ as $\epsilon\rightarrow0$, where now $\epsilon=(m/M)^{1/2}$.

Certainly the most interesting example of multicomponent quantization we have considered is our original problem of spin-orbit coupling. Space does not permit us to present all our calculations on this subject; instead, we will simply present some salient conclusions, and promise the details for the future. In the Pauli equation including the spin-orbit term $\mathbf{L}\cdot\mathbf{S}$, the spinor eigenvector depends on the orbital angular momentum $\mathbf{L}$. It is therefore a nontrivial spinor field over phase space, one which cannot be represented as a lift from configuration space. The correction term λ_{12} in the Hamiltonian does not vanish, and in fact is essential to get the right eigenvalues. The Berry's-phase term in the Hamiltonian in the unprimed coordinates $\lambda_{1B}(z)$ vanishes for this problem, and this fact led us originally to suppose that one would not need the noncanonical, primed coordinates. Later we realized that even in this case, the primed coordinates are essential for complete understanding, for, although Berry's 1-form vanishes when taken along the flow of the classical ray Hamiltonian, it does not vanish when taken along the flow of other conserved quantities, such as angular momentum.

The role of angular momentum is very interesting in this problem. Neither the orbital nor spin angular momentum of the multicomponent wave system can be expressed as a symbol in the phase space of a single polarization because they are not diagonalized by the same matrix $\hat{\mathbf{U}}$, which diagonalizes the Hamiltonian. Thus one cannot say what the orbital angular momentum is in the classical phase space. However, the total angular momentum $\mathbf{J}=\mathbf{L}+\mathbf{S}$ is representable in the classical phase space of a single polarization, and is conserved. In fact, the classical orbit lies in a plane perpendicular to $\mathbf{J}$, and H, J^2, and J_z form a convenient triplet of conserved quantities with which to apply the Liouville method.

The wave functions are also interesting. When the 3-torus in phase space is mapped onto the two-dimensional Poincaré sphere, the image is a one-dimensional line of constant latitude. Thus monopole strings can be avoided on any individual Lagrangian manifold. But when the whole family of states corresponding to all possible values of the magnetic quantum number are considered, then one encounters monopole strings and must use two gauges. Thus there are two different expressions for the wave functions, depending on the magnetic quantum number. These expressions reproduce the asymptotic behavior of the Clebsch-Gordan coefficients, in two different ways. Altogether the spin-orbit problem provides a rich and detailed example of the considerations raised in this paper, with many interesting surprises.

We also hope to apply some of these ideas to the propagation and quantization of electromagnetic waves in plasmas. We will report on these developments in the future.

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Note added. We would like to call the reader's attention to several references dealing with some of the same topics as this paper. In a series of papers, Kuratsuji and Iida [Prog. Theor. Phys. **74**, 439 (1985); Phys. Lett. **111A**, 220 (1985); Phys. Rev. Lett. **56**, 1003 (1986); Phys. Lett. B **184**, 242 (1987); and Phys. Rev. D **37**, 441 (1988)] have used path integrals to study coupled quantum systems, in which one (fast) subsystem is driven adiabatically by the other (slow) subsystem. They find that Berry's phase is naturally incorporated into the effective Lagrangian for the slow component, which appears in the phase of the path integral. These authors have taken semiclassical limits, and have emphasized the resulting modification of the classical symplectic form due to the incorporation of Berry's phase, much as in our Eq. (4.24). They have also stated a semiclassical quantization condition, which uses action integrals just as in our Eq. (4.25). Their derivation of this quantization condition is based on periodic-orbit sums as in the Gutzwiller trace formula; since they do not treat amplitude determinants in detail, their derivation as it stands is only valid for systems of one degree of freedom. But their results are, in fact, valid for systems of higher dimension, as is shown in detail in this paper. Kuratsuji and Iida do not explicitly compute or display the term λ_{12} shown in our Eq. (3.23), which is just as necessary as the Berry's-phase correction to the symplectic form to get the correct eigenvalues, but they do discuss some examples based on coherent states, in which the term λ_{12} seems to be hidden in the coherent-state version of the classical Hamiltonian. They also discuss the modified Poisson bracket, obtained by inverting the matrix of the symplectic form, as in our Appendix B. Work related to this paper is also reported by Karasev [Funct. Anal. Appl. **24**, 102 (1990)], who considers various ranges for both $\hbar$ and the adiabaticity parameter in coupled quantum systems. Karasev uses symbol matrices much as we do, and displays the $O(\hbar)$ corrections to the ray Hamiltonian, expressed in terms of projection operators. He also gives expressions for the wave functions as integrals over coherent states. Karasev's work is more mathematically rigorous than this paper or the other references we cite.

APPENDIX A: THE WEYL TRANSFORM

This appendix summarizes our conventions for the Weyl transform and gives the main formulas we use. We have found McDonald [33] to be a good reference for further details.

The Weyl transform maps operators into their corresponding "symbols," which are functions of (x,k), and which represent those operators just as the classical q and p represent the quantum operators $\hat{q}$ and $\hat{p}$. The symbol $A(x,k)$ of the operator $\hat{A}$ is given by

$$A(x,k)=\int ds\, e^{-iks/\epsilon}\left\langle x+\frac{s}{2}\left|\hat{A}\right|x-\frac{s}{2}\right\rangle , \tag{A1}$$

where ϵ is the same ordering parameter as in the main text. The unique inverse of the Weyl transform is given by

$$\langle x|\hat{A}|x'\rangle=\frac{1}{(2\pi\epsilon)^N}\int dk\, e^{ik(x-x')/\epsilon}A\left(\frac{x+x'}{2},k\right) . \tag{A2}$$

For example, the symbols of $\hat{x}$ and $\hat{k}$ are x and k, respectively. An important property of the Weyl correspondence is its reality: if the Weyl symbol of $\hat{A}$ is $A(x,k)$, then the Weyl symbol of $\hat{A}^\dagger$ is $A(x,k)^*$.

If $\hat{A},\hat{B},\hat{C}$ are operators $A(x,k),B(x,k),C(x,k)$ their symbols, and if $\hat{C}=\hat{A}\hat{B}$, then according to the Weyl product rule or Moyal formula [34]

$$C(x,k)=A(x,k)\exp\left[\frac{i\epsilon}{2}\left[\frac{\overleftarrow{\partial}}{\partial x}\frac{\overrightarrow{\partial}}{\partial k}-\frac{\overleftarrow{\partial}}{\partial k}\frac{\overrightarrow{\partial}}{\partial x}\right]\right]B(x,k) , \tag{A3}$$

where the arrows indicate the directions in which the operands of the partial differential operators lie. When the exponential is expanded, this formula becomes

$$C(x,k)=A(x,k)B(x,k)+\frac{i\epsilon}{2}\{A,B\}+O(\epsilon^2) , \tag{A4}$$

where $\{A,B\}$ is the (x,k) Poisson bracket. Similarly, the commutator relation $\hat{C}=[\hat{A},\hat{B}]$, when expressed in terms of symbols, becomes

$$C(x,k)=i\epsilon\{A,B\}+O(\epsilon^3) . \tag{A5}$$

For the purposes of this paper, the higher-order correction terms in Eqs. (A4) and (A5) are not needed.

APPENDIX B: NONCANOINCAL COORDINATES IN CLASSICAL MECHANICS

All the modern mathematical treatments of classical mechanics, such as Arnold [19] or Abraham and Marsden [35], formulate their results in a coordinate independent manner, and therefore in a sense also cover noncanonical coordinates. A considerably less formalistic treatment of noncanonical coordinates may also be found in Cary and Littlejohn [36]. In this appendix, we simply summarize notation and quote the principal formulas which are of use in the main text.

Hamilton's equations are equivalent to the variational principle

$$\delta\int p\,dq-H(q,p)dt=0 . \tag{B1}$$

This is distinct from Hamilton's principle in the usual sense in mechanics, not because of the integrand, which is just $L\,dt$ (L is the Lagrangian), but because both q and p are varied independently. Thus Eq. (B1) is a variational principle in phase space, and can be transformed to any new coordinates in phase space, even noncanonical ones.

It is not restricted to the point transformations of ordinary Lagrangian mechanics.

We let $z = (q,p)$, so that z is a $2N$ vector, and we define another $2N$ vector $\xi = (p,0)$, so that the variational principle can be written

$$\delta \int \xi_a(z)dz^a - H(z)dt = 0 \ . \tag{B2}$$

Here we let indices $a,b,\ldots$ run over $1,\ldots,2N$. Next we write $z' = z'(z)$ for any new coordinates on phase space. Transforming Eq. (B2) to the new coordinates, we have

$$\delta \int \xi'_a(z')dz'^a - H'(z')dt = 0 \ , \tag{B3}$$

where ξ has transformed as a covariant vector

$$\xi'_a(z') = \frac{\partial z^b}{\partial z'^a}\xi_b(z) \tag{B4}$$

and H as a scalar

$$H'(z') = H(z) \ . \tag{B5}$$

Furthermore, the equations of motion are left unchanged if any exact differential is added to the integrand of the variational principle. We call this is "gauge transformation in phase space," and its effect on ξ is

$$\xi_a(z) \rightarrow \xi_a(z) + \frac{\partial g(z)}{\partial z^a} \ , \tag{B6}$$

where $g(z)$ is the gauge scalar.

Thus the form shown in Eqs. (B2) and (B3) is generally covariant in phase space, and with the understanding of the transformation laws (B4) and (B5), we can drop the primes, reinterpreting z as the symbol for arbitrary coordinates in phase space, canonical or otherwise.

The variational principle implies equations of motion of the form

$$\Omega_{ab}\dot{z}^b = \frac{\partial H}{\partial z^a} \ , \tag{B7}$$

where

$$\Omega_{ab} = \frac{\partial \xi_b}{\partial x^a} - \frac{\partial \xi_a}{\partial z^b} \ . \tag{B8}$$

We introduce the inverse matrix J^{ab} of Ω_{ab},

$$J^{ab}\Omega_{bc} = \delta_c^a \ , \tag{B9}$$

in terms of which the equations of motion can be written

$$\dot{z}^a = J^{ab}\frac{\partial H}{\partial z^b} = \{z^a, H\} \ . \tag{B10}$$

Combined with the chain-rule property of the Poisson bracket, this equation implies

$$J^{ab} = \{z^a, z^b\} \ , \tag{B11}$$

so that for any two functions $f(z), g(z)$, expressed in terms of the possibly noncanonical coordinates z, we have

$$\{f,g\} = \frac{\partial f}{\partial z^a}J^{ab}\frac{\partial g}{\partial z^b} \ . \tag{B12}$$

Both Ω_{ab} and J^{ab} are invariant under gauge transformations in phase space; these objects are antisymmetric tensors in phase space of, respectively, the covariant and contravariant kinds.

Canonical coordinates are characterized by the fact that $J^{ab} = -\Omega_{ab} = \Gamma_{ab}$, where Γ is the constant matrix

$$\Gamma = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & \mathbf{0} \end{bmatrix} \ . \tag{B13}$$

In noncanonical coordinates, the components of J and Ω are generally functions of z.

Finally, the principal differential forms of interest in phase space are the symplectic 1-form

$$\xi = \xi_a dz^a \tag{B14}$$

and the symplectic 2-form

$$\omega = d\xi = \tfrac{1}{2}\Omega_{ab}dz^a \wedge dz^b \ . \tag{B15}$$

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