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Geometric Phases and the Bohr-Sommerfeld Quantization of Multicomponent Wave Fields

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Geometric phases play an important role in the asymptotic behavior of multicomponent wave fields, such as electromagnetic waves in plasmas or quantum-mechanical spinors, particularly in the problem of Bohr-Sommerfeld quantization. The proper gauge independence of the eigenvalues and asymptotic wave functions can be understood in terms of gauge-invariant but noncanonical coordinates on the classical phase space.

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Multicomponent wave fields and their asymptotic (short wavelength) behavior are important in physics. They include optical waves, electromagnetic waves in plasmas, elastic waves in solids, and various quantum-mechanical waves, including nuclear wave functions in the Born-Oppenheimer approximation. Aspects of the asymptotic analysis of such waves have been treated by a number of authors,[1-5] but essential elements, including the role of geometric phases in the Bohr-Sommerfeld quantization conditions and in the construction of wave functions, have received insufficient attention. It seems, in fact, that a general, geometrically clear, and manifestly gauge-invariant statement of the Bohr-Sommerfeld quantization conditions for such waves has never been made. For reference and to establish notation, we begin by summarizing the asymptotic behavior of scalar wave equations.

Consider a scalar wave $\psi(x)$, with $x=(x_1,\ldots,x_n)$, satisfying a wave equation $\hat{D}\psi=0$, where $\hat{D}$ is a linear operator. $\hat{D}$ can be regarded as a function of $\hat{x}$ (= multiplication by x), $\hat{k}=-i\epsilon\partial/\partial x$, where ϵ is the WKB ordering parameter. In quantum applications, ϵ is to be identified with $\hbar$, and k with the momentum p. The classical counterparts, or "symbols," of the operators $\hat{x}$, $\hat{k}$, and $\hat{D}$ are the functions x, k, and $D(x,k)$, where the one-to-one correspondence between operators and functions on the classical (x,k) phase space is given by the Weyl correspondence.[6] For example, in the usual Schrödinger equation, we have $D(x,p)=p^2/2m+V(x)-E$. The WKB approximation on ψ proceeds by setting $\psi(x)=A(x)e^{iS(x)/\epsilon}$ and substituting this into $\hat{D}\psi=0$. Expanding in ϵ, one finds the Hamiltonian-Jacobi equation $D(x,k)=0$ for S, and the amplitude transport equation $(\partial/\partial x)[A^2\partial D(x,k)/\partial k]=0$ for A, where in both equations D is evaluated at $k=\partial S/\partial x$. It is common to work only to the lowest two orders in ϵ, as we do here.

As for multicomponent wave fields, let the wave function be $\psi_\alpha(x)$, and let it satisfy the wave equation $\hat{D}_{\alpha\beta}\psi_\beta=0$. Here α,β are "spinor" indices, indexing the components of the wave field, and $\hat{D}_{\alpha\beta}$ is a matrix of "orbital" operators, i.e., functions of $\hat{x},\hat{k}$. This terminology is useful even for classical waves, such as electromagnetic waves in plasmas. We assume that $\hat{D}_{\alpha\beta}$ is Hermitian, $(\hat{D}_{\alpha\beta})^\dagger=\hat{D}_{\beta\alpha}$. The multicomponent WKB ansatz is $\psi_\alpha(x)=A_\alpha(x)e^{iS(x)/\epsilon}$, where the generally complex amplitude $A_\alpha(x)$ is now a spinor. The derivation of the WKB equations for S and A_α is more difficult than in the scalar case, but approaches have been worked out by several authors.[1-3]

The results are the following. Let the "dispersion tensor," $D_{\alpha\beta}(x,k)$, be the Hermitian matrix of Weyl symbols of $\hat{D}_{\alpha\beta}$, with eigenvalues $\lambda_0^{(\mu)}(x,k)$ and orthonormal eigenvectors $\tau_\alpha^{(\mu)}(x,k)$, so that $D_{\alpha\beta}\tau_\beta^{(\mu)}=\lambda_0^{(\mu)}\tau_\alpha^{(\mu)}$. The index μ is the "polarization" index and is not summed; it is placed in parentheses to distinguish it from the spinor-component indices α,β. The subscript 0 on λ will be explained momentarily. The wave function ψ_α is a linear combination of independent polarizations. The ac-

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tion S of the μth polarization satisfies the Hamilton-Jacobi equation $\lambda_0^{(\mu)}(x,k)=0$, with $k=\partial S/\partial x$, so that $\lambda_0^{(\mu)}(x,k)$ is the classical ray Hamiltonian for the μth polarization. The corresponding spinor amplitude is related to the eigenvector by

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

where B is real and satisfies the amplitude transport equation $(\partial/\partial x)[B^2\partial\lambda_0^{(\mu)}(x,k)/\partial k]=0$, where γ is a phase, and where again $k=\partial S/\partial x$. We ignore the important problem of nearly degenerate polarizations or conical intersections, which lead to mode conversion or coupling between polarizations.

The phase γ is an important element in multicomponent WKB theory, not present in the scalar problem. Along a ray of the Hamiltonian $\lambda_0(x,k)$ [we drop the polarization index (μ) for convenience] this phase satisfies[1-3]

$$\dot\gamma=i\tau_\alpha^*\{\tau_\alpha,\lambda_0\}+(i/2)D_{\alpha\beta}\{\tau_\alpha^*,\tau_\beta\}\,. \tag{1}$$

The first term is (by now) easily recognized as an example of Berry's phase,[7] since the Poisson bracket $\{\tau_\alpha,\lambda_0\}$ is the derivative $\dot\tau_\alpha$ of the eigenvector along the ray. Thus, the first term contributes $i\int\tau^\dagger d\tau$ to the phase γ. The fact that this contribution to the phase is anholonomic was recognized by Budden and Smith,[4] who dealt with several special examples of dispersion tensors, but was overlooked by several later authors,[1-3] who nevertheless did treat general dispersion tensors. Equation (1) was rederived by Yabana and Horiuchi,[5] who did recognize Berry's phase in the first term. In comparing (1) with Berry's original analysis,[7] we see that Berry's parameter space in his adiabatic process can be identified here with the $2n$-dimensional (x,k) phase space, and that the differential one-form $i\tau^\dagger d\tau$ is the connection for parallel transport of spinors through phase space. In the WKB problem, spinors are transported along the rays or orbits of the ray Hamiltonian.

The problem of the Bohr-Sommerfeld quantization of multicomponent wave fields, which in its modern form is well understood for scalar waves, has been considered in the one-dimensional ($\dim x=n=1$) case by Berk and Pfirsch[1] and by Yabana and Horiuchi.[5] The phase γ contributes to the quantization condition at the same level as the Maslov index, with the first term of (1) effectively causing a modification in the computation of the area of the orbit by the inclusion of Berry's angle flux intercepted by the orbit. The second term of (1), however, is not "geometrical," i.e., it cannot be represented in terms of a differential form on phase space, it does depend on the rate at which the path is traversed, etc. As a result, the quantization condition is somewhat less elegant than in the scalar theory. The multidimensional case ($n>1$) has been considered by Tabana and Horiuchi,[5] who imagine solving the Hamilton-Jacobi equation in λ_0 for S by separation of variables. Unfortunately, these authors are able to take account of the phase corrections in (1) only for special dispersion tensors. The results are therefore not general, and in any case, lack the geometrical beauty of torus quantization known for the scalar case.

We now introduce an alternative approach, based on the ideas of Friedland and Kaufman,[8] which is general (any n), which is manifestly gauge invariant, and which is geometrically as clear as the scalar case. We introduce a unitary matrix $\hat U$ of orbital operators, $(\hat U_{\alpha\beta})^\dagger\hat U_{\alpha\nu}=\delta_{\beta\nu}$, such that $\hat U^\dagger\hat D\hat U=\hat\Lambda$ is diagonal. If such a $\hat U$ can be found, then all the polarizations are decoupled, and each polarization, say, $\phi^{(\mu)}(x)$, satisfies the scalar wave equation $\hat\lambda^{(\mu)}\phi^{(\mu)}=0$ (no sum on μ), where $\hat\lambda^{(\mu)}$ is the orbital operator on the diagonal of $\hat\Lambda$. Scalar WKB theory can be applied to these scalar wave equations, and all known results, such as torus quantization, periodic-orbit expansions, Van Vleck expressions for Green's functions, wave-packet methods, etc., follow immediately. The scalar WKB theory is expressed in terms of the classical ray Hamiltonian $\lambda^{(\mu)}(x,k)$, the symbol of $\hat\lambda^{(\mu)}$. Furthermore, if problems such as caustics or wave chaos make the WKB analysis difficult, there is no need to apply it; one can always work directly with the scalar wave equation itself. This is the approach commonly taken in the Born-Oppenheimer approximation, which is a special case of the techniques described here.

Given $\hat D$, we solve for the unknown $\hat U$ which will diagonalize it by using the Weyl correspondence, and by expanding symbols in power of ϵ. Under the Weyl correspondence, the operator product $\hat B\hat C$ is mapped into[6,9] $B(x,k)C(x,k)+(i\epsilon/2)\{B,C\}+O(\epsilon^2)$, and the operator commutator $[\hat B,\hat C]$ is mapped into $i\epsilon\{B,C\}+O(\epsilon^3)$. These are the principal rules we need for the calculation. For example, in order to satisfy $\hat U^\dagger\hat U=$identity, the symbol matrix $U_{\alpha\beta}(x,k)$ is not exactly a unitary matrix. Instead, we write $U=U_0+\epsilon U_1+\cdots$ for the symbol matrix, finding that U_0 is unitary, while the correction U_1 satisfies

$$U_1=-iU_0(G+\tfrac14\{U_0^\dagger,U_0\})\,, \tag{2}$$

where G is a Hermitian matrix, not otherwise determined by the requirement that $\hat U$ be unitary.

Similarly, we use the Weyl correspondence to transcribe the condition $\hat U^\dagger\hat D\hat U=\hat\Lambda$ into symbols, demanding that $\hat\Lambda$ and hence its symbol matrix $\Lambda_{\mu\nu}$ be diagonal, $\Lambda_{\mu\nu}=\lambda^{(\mu)}\delta_{\mu\nu}$, and expanding, $\lambda^{(\mu)}=\lambda_0^{(\mu)}+\epsilon\lambda_1^{(\mu)}+\cdots$. At order zero, we find that $\lambda_0^{(\mu)}$ is the eigenvalue of the symbol matrix D, exactly as in earlier paragraphs, and that U_0 diagonalizes D, so that we can set $\tau_\alpha^{(\mu)}=U_{0\alpha\mu}$. As for the correction terms in the symbol of $\hat\lambda^{(\mu)}$, we find

$$\lambda_1=\lambda_{11}+\lambda_{12}$$
$$=-i\tau_\alpha^*\{\tau_\alpha,\lambda_0\}-(i/2)(D_{\alpha\beta}-\lambda_0\delta_{\alpha\beta})\{\tau_\alpha^*,\tau_\beta\}\,, \tag{3}$$

where again we drop polarization indices. The two ma-

jor terms of this equation obviously correspond to the terms in (1), except that here they appear as part of the ray Hamiltonian, not the phase. Thus, by using the total ray Hamiltonian $\lambda=\lambda_0+\epsilon\lambda_1$, scalar WKB theory can be applied immediately. For example, for the bound states of integrable problems, we must seek the invariant tori of this Hamiltonian; for periodic-orbit expansions, we must seek the periodic orbits of this Hamiltonian. The wave function now has the form $\psi_\alpha=\tau_\alpha Be^{iS/\epsilon}$, where S and B are the action and amplitude of the classical system described by the total Hamiltonian $\lambda=\lambda_0+\epsilon\lambda_1$.

The gauge transformations in Berry's adiabatic theory[7] are changes in phase conventions for the vectors τ; here we write $\tau\rightarrow e^{i\theta}\tau$ for a gauge transformation, where $\theta=\theta(x,k)$. The term λ_{11} of (3) can be written $-i\tau^\dagger\dot{\tau}$, where the time derivative is computed along the trajectories of λ_0. It is gauge dependent in the standard way in Berry's adiabatic theory. The term λ_{12}, although it is expressed in terms of τ, is gauge invariant. Thus, the classical ray Hamiltonian $\lambda(x,k)$ is gauge dependent. This fact must be taken into account when constructing eigenvalues and wave functions.

Normally, gauge dependence is not an issue in scalar WKB theory, and ray Hamiltonians are gauge invariant. An exception is the scalar Schrödinger equation for a particle in a magnetic field, for which the classical Hamiltonian $(\mathbf{p}-e\mathbf{A}/c)^2/2m$ is gauge dependent (in the sense of $\mathbf{A}\rightarrow\mathbf{A}+\nabla g$). (We use boldface for three vectors.) If we find, say, an invariant torus of this Hamiltonian, having some representation in the canonical $(\mathbf{x},\mathbf{p})$ coordinates, then we can construct a WKB wave function $\psi(\mathbf{x})$ from it in the usual way. If the wave function is to represent a definite physical state, then it must transform under the gauge transformation according to $\psi(\mathbf{x})\rightarrow e^{ieg(\mathbf{x})/\hbar c}\psi(\mathbf{x})$. But this transformation law cannot be achieved if we hold the torus fixed, in the sense of its representation in terms of the $(\mathbf{x},\mathbf{p})$ coordinates. This is obvious: A torus which is invariant in one gauge will not be invariant in another, since the Hamiltonian itself changes under the gauge transformation. On the other hand, introducing the kinetic momentum $\mathbf{p}'=\mathbf{p}-e\mathbf{A}/c$, if we hold the representation of the torus in the $(\mathbf{x},\mathbf{p}')$ coordinates fixed, then the WKB wave function has the proper transformation law under the gauge transformation. Thus, definite physical states are represented by tori (or other Lagrangian manifolds) whose representation in the noncanonical but gauge-invariant coordinates $(\mathbf{x},\mathbf{p}')$ is fixed.

Similarly, in the case of the multicomponent wave function, a physical state described by $\psi_\alpha(x)$ must be invariant under $\tau\rightarrow e^{i\theta}\tau$. But if an invariant torus (or other Lagrangian manifold) of the Hamiltonian $\lambda(x,k)=\lambda_0+\epsilon\lambda_1$, supporting an asymptotic wave function, is held fixed during the gauge transformation, in the sense of its representation in terms of the (x,k) coordinates on phase space, then the wave function $\psi_\alpha(x)$ will not be gauge invariant. Indeed, since the Hamiltonian itself changes, the torus will generally not remain invariant. If, however, we introduce new, primed phase-space coordinates,

$$z_j'=z_j-i\epsilon\tau_\alpha^*\{\tau_\alpha,z_j\}\,, \tag{4}$$

where $z=(x,k)$, $z'=(x',k')$, $j=1,\ldots,2n$, then a Lagrangian manifold which is fixed in the primed coordinates does correspond to a gauge-invariant wave function, and hence to a definite physical state. The primed coordinates z' are generalizations of the primed kinetic momentum $\mathbf{p}'$ of the preceding paragraph, and can be regarded as symbols of covariant derivative operators. These facts can be established in a straightforward manner.

The primed coordinates are useful for describing gauge-invariant objects, but they are noncanonical. For example, if we transform the ray Hamiltonian to the primed coordinates, we find

$$\lambda'(x',k')=\lambda(x,k)=\lambda_0(x',k')+\epsilon\lambda_{12}(x',k')\,. \tag{5}$$

The gauge-dependent term λ_{11} has been transformed away, and the new Hamiltonian λ' is now gauge invariant. But since the primed coordinates are noncanonical, the expressions for the symplectic one- and two-forms are modified. To within an exact differential, the symplectic one-form is $k'dx'+i\epsilon\tau^\dagger d\tau$, showing that Berry's phase contributes to the computation of action integrals in the primed coordinates; and the symplectic two-form is $dk'\wedge dx'+i\epsilon d\tau^\dagger\wedge d\tau$. By inverting the component matrix of the symplectic two-form,[10] we can compute the fundamental Poisson brackets in the primed coordinates. The modified formula for the Poisson bracket is gauge invariant since the two-form itself is. Since both the Hamiltonian and the Poisson bracket are gauge invariant, the classical equations of motion $\dot{z}_j'=\{z_j',\lambda'\}$ are gauge invariant also.

We see that every multicomponent wave field will give rise to some gauge-invariant but noncanonical formula for the Poisson bracket. Such noncanonical Poisson brackets have proven to be of value in understanding the classical motion of charged particles in magnetic fields,[11] and are indispensible in sophisticated applications of classical mechanics.[12] They are also of considerable intrinsic interest.

Let us now detail how we could compute the Bohr-Sommerfeld eigenvalues for a multicomponent wave equation. First we compute the dispersion tensor, its eigenvalues λ_0 and eigenvectors τ, and the correction term λ_{12}. Next we compute the transformation (4) to the primed coordinates, and the symplectic form and fundamental Poisson brackets in those coordinates. Assuming the ray Hamiltonian $\lambda'=\lambda_0+\epsilon\lambda_{12}$ is integrable, we find its invariant tori. For example, if we can find n constants of motion in involution (according to the noncanonical but gauge-invariant Poisson bracket), then their level sets, if bounded, are tori; or we can create an

invariant Lagrangian manifold by ray tracing, in which we use the gauge-invariant equations of motion in the primed coordinates. The quantized tori are selected from the others by computing the action integrals around basis contours; the action differential includes the Berry's phase term $i\tau^\dagger d\tau$, which yields a gauge-invariant result when integrated around the closed basis contours. Thus, the actions are gauge invariant. Then the value of any observable quantity (such as the energy or frequency) which is constant on a quantized torus is an eigenvalue of the corresponding wave operator.

As for the wave functions, these cannot be constructed by purely gauge-invariant means, since if $\psi_a(x)$ is gauge invariant but $\tau_a(x,k)$ is not, then the rest of the wave function, $B(x)e^{iS(x)/\epsilon}$, cannot be gauge invariant either. Nevertheless, the gauge-invariant, primed coordinates are useful for finding an invariant torus or other Lagrangian manifold in the first place, properly quantized if necessary. The representation of the Lagrangian manifold is then transformed to the unprimed, canonical coordinates, in which $S(x)=\int k\,dx$ is computed. In general, it will be necessary to use more than one (x,k)-coordinate patch on phase space, since in any particular gauge there will be singularities (monopole strings) in some region of phase space or of an individual torus. The wave functions are patched together by gauge transformations in the overlap regions.

We have explored several examples illustrating these calculations. The most interesting problem we have examined is that of spin-orbit coupling of a Pauli spinor. This is not just a model problem, since asymptotic representations of the density of states (i.e., periodic-orbit expansions[13,14]) have proven useful in understanding shell structure in nuclear physics,[15–17] and spin-orbit forces between nuclei are significant. Indeed, this problem was the original motivation for the work reported in this Letter. The spin-orbit calculation is rich, and gives not only illustrations of all the considerations raised above, but some others as well, such as the role of conservation laws in the asymptotic analysis. We will report on this and other examples in detail in the future.

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