Semiclassical theory of spin-orbit coupling

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Newly developed methods for finding the semiclassical or WKB eigenvalues and eigenfunctions for vector wave fields are applied to spinning particles moving in central potentials subject to spin-orbit forces. The new methods are like the familiar Bohr-Sommerfeld or Einstein-Brillouin-Keller quantization methods for scalar wave fields, but involve additional issues relating to Berry's phase, gauge structures, and monopolelike singularities. All these extra issues occur in the asymptotics of spin-orbit coupling. The role of angular momentum and conservation laws is particularly interesting, due to the role played by gauge fields in the classical-quantum correspondence. The work presented is a contribution to ongoing semiclassical studies of shell structure in nuclei and other fermion systems such as metal clusters, as well as an example of the general methods of semiclassical vector wave quantization.

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I. INTRODUCTION

This paper contains a study of Bohr-Sommerfeld (i.e., semiclassical, WKB, Einstein-Brillouin-Keller, or torus) quantization for a vector wave field in several spatial dimensions. The wave field considered is the $(2s+1)$-component spinor wave function for a particle of spin s subject to spin-orbit forces. The necessary theory for Bohr-Sommerfeld vector wave quantization has only recently been brought to a satisfactory condition, in the sense of possessing the same geometrical clarity and elegance as Bohr-Sommerfeld quantization for scalar wave fields. The new theory involves a number of elements not present in the case of scalar waves, including Berry's phase, gauge structures, monopolelike singularities, and mode conversion (or Landau-Zener transitions). All these elements except mode conversion are important in the present study of spin-orbit interactions. Therefore part of the significance of this work is that it is an explicit example, worked out in full detail, of the new techniques of vector wave quantization.

A second point of significance of this work is that it is part of a series of studies investigating the role of classical periodic orbits in organizing and explaining the shell structure of many-particle fermion systems, such as nuclei and metal clusters. Such studies are necessarily semiclassical in nature, and the present work shows explicitly how certain semiclassical methods can be extended to spinning particles with significant spin interactions (we have worked specifically on spin-orbit effects in nucleons, but generalizations are easy).

Semiclassical or WKB techniques have long been applied to vector wave equations, and many specific examples from many areas of physics have been worked out. The subject was treated from a fairly general standpoint in 1975 by Bernstein [1], who dealt with general linear wave equations, both differential and integral, in any number of spatial dimensions. Bernstein derived the generalizations of the Hamilton-Jacobi and amplitude transport equations, familiar in scalar WKB theory, in a form appropriate for vector wave equations. Bernstein did not, however, consider the problem of Bohr-Sommerfeld quantization. This problem was later considered in one dimension by Berk and Pfirsch [2] and in one and several dimensions by Yabana and Horiuchi [3]. These authors found a quantization condition for one-dimensional problems, but had difficulty in generalizing it to more than one dimension. Furthermore, the one-dimensional quantization condition lacked the elegance and geometrical simplicity of the analogous quantization condition for scalar waves. Yabana and Horiuchi recognized the importance of Berry's phase in vector wave propagation, but did not incorporate it into the quantization condition in a fully symmetrical way.

A real breakthrough in the problem of semiclassical quantization of vector wave fields was made by Kuratsuji and Iida [4], who approached the subject from the standpoint of path integrals rather than WKB theory. This approach has the advantage that it quickly leads to the realization that Berry's phase must be incorporated into the symplectic form in the classical phase space, from which point it influences not only the phase of the wave function (a fairly obvious conclusion), but also the classical dynamics of the rays, the definitions of the fundamental Poisson brackets, and the meaning of Lagrangian manifolds in phase space. In our opinion, this is the most significant and nontrivial feature of Bohr-Sommerfeld vector wave quantization, which distinguishes it from the scalar case. Kuratsuji and Iida made several studies of the quantization condition, from the standpoint of a path integral and coherent-state formalism. Regrettably, our own recent papers [5] on this subject have not given proper credit to their important work.

Parallel developments seem to have been made by mathematicians, who have studied $U(n)$ bundles and connections over Lagrangian manifolds. We are particularly aware of the work of Karasev [6], who treats many of the same subjects as Kuratsuji and Iida and ourselves. This work is somewhat technical for nonmathematicians, so it is difficult for us to evaluate it, nor are we aware of any

physical applications. But in many respects it does seem to reach equivalent conclusions.

Our own contribution to the subject of vector wave quantization proceeds from the standpoint of WKB theory. In our work [5] we rediscovered the modified symplectic form of Kuratsuji and Iida, and also explored such things as amplitude determinants, explicit formulas for wave functions, gauge invariance, and monopolelike singularities. All these features make their appearance in the present study of spin-orbit interactions. We also provided a critique of the older WKB approaches of Bernstein, showing why they make it difficult to formulate a quantization condition, and we developed new approaches to the WKB analysis, based on the Wigner function, that circumvent the difficulties.

In some respects the comparison of our work with that of Kuratsuji and Iida is not straightforward, since it involves the translation of results from path-integral and coherent-state theory into those of WKB theory. In particular, there is an extra first-order term in our ray Hamiltonian (denoted in λ_{12} in Ref. [5]), which is not manifestly evident in the results of Kuratsuji and Iida. This extra term was not new with us, but was present already in Bernstein's theory [1]. It was later transformed into Poisson bracket form by Kaufman, Ye, and Hui [7], and further examined by Yabana and Horiuchi [3]. This term is of the same order of magnitude as the Maslov terms and the Berry's-phase terms, and is absolutely necessary to get the correct eigenvalues, as the calculations of this paper show. Recently Fukui [8] has made progress in reconciling the two approaches, concentrating especially on the extra term in question.

Our motivation for examining spin-orbit effects derives from a series of earlier studies of the semiclassical behavior of nucleons in various model nuclear potentials. The first of these is a paper by Carbonell, Brut, Arview, and Touchard [9], which examines spherically symmetric nuclear potentials from a classical and semiclassical standpoint. This was followed by a study by the same authors of oblate and prolate potentials [10], and by Frisk and Arvieu [11] on rotating potentials.

Part of the motivation for these studies was to use classical periodic orbits as a tool for understanding shell structure in nuclei, including deformed and rotating nuclei which typically exhibit a mixture of regular and chaotic behavior in their classical dynamics. The role of periodic orbits in shell structure is an old one, for which a basic reference is Bohr and Mottelson [12]. The theory seems first to have been developed from a deep standpoint in the work of Balian and Bloch [13], although at the time of their work the distinction between regular and chaotic classical dynamics was not fully appreciated, and Berry's phase was not appreciated at all. Since that time the subject has been developed by a number of authors, including Strutinskii and Magner [14], Frisk [15], and others. This theory has also been applied to problems outside of nuclear physics, such as in the recent work by Nishioka [16] on metal clusters. Most of these studies have dealt with the scalar Schrödinger equation and have neglected spin; an exception is some early work by Balian and Bloch, on which we will comment below.

More recently, Arvieu, Rozmej, and Ploszajczak [17] have incorporated spin-orbit effects into their models of nuclear potentials by treating the spin as a classical vector confined to a sphere of constant radius. In this manner one can construct classical models and study periodic orbits, order, and chaos, etc. However, in treating the spin classically, one is in effect assuming that the spin quantum number is large; the fact that in reality it is not large presumably introduces errors that are larger than the usual ones expected in semiclassical theories. It is not clear whether these errors are important or not but treating the spin variable as a continuum is certainly one approach to incorporating spin in semiclassical theories. It is to be contrasted with the approach taken in this paper, in which the spin variables are retained in discrete form and the spin quantum number is not assumed to be large.

There are other semiclassical treatments of spin-orbit effects in the literature. One is by Balian and Bloch [18], who treated the spatial or orbital variables by semiclassical means, while retaining the discrete nature of the spin variables. This is exactly as in this paper. Balian and Bloch recognized that their approximations implied an adiabatic motion of the spin variables, which are driven by the slow classical variables describing the orbital dynamics. They developed semiclassical expansions for the energy-dependent Green's function, proceeding by an amplitude-phase representation for the wave function, much as in a special case of Bernstein's theory [1]. They did not consider the problem of Bohr-Sommerfeld quantization (except insofar as it is implicitly contained in the poles of the Green's function).

Another aspect of the problem was treated by Balazs and Pauli [19], who used the Wigner function, generalized into a matrix in the spin coordinates, to compute various quantities of interest for spin-$\frac{1}{2}$ particles. In particular, they studied spin-orbit effects in central-force potentials, as in this paper. These authors carried out most of their calculations in terms of the exact eigenfunctions for the spherically symmetric case, but at the end introduced semiclassical (Thomas-Fermi) approximations and discussed variational principles. One of their results was the discovery of two classical fluids governed by two classical Hamiltonians, much as we will also find in our calculations below. Balazs and Pauli did not consider the Bohr-Sommerfeld quantization problem.

In this paper we consider spin-orbit effects in central potentials, and derive explicit results both for eigenvalues and eigenfunctions. The calculation is in a sense a "straightforward" application of the methods of Ref. [5], in that no new general principles are introduced. But the analysis takes a number of surprising twists and turns, ultimately reinforcing our belief in the fundamental importance of Berry's phase and the modified symplectic structure of Kuratsuji and Iida. We will show that both the eigenvalues and the eigenfunctions computed by our theory are the correct asymptotic forms of the exact solutions. Our theory for the wave functions, in particular, automatically generates the correct asymptotics of the spherical harmonics and the Clebsch-Gordan coefficients.

The example we study in this paper is integrable, so it

presents nothing new from the standpoint of chaos theory. But chaotic systems have been discussed in Ref. [5], in which we showed that they present no more (or less) difficulty than in the case of scalar waves. If the spherically symmetric potential of this paper is replaced by an axially symmetric one, then chaotic orbits do arise. We have performed calculations for this case, and have derived the noncanonical symplectic form and studied the classical dynamics. We have found in these studies that mode conversion (nonadiabatic spin flips) are important, and this discovery has led us to examine multidimensional mode conversion or Landau-Zener transitions from a general standpoint. A preliminary report on this work is given in Ref. [20]. These calculations on axially symmetric potentials are of greater importance for real nuclear problems than the spherically symmetric potentials studied in this paper, and we will report on them at greater length in the future.

There are some obvious questions that arise when one considers what must be involved in a semiclassical treatment of spin-orbit coupling, comparing to what is known in the standard semiclassical treatment of (spinless) central-force motion. For example, for spinless particles, the classical orbits lie in planes perpendicular to the classical angular-momentum vector **L**. But with spin-orbit effects included, the quantum operator **L** is not conserved; only **J** is conserved. Does this mean that the classical orbits no longer lie in a plane? And concerning **J**, is there a conserved classical vector which corresponds to it? These questions and others like them cannot even be properly addressed without an appreciation for the role of Berry's phase in the semiclassical mechanics of vector waves. Therefore we will let the following analysis speak for itself, mentioning only that the study of conserved quantities in general and angular momentum in particular is one of the most interesting aspects of the following calculation.

II. ELEMENTS OF THE CALCULATION

We consider a particle of spin s governed by the quantum Hamiltonian

$$H=\frac{p^2}{2M}+V(r)+f(r)\mathbf{L}\cdot\mathbf{S}\ , \tag{2.1}$$

where M is the mass, where the potential V is spherically symmetric, where $\mathbf{L}=\mathbf{r}\times\mathbf{p}$, and where $\mathbf{S}$ is the vector of dimensionless spin operators, satisfying the commutation relations,

$$[S_i,S_j]=\epsilon_{ijk}S_k \tag{2.2}$$

(without the $\hbar$). We will generally use Latin indices i,j,k, etc., which run over 1,2,3, to index vectors in configuration space. In atomic problems, one would normally take

$$f(r)=\frac{\hbar}{2M^2c^2}\frac{1}{r}\frac{dV}{dr}\ , \tag{2.3}$$

but for the purposes of this paper $f(r)$ need not be specified.

In the asymptotic analysis of the Hamiltonian of Eq. (2.1), we will assume that the typical wavelength of the spatial part of the wave function is small in comparison to the scale length of the system. Apart from the fact that the wave function has several components (namely, $2s+1$), this is the usual WKB assumption. It is equivalent to assuming that the spatial quantum numbers (n,l,m) are large in comparison to unity, and, in particular, large in comparison to the spin quantum number s, which we treat as of order unity. On the other hand, WKB theory often gives good results even when its nominal conditions of validity are breaking down, so, even when quantum numbers are small, we can hope that our results will be better than just qualitative.

Following the program presented in Ref. [5], we write the wave equation in the form $\hat{D}\psi=0$, where $\hat{D}=\hat{H}-E$, and we regard both $\hat{D}$ and $\hat{H}$ as $(2s+1)\times(2s+1)$ matrices of orbital operators (E stands for E times the spinor identity matrix). We use carets to emphasize that operators are being referred to, not classical functions. Next we use the Weyl correspondence to transcribe these orbital operators into their symbols or classical counterparts, and obtain the dispersion matrix,

$$D_{\alpha\beta}=\left[\frac{p^2}{2M}+V(r)-E\right]\delta_{\alpha\beta}+f(r)(\mathbf{L}\cdot\mathbf{S})_{\alpha\beta}\ . \tag{2.4}$$

In this equation, r,p,L, etc., are classical quantities. Similarly, $D_{\alpha\beta}$ in Eq. (2.4) is a component of a $(2s+1)\times(2s+1)$ Hermitian matrix $\mathbf{D}$ which is a function of (r,p); thus, $\mathbf{D}=\mathbf{D}(\mathbf{r},\mathbf{p})$ is a field of Hermitian matrices over the six-dimensional classical phase space. Throughout this paper, we use Greek indices to run over $-s,\ldots,+s$, representing spinors. We sum over repeated indices, as in Eq. (2.4), with the exception of the polarization indices to be introduced momentarily.

In this paper we treat the WKB expansion as a development in $\hbar$, which is straightforwardly carried out as detailed in Ref. [5], with one exception. The exception is that we treat the spin-orbit term in the Hamiltonian of Eq. (2.1) as of order $\hbar^0$, just like the kinetic and potential energies, in spite of the fact that $\hbar$ occurs in $f(r)$, as shown in Eq. (2.3). We justify this approach by noting that spin-orbit effects are considered large in nuclear problems, and also by arguing that there is no harm from a purely mathematical standpoint in treating all the terms of the Hamiltonian as of the same order. A similar approach was taken by Balian and Bloch [18]; it allows us to circumvent the difficulties associated with a dispersion tensor which is degenerate at lowest order.

To proceed with the semiclassical analysis, we require the eigenvalues $\lambda_0^{(\mu)}$ and eigenvectors $\tau^{(\mu)}$ of the dispersion matrix $D_{\alpha\beta}$, where μ is a polarization index (in the terminology and notation of Ref. [5]). That is,

$$D_{\alpha\beta}\tau_\beta^{(\mu)}=\lambda_0^{(\mu)}\tau_\alpha^{(\mu)}\ . \tag{2.5}$$

Polarization indices are placed in parentheses to emphasize that they distinguish the eigenvalues and eigenvectors, and are not spinor indices. For example, for fixed value of μ, $\tau^{(\mu)}$ is a spinor, with components $\tau_\alpha^{(\mu)}$. (This distinction is partly phychological, because sometimes a polarization index can be interpreted as a spinor

index, and will be so written. It depends on which aspect we wish to emphasize.)

Since the first major term in Eq. (2.4) is already diagonal, the problem of determining the eigenvalues and eigenvectors of $D_{\alpha\beta}$ reduces to finding those of $\mathbf{L}\cdot\mathbf{S}$. In the theory of Berry's phase [21], a popular model problem is that of the adiabatic evolution of a spinning particle in a time-dependent magnetic field, for which the Hamiltonian is proportional to $\mathbf{B}\cdot\mathbf{S}$. Therefore with $\mathbf{B}$ replaced by $\mathbf{L}$, most of the known results for this standard problem can be applied to our calculation. These standard results have been collected and organized in Appendix A; it turns out we will need all of them.

The eigenvalues are immediate; they are given by

$$\lambda_0^{(\mu)}(\mathbf{r},\mathbf{p})=\frac{p^2}{2M}+V(r)-E+\mu L f(r)\ , \tag{2.6}$$

where $\mu=-s,\ldots,+s$, and where $L=|\mathbf{L}|$. The dispersion tensor is degenerate on the surface $L=0$, which is the mode-conversion surface [we will not worry about any possible vanishings of $f(r)$]. This surface has codimension 2 or dimension 4 in phase space, in spite of the fact that the vanishing of L requires the simultaneous vanishing of the three components of $\mathbf{L}$, for these three components are not independent when $\mathbf{L}=0$. (Alternatively, we can have $\mathbf{L}=0$ only if $\mathbf{r}$ and $\mathbf{p}$ are parallel. This implies four free parameters.) In this paper we will stay away from the mode-conversion surface, i.e., we will assume $L\neq 0$, so that the asymptotic expansion developed in Ref. [5] will be valid. This is also in accordance with the assumptions discussed earlier, i.e., that the spatial quantum numbers are large. In any case, we note that the degeneracy of the dispersion matrix at $L=0$ is $(2s+1)$-fold; for $s>\frac{1}{2}$, this is not a generic degeneracy.

The eigenvectors $\tau^{(\mu)}$ of $D_{\alpha\beta}$ are determined in the usual way in the theory of Berry's phase by using rotation operators, as discussed in Appendix A. We write $\hat{\boldsymbol{l}}=\mathbf{L}/L$ and (θ_l,ϕ_l) for the spherical angles of $\mathbf{L}$ or $\hat{\boldsymbol{l}}$, and regard $\tau^{(\mu)}$ as a function of either (θ_l,ϕ_l) or $\hat{\boldsymbol{l}}$ or $\mathbf{L}$ or $(\mathbf{r},\mathbf{p})$ by progressively lifting from the unit $\hat{\boldsymbol{l}}$ sphere to $\mathbf{L}$ space to the full phase space. In the two gauges discussed in Appendix A, north standard gauge and south standard gauge, the monopole string lies, respectively, at the south and north poles of the unit $\hat{\boldsymbol{l}}$ sphere. When lifted into phase space, the monopole string is the surface specified by $\mathbf{L}=L_z\hat{\mathbf{z}}$, with $L_z<0$ or $L_z>0$, depending on the gauge. These surfaces have codimension 2 or dimension 4 in the phase space, the same as the mode-conversion surface. We will henceforth drop the polarization index (μ) on λ and τ and other quantities which depend on it, it being understood that we are working with a definite polarization μ.

In the theory developed in Ref. [5], the eigenvalue λ_0 is only the lowest-order term in the classical Hamiltonian corresponding to a given polarization. The first-order correction is written $\hbar\lambda_1=\hbar(\lambda_{1B}+\lambda_{12})$, where λ_{1B} is the Berry's phase term,

$$\lambda_{1B}=-i\tau^{\dagger}\{\tau,\lambda_0\}\ , \tag{2.7}$$

and where λ_{12} has no name and is given by

$$\lambda_{12}=-\frac{i}{2}(D_{\alpha\beta}-\lambda_0\delta_{\alpha\beta})\{\tau_\alpha^*,\tau_\beta\}\ . \tag{2.8}$$

In these expressions, the curly bracket is the Poisson bracket.

In our problem the Berry's phase contribution to the Hamiltonian vanishes, for the eigenvectors τ depend only on the angular momentum $\mathbf{L}$, and the eigenvalue λ_0 given in Eq. (2.6), being rotationally symmetric, Poisson commutes with $\mathbf{L}$. Another way to say this is that since $\mathbf{L}$ is constant along the orbits generated by λ_0, the eigenvector $\tau(\mathbf{L})$ is also constant, so there is no transport on the unit $\hat{\boldsymbol{l}}$ sphere, and no accumulated Berry's phase. We will return later to the implications of this fact.

As for λ_{12}, it is gauge invariant, as noted on general grounds in Ref. [5], so it must be possible to compute it without knowing explicit forms for τ in some gauge. Such indeed is the case. Once again we call on the fact that τ depends only on $\mathbf{L}$, to write

$$\{\tau_\alpha^*,\tau_\beta\}=\epsilon_{ijk}L_i\frac{\partial\tau_\alpha^*}{\partial L_j}\frac{\partial\tau_\beta}{\partial L_k}\ , \tag{2.9}$$

and we use Eq. (A22) for the derivatives. The result involves the vector potential $\mathbf{A}(\mathbf{L})$, which represents Berry's 1-form on angular-momentum space, and is therefore gauge dependent. But when we contract this with either $\delta_{\alpha\beta}$ or $D_{\alpha\beta}$, the gauge-dependent terms drop out, and we are left with

$$\lambda_{12}=\tfrac{1}{2}f(r)[\mu^2-s(s+1)]\ . \tag{2.10}$$

The details of this calculation are summarized in Appendix B.

Altogether, we have obtained the following classical Hamiltonian describing the evolution of the rays in phase space for polarization μ:

$$H(r,p)=\frac{p^2}{2M}+V(r)+f(r)\left[\mu L+\frac{\hbar}{2}[\mu^2-s(s+1)]\right], \tag{2.11}$$

where we have set $\lambda(\mathbf{r},\mathbf{p})=H(\mathbf{r},\mathbf{p})-E$, and where the classical H depends implicitly on (μ).

A physical interpretation of the polarization index μ is obtained if we compare this result with the result of an exact quantum treatment of Eq. (2.1), in which we set $\mathbf{J}=\mathbf{L}+\hbar\mathbf{S}$ and restrict to a subspace of constant j and l. In this case the spin-orbit term takes the form,

$$f(r)\mathbf{L}\cdot\mathbf{S}=\tfrac{1}{2}\hbar f(r)[j(j+1)-l(l+1)-s(s+1)]\ . \tag{2.12}$$

On the other hand, standard analysis in scalar (one-component) WKB theory [22] for spherically symmetric problems leads us to expect that L is quantized according to $L=(l+\frac{1}{2})\hbar$; substituting this into Eq. (2.11) and comparing with Eq. (2.12), we find that the two results agree exactly if we take

$$\mu=j-l\ . \tag{2.13}$$

This shows that the polarization index is essentially a label for the total angular momentum j, given a value of

the orbital angular momentum l. Furthermore, the range of values on μ is exactly the correct one for the coupling $\mathbf{J}=\mathbf{L}+\hbar\mathbf{S}$, i.e., $\mu=-s,\ldots,+s$ implies $j=l-s,\ldots,l+s$. This calculation also shows that the correction term λ_{12} to the ray Hamiltonian, which was not appreciated in earlier multicomponent WKB theories [1], is essential to get the correct eigenvalues.

III. DO WE NEED BERRY'S PHASE OR NONCANONICAL COORDINATES?

In Ref. [5] considerable attention was given to the fact that the total ray Hamiltonian λ is in general gauge dependent because of the Berry's phase term $\lambda_{1B}=-i\tau^{\dagger}\{\tau,\lambda_0\}$. In particular, it was argued that a proper understanding of the gauge invariance of both eigenvalues and eigenfunctions requires the introduction of a new set of phase-space coordinates $z'=(\mathbf{r}',\mathbf{p}')$, defined in terms of the old set $z=(\mathbf{r},\mathbf{p})$ by

$$z_a'=z_a-i\hbar\tau^{\dagger}\{\tau,z_a\}\ , \tag{3.1}$$

where (for the present problem) $a=1,\ldots,6$. The new, primed coordinates are noncanonical, but they have a number of advantages over the unprimed, canonical coordinates, such as the fact that the Berry's phase term in the ray Hamiltonian vanishes when the Hamiltonian is expressed in terms of them. This causes the ray Hamiltonian to be gauge invariant, as discussed in Ref. [5]. In fact, the original motivation for introducing the noncanonical coordinates z' was to get rid of the Berry's phase term, in order to obtain a ray Hamiltonian that is gauge invariant.

In the present problem, however, the Berry's phase term in the ray Hamiltonian has already vanished, as noted below Eq. (2.8), so the ray Hamiltonian is gauge invariant even in the canonical coordinates $z=(\mathbf{r},\mathbf{p})$. This fact is an ideosyncracy of the present problem and does not hold generally (for example, λ_{1B} does not vanish in the Stern-Gerlach problem discussed in Ref. [5]). Nevertheless, since our ray Hamiltonian is already gauge invariant, we are led to question whether we really need to bother with Berry's phase or noncanonical coordinates, as detailed in Ref. [5]. That is, the ray Hamiltonian in Eq. (2.11) describes the evolution of a single polarization μ and can be thought of as the symbol of a wave operator for a scalar-wave equation; therefore it seems logical simply to solve the Hamilton-Jacobi equation corresponding to Eq. (2.11) in canonical coordinates and to construct eigenvalues and eigenfunctions in the usual way.

The results of doing this are that one does obtain the correct eigenvalues, but the multiplicities are wrong and the wave functions, even though they correspond to a definite and complete set of quantum numbers, are gauge dependent. A proper understanding of the latter two defects in the calculation requires both Berry's phase and the noncanonical coordinates z', and provides a considerable reinforcement for their importance in multicomponent WKB theory, even in a problem such as this one, for which $\lambda_{1B}=0$. We will now proceed with the standard WKB analysis of Eq. (2.11) in canonical coordinates, initially taking a somewhat devil's advocate point of view, and show finally what goes wrong and why.

The Hamiltonian in Eq. (2.11) is integrable, and the corresponding Hamilton-Jacobi equation is separable in spherical coordinates. The calculation of the solution $S(\mathbf{r})$ of the Hamilton-Jacobi equation, the actions I_i, and the eigenvalues proceeds much as in any textbook example of central-force motion. In particular, the invariant tori are level sets in phase space of the commuting constants of motion (H,L^2,L_z), and the basis contours Γ_i, around which the actions are computed according to

$$I_i=\frac{1}{2\pi}\oint_{\Gamma_i}\mathbf{p}\cdot d\mathbf{r}\ , \tag{3.2}$$

are the contours on the torus obtained by holding all but one of the coordinates (r,θ,ϕ) at a time fixed. We will call these contours $(\Gamma_r,\Gamma_\theta,\Gamma_\phi)$, and the corresponding actions (I_r,I_θ,I_ϕ). The actions are quantized according to $I_i=(n_i+m_i/4)\hbar$, where n_i is the quantum number and m_i is the Maslov index [23], the Hamiltonian is expressed as a function of the actions, and the energy eigenvalues result. It is a standard calculation in EBK or torus quantization [24,25].

For the moment, however, we do not need the explicit form of the solution $S(\mathbf{r})$ of the Hamilton-Jacobi equation, and a slightly different approach to the computation of the eigenvalues has several advantages. Our approach will differ from the usual one in that we will use different basis contours on the 3-torus than $(\Gamma_r,\Gamma_\theta,\Gamma_\phi)$. We begin by noting that (H,L^2,L_z) Poisson commute with one another, so that their level sets in phase space are Lagrangian invariant tori, in accordance with a theorem proved by Arnold [26]. (This theorem is really a modern version of a theorem due to Liouville, which is discussed by Whittaker [27]. It is the basis for what we called the Liouville method of solving the Hamilton-Jacobi equation in Ref. [5].) Next, we note that the orbits in phase space created by treating each of the observables (H,L^2,L_z) as a Hamiltonian lie on the tori, because all three observables are constants of each other's flows. Therefore if any of these orbits forms a closed curve, it can be used to construct a basis contour on the torus on which it lies. From the basis contours, actions and eigenvalues can be computed, just as above, but without having to deal directly with the Hamilton-Jacobi equation. We will now carry out these calculations in a little detail, because similar calculations will be needed in Sec. [5], in the less familiar context of noncanonical coordinates.

One basis contour can be obtained from the orbits generated by $L_z=\hat{\mathbf{z}}\cdot(\mathbf{r}\times\mathbf{p})$. These orbits are the solutions of

$$\begin{aligned}\frac{d\mathbf{r}}{dt_3}&=\{\mathbf{r},L_z\}=\hat{\mathbf{z}}\times\mathbf{r}\ ,\\ \frac{d\mathbf{p}}{dt_3}&=\{\mathbf{p},L_z\}=\hat{\mathbf{z}}\times\mathbf{p}\ ,\end{aligned} \tag{3.3}$$

where t_3 is not time but just the parameter of the orbits. These orbits are just rotations about the $\hat{\mathbf{z}}$ axis, as shown by the general solution,

$$\mathbf{r}(t_3)=R(\hat{\mathbf{z}},t_3)\mathbf{r}_0,\quad \mathbf{p}(t_3)=R(\hat{\mathbf{z}},t_3)\mathbf{p}_0\ , \tag{3.4}$$

where $R(\hat{\mathbf{z}},t_3)$ represents the rotation in axis-angle form (i.e., $\hat{\mathbf{z}}$ is the axis and t_3 is the angle). Therefore after elapsed parameter $t_3=2\pi$, any one of these orbits traces out a closed contour on the torus, for which we write Γ_3. The corresponding action is easily computed by Eq. (3.2),

$$I_3=\frac{1}{2\pi}\int_0^{2\pi}\mathbf{p}(t_3)\cdot\frac{d\mathbf{r}(t_3)}{dt_3}dt_3$$
$$=\frac{1}{2\pi}\int_0^{2\pi}\hat{\mathbf{z}}\cdot(\mathbf{r}\times\mathbf{p})dt_3=L_z\ , \tag{3.5}$$

since L_z is constant along its own orbits and comes out of the integral. When we rotate about the $\hat{\mathbf{z}}$ axis, both θ and r are held constant, and only ϕ varies; therefore the contour Γ_3 is the same as the contour Γ_ϕ which emerges from the Hamilton-Jacobi equation. Similarly, the actions satisfy $I_\phi=I_3=L_z$.

Similarly, the observable L^2 also generates orbits which are closed curves in phase space. Now Hamilton's equations are

$$\frac{d\mathbf{r}}{dt_2}=\{\mathbf{r},L^2\}=2\mathbf{L}\times\mathbf{r}=2L\hat{\mathbf{l}}\times\mathbf{r}\ ,$$
$$\frac{d\mathbf{p}}{dt_2}=\{\mathbf{p},L^2\}=2\mathbf{L}\times\mathbf{p}=2L\hat{\mathbf{l}}\times\mathbf{p}\ , \tag{3.6}$$

where t_2 is not time but just the parameter of the L^2 orbits. Since $\{\mathbf{L},L^2\}=0$, $\mathbf{L}$ and $\hat{\mathbf{l}}$ are constant along the L^2 orbits, and the solution consists of rotations about the $\hat{\mathbf{l}}$ axis by angle $2Lt_2$,

$$\mathbf{r}(t_2)=R(\hat{\mathbf{l}},2Lt_2)\mathbf{r}_0,\quad \mathbf{p}(t_2)=R(\hat{\mathbf{l}},2Lt_2)\mathbf{p}_0\ . \tag{3.7}$$

Therefore after elapsed parameter $t_2=\pi/L$, any one of these orbits forms a closed contour on the torus, for which we write Γ_2. The corresponding action is

$$I_2=\frac{1}{2\pi}\int_0^{\pi/L}\mathbf{p}(t_2)\cdot\frac{d\mathbf{r}(t_2)}{dt_2}dt_2$$
$$=\frac{1}{2\pi}\int_0^{\pi/L}2L^2dt_2=L\ . \tag{3.8}$$

During the L^2 evolution, the variable ϕ increases monotonically if $L_z>0$ and decreases monotonically if $L_z<0$, the variable θ oscillates between its turning points, and the variable r is held fixed. Therefore we have $\Gamma_2=\Gamma_\theta+\Gamma_\phi$ if $L_z>0$ and $\Gamma_2=\Gamma_\theta-\Gamma_\phi$ if $L_z<0$. These equations relate the basis contour Γ_2 to those which occur in the separation of the Hamilton-Jacobi equation. Similarly, the actions satisfy $I_2=I_\theta+|I_\phi|$, or $I_\theta=L-|L_z|$.

To obtain a final basis contour, we examine the orbits of H, which are described by Hamilton's equations in the usual sense,

$$\frac{d\mathbf{r}}{dt}=\{\mathbf{r},H\}=\frac{\mathbf{p}}{M}+\mu f(r)\hat{\mathbf{l}}\times\mathbf{r}\ ,$$
$$\frac{d\mathbf{p}}{dt}=\{\mathbf{p},H\}$$
$$=-\frac{\mathbf{r}}{r}\left[V'(r)+f'(r)\left[\mu L+\frac{\hbar}{2}[\mu^2-s(s+1)]\right]\right]$$
$$+\mu f(r)\hat{\mathbf{l}}\times\mathbf{p}\ , \tag{3.9}$$

where $t=t_1$ is time. The motion is not purely potential motion because of the terms involving $\hat{\mathbf{l}}\times\mathbf{r}$ and $\hat{\mathbf{l}}\times\mathbf{p}$, but the orbit as seen in configuration space does lie in a plane perpendicular to $\mathbf{L}$. The orbit is not, in general, closed, and so does not by itself form a basis contour on the torus in phase space. Such a basis contour can be constructed, however, by combining the H evolution with the L^2 evolution, which by Eq. (3.7) consists of rotations in the plane of the orbit. In particular, by combining these two evolutions, we can cause the direction of $\mathbf{r}$ to remain constant, while only its magnitude r varies. The resulting contour Γ_1 is the same as the contour Γ_r resulting from a separation of the Hamilton-Jacobi equation. The variable r satisfies equations of motion that can be derived from the effective radial Hamiltonian,

$$H_{\rm rad}(r,p_r)=\frac{1}{2M}\left[p_r^2+\frac{L^2}{r^2}\right]+V(r)$$
$$+f(r)\left[\mu L+\frac{\hbar}{2}[\mu^2-s(s+1)]\right]\ . \tag{3.10}$$

The final action $I_1=I_r$ is just $(1/2\pi)\oint p_r dr$, computed in the usual way for one dimensional problems. It cannot be obtained in explicit form without knowing the functional forms of $V(r)$ and $f(r)$.

The actions are quantized according to

$$I_1=I_r=(n-l-\tfrac{1}{2})\hbar\ ,$$
$$I_2=I_\theta+|I_\phi|=L=(l+\tfrac{1}{2})\hbar\ , \tag{3.11}$$
$$I_3=I_\phi=L_z=m\hbar\ ,$$

where the Maslov indices are determined by counting turning points, and where the quantum numbers (n,l,m) have been defined so as to agree with the usual notation in the case of the spinless hydrogen atom, i.e., when $V(r)=-k/r$, $f(r)=0$. The energy eigenvalues are determined by expressing the Hamiltonian as a function of the quantized actions; the Hamiltonian turns out to be independent of I_3, so the energy levels E_{nl} are independent of m. Of course, the energy levels do depend on the polarization index μ, which is a parameter of the Hamiltonian, and which by Eq. (2.13) can be regarded as just another notation for the total angular-momentum quantum number j. To emphasize this dependence, we can also write the energy levels as $E_{nl}^{(\mu)}$ or E_{njl}.

Furthermore, the energy levels so determined are the correct semiclassical energy levels for the original quantum Hamiltonian of Eq. (2.1). We can say this without knowing the functional form of $V(r)$ or $f(r)$ and without

having any prior multicomponent WKB theory to fall back on, because the original quantum Hamiltonian in Eq. (2.1) is separable, and can be reduced to a scalar (one-component) radial equation. To do this, we choose quantum numbers (j,l,m_j), where m_j is the quantum number of J_z, and we write the exact eigenfunction of the Hamiltonian in Eq. (2.1) in the form,

$$\psi_\alpha^{jlm_j}(r,\theta,\phi)=\frac{1}{r}\Phi(r)Y_{l,m_j-\alpha} \times(\theta,\phi)\langle l,m_j-\alpha,s,\alpha|j,m_j\rangle \ , \tag{3.12}$$

where α is a spinor index (not summed), where the Dirac bracket is a Clebsch-Gordan coefficient in the form $\langle j_1 m_1 j_2 m_2|j_3 m_3\rangle$, and where Y_{lm} is a spherical harmonic. Substituting this into the original quantum Hamiltonian in Eq. (2.1) and separating variables, we find a radial Schrödinger equation for Φ,

$$\hat{H}_{\rm rad}\Phi=E\Phi \ , \tag{3.13}$$

in which $\hat{H}_{\rm rad}$ is exactly the same as in Eq. (3.10), except that it is reinterpreted as a quantum operator on radial wave functions with $p_r=-i\hbar\partial/\partial r$, and the constants L, L^2, and μ are replaced, respectively, by $(l+\frac{1}{2})\hbar$, $l(l+1)\hbar^2$, and $j-l$. This radial Schrödinger equation can be subjected to a one-dimensional WKB analysis, which leads to exactly the same energy levels E_{jln} discussed in the preceding paragraph, apart from the difference between $(l+\frac{1}{2})^2$ and $l(l+1)$. This latter difference is the usual one that arises in treating radial equations [22,28]; it is of relative order $\hbar^2$ and can therefore be considered outside the scope of standard WKB theory, although it is usually agreed that $(l+\frac{1}{2})^2$ gives better answers.

Although the semiclassical analysis presented so far does give the correct semiclassical eigenvalues E_{njl}, it does not give the correct multiplicities of the degenerate levels. Multiplicities are determined in a semiclassical analysis by counting the number of invariant quantized tori which have a given energy. In the present case, since the energies do not depend on the quantum number m, we must count the allowed m values. Because of the classical inequality

$$-L\le L_z\le +L \ , \tag{3.14}$$

and because of the quantized values of the actions L and L_z given in Eq. (3.11), we have $m=-l,\ldots,+l$, for a total of $2l+1$ values. This is exactly as in any textbook treatment of any central-force problem by scalar WKB theory, but it is unfortunately incorrect for the spin-orbit problem, for which the degeneracy of E_{njl} is $2j+1=2(l+\mu)+1$.

The reason we have obtained the wrong multiplicities has to do with monopole strings, i.e., the singularities in phase space of the eigenvectors $\tau^{(\mu)}(\mathbf{r},\mathbf{p})$. Although these eigenvectors have appeared nowhere so far in our semiclassical analysis of the Hamiltonian in Eq. (2.11), nevertheless they were involved in the derivation of that Hamiltonian, in which one of the assumptions made was that the amplitude of the WKB wave function, including the eigenvector τ, was slowly varying. Unfortunately, this assumption is not valid near a monopole string, where τ is rapidly varying, and therefore the invariant tori which are close to the monopole string cannot be used to construct valid wave functions. This means that the count of linearly independent wave functions of a given energy, i.e., the multiplicity of the energy level, cannot be determined from an inequality such as Eq. (3.14), because some of the tori in the range $m=-l,\ldots,+l$ do lie close to the monopole string. For example, in north standard gauge, the m values near $-l$ cannot be trusted, because the string lies at the south pole of the unit $\hat{l}$ sphere; and in south standard gauge, the m values near $+l$ cannot be trusted, because the string lies at the north pole.

But now one is likely to object that this cannot be the true explanation for the incorrect multiplicity, because the monopole string can be placed anywhere we want by means of a gauge transformation. For example, why do we not construct wave functions over the northern hemisphere, i.e., for positive-m values, using north standard gauge, and over the southern hemisphere, i.e., for negative-m values, using south standard gauge? We can overlap a little at the equator, so that some tori are represented in both gauges. It would then seem that we still have $2l+1$ linearly independent wave functions, which again is the wrong answer.

The flaw in this counterargument is that the wave function associated with a given torus depends not only on that torus, but also on the gauge. Therefore when we overlap at the equator, using two gauges for some tori, then the two wave functions corresponding to a given torus will not be the same, even to within a multiplicative factor. Therefore the count of linearly independent wave functions is not the same as the count of tori. (Actually, there is a certain important sense, to be explained later, in which even the count of tori is not what it seems, i.e., $2l+1$.)

Let us examine the gauge dependence of the WKB wave functions more closely. As shown in Ref. [5], the wave functions have the form,

$$\psi_\alpha(\mathbf{r})=\tau_\alpha(\mathbf{r},\mathbf{p})B(\mathbf{r})e^{iS(\mathbf{r})/\hbar} \ , \tag{3.15}$$

where $\mathbf{p}=\mathbf{p}(\mathbf{r})=\nabla S(\mathbf{r})$, and where $B(\mathbf{r})$ is the scalar amplitude. The action function $S(\mathbf{r})$ is determined by solving the Hamilton-Jacobi equation for the Hamiltonian of Eq. (2.11), either by separation of variables or some other method. The action function is parametrized by the torus in question, which in turn is specified by the actions $\mathbf{I}=(I_1,I_2,I_3)$, and may more properly be written $S(\mathbf{r},\mathbf{I})$. For given values of $\mathbf{I}$, i.e., for a given torus, S is gauge invariant, since the Hamiltonian of Eq. (2.11) is gauge invariant due to the vanishing of the Berry's phase term λ_{1B}. Therefore the amplitude, which is given by

$$B(\mathbf{r})=\left|\frac{\partial^2 S(\mathbf{r},\mathbf{I})}{\partial\mathbf{r}\partial\mathbf{I}}\right|^{1/2} \ , \tag{3.16}$$

is also gauge invariant.

We see that the only gauge-dependent contribution to the wave function comes from τ_α, which transforms according to $\tau_\alpha\rightarrow e^{ig}\tau_\alpha$, where g is the gauge scalar. As dis-

cussed in Appendix A, both τ_α and g depend essentially only on $\hat{l}$, but can be lifted into functions of $\mathbf{L}$ or $(\mathbf{r},\mathbf{p})$. The function $\tau_\alpha(\mathbf{r},\mathbf{p})$ in Eq. (3.15) is such a lift. Therefore as we let $(\mathbf{r},\mathbf{p})$ move around on the invariant torus, the eigenvector $\tau_\alpha(\mathbf{r},\mathbf{p})$ will change only if $\hat{l}$ changes. In fact, $\hat{l}$ does change as we move around on the torus, but not as much as one might expect, given that the torus is three dimensional. For it turns out that $\hat{l}$ is constant along two directions on the torus, and varies only in the third. The three directions in question are those specified by the flows of (H,L^2,L_z) given, respectively, by Eqs. (3.9), (3.6), and (3.3). Along the L^2 flow and the H flow, $\hat{l}$ is constant because $\mathbf{L}$ is constant, since $\{\mathbf{L},L^2\}=0$ and $\{\mathbf{L},H\}=0$. Therefore τ_α is also constant along these flows. Along the L_z flow, however, $\mathbf{L}$ is not constant, but rather satisfies

$$\frac{d\mathbf{L}}{dt_3}=\{\mathbf{L},L_z\}=\hat{\mathbf{z}}\times\mathbf{L}\ . \tag{3.17}$$

Therefore along the L_z flow on the torus, the vector $\hat{l}$ traces out a small circle of constant latitude, as illustrated in Fig. 1.

In Ref. [5] it was pointed out that in a general two-component WKB problem, there is a mapping from any N-dimensional Lagrangian manifold onto the Poincaré sphere, where N is the number of degrees of freedom, given by any specific eigenvector of the dispersion matrix computed over the Lagrangian manifold. In the generic case, we expect this mapping to cover a one-dimensional region of the Poincaré sphere if $N=1$, and a two-dimensional region if $N\geq 2$. In the spin-orbit problem, we have $N=3$, but the mapping only covers a one-dimensional region. This is a reflection of the fact that the spin-orbit problem is not generic.

In any case, since the eigenvector τ_α is not constant as we move around on the torus, different parts of the torus can be subjected to different changes of phase under a gauge transformation. Therefore the wave function $\psi_\alpha(\mathbf{r})$ of Eq. (3.15) also suffers different changes of phase at different spatial points, and a gauge transformation transforms $\psi_\alpha(\mathbf{r})$ into a new function, which is generally linearly independent of the old one. This substantiates our earlier claim that the count of linearly independent wave functions is not necessarily or obviously the same as the count of tori.

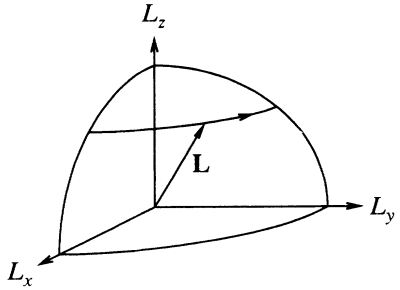

FIG. 1. The angular-momentum vector $\mathbf{L}$ is not constant on the invariant torus specified by fixed values of L_z, L^2, and H, but rather traces out a small circle of constant latitude, since $\mathbf{L}$ does not commute with L_z.

But now another question arises. A given torus corresponds to definite values of the quantum numbers $(njlm)$, which form a complete set and should therefore specify a definite physical state. How then can the wave function be gauge dependent? We might expect the wave function to suffer an overall change of phase under a gauge transformation, but not to be changed into a linearly independent function.

A little thought causes us to be suspicious of the quantum number m, corresponding to the operator $\hat{L}_z$, since we know that in the exact quantum Hamiltonian of Eq. (2.1) $\hat{L}_z$ is not conserved, nor is any other component $\hat{\mathbf{L}}$. It is only the total angular momentum $\hat{\mathbf{J}}=\hat{\mathbf{L}}+\hbar\hat{\mathbf{S}}$ which is conserved. But the classical Hamiltonian of Eq. (2.11), representing a single polarization, does satisfy the classical equation $\{\mathbf{L},H\}=0$. How, then, is the conserved operator $\hat{\mathbf{J}}$ represented within the semiclassical description of a single polarization? And how are the nonconserved operators $\hat{\mathbf{L}}$ and $\hat{\mathbf{S}}$ represented, if at all? In particular, is the operator $\hat{\mathbf{L}}$ represented by the classical vector $\mathbf{L}=\mathbf{r}\times\mathbf{p}$? Finally, how is it that we seem to find semiclassically a simultaneous eigenstate of $(\hat{H},\hat{J}^2,\hat{L}^2,\hat{L}_z)$, when $\hat{L}_z$ does not commute with $\hat{H}$? We turn now to a closer examination of these questions, which will greatly reinforce our belief in the general importance of Berry's phase and the noncanonical coordinates discussed in Ref. [5].

IV. CONSERVED QUANTITIES AND ANGULAR MOMENTUM

In scalar WKB theory, the relationship between the classical and quantum expressions for conserved quantities is straightforward. That is, if $\hat{F}$ is an operator which commutes with the Hamiltonian $\hat{H}$, $[\hat{F},\hat{H}]=0$, then the corresponding Weyl symbols $F(\mathbf{r},\mathbf{p}),H(\mathbf{r},\mathbf{p})$ satisfy $\{F,H\}=0$ with a relative error of $O(\hbar^2)$.

In multicomponent WKB theory, however, things are more complicated. Let us for the moment forget about the spin-orbit problem and speak in general terms, using the notation of Ref. [5]. We also restore polarization indices for the time being. Writing the wave equation in the form $\hat{\mathbf{D}}\psi=0$ or $\hat{D}_{\alpha\beta}\psi_\beta=0$, where $\hat{\mathbf{D}}$ is a matrix of orbital operators with components $\hat{D}_{\alpha\beta}$, we will regard another matrix of orbital operators $\hat{\mathbf{F}}$ to be a conserved quantity if $[\hat{\mathbf{F}},\hat{\mathbf{D}}]=0$, i.e.,

$$\hat{F}_{\mu\alpha}\hat{D}_{\alpha\nu}-\hat{D}_{\mu\alpha}\hat{F}_{\alpha\nu}=0\ . \tag{4.1}$$

When we apply multicomponent WKB theory, $\hat{\mathbf{D}}$ is diagonalized by a unitary matrix of orbital operators $\hat{\mathbf{U}}$,

$$\hat{\mathbf{U}}^\dagger\hat{\mathbf{D}}\hat{\mathbf{U}}=\hat{\mathbf{\Lambda}}=\begin{pmatrix}\hat{\lambda}^{(1)} & & \\ & \hat{\lambda}^{(2)} & \\ & & \ddots\end{pmatrix}$$
$$=(\text{a diagonal matrix})\ . \tag{4.2}$$

The individual polarizations then evolve according to the operators $\hat{\lambda}^{(\mu)}$ on the diagonal of $\hat{\mathbf{\Lambda}}$. Evidently, the effect

of the transformation of Eq. (4.2) is to block diagonalize the wave operator $\hat{\mathbf{D}}$, much as is done in applications of group theory to quantum mechanics, except that here semiclassical methods are used to determine $\hat{\mathbf{U}}$.

Now we ask, can the action of $\hat{\mathbf{F}}$ be represented by some operator, say, $\hat{f}^{(\mu)}$, within the subspace consisting of a single polarization μ? The answer will be yes if $\hat{\mathbf{F}}$ does not mix polarizations, i.e., if $\hat{\mathbf{F}}$ is diagonalized by the same $\hat{\mathbf{U}}$ as $\hat{\mathbf{D}}$ itself,

$$\hat{\mathbf{U}}^{\dagger}\hat{\mathbf{F}}\hat{\mathbf{U}}=\begin{bmatrix}\hat{f}^{(1)} & & \\ & \hat{f}^{(2)} & \\ & & \ddots\end{bmatrix} =\text{a diagonal matrix} . \tag{4.3}$$

Then we can conjugate Eq. (4.1) with $\hat{\mathbf{U}}$ to show that

$$[\hat{f}^{(\mu)},\hat{\lambda}^{(\mu)}]=0 , \tag{4.4}$$

i.e., that the operator $\hat{f}^{(\mu)}$ on the diagonal is a conserved operator within its polarization. This can be transcribed into symbols, giving $\{f^{(\mu)},\lambda^{(\mu)}\}=0$, exactly as in scalar WKB theory.

Let us now return to the spin-orbit problem, and apply these ideas to the total angular momentum, identifying $\hat{\mathbf{F}}$ with a component $\hat{\mathbf{J}}_i$ of $\hat{\mathbf{J}}$. That is, we write

$$\hat{J}^{i}_{\alpha\beta}=\hat{L}_i\delta_{\alpha\beta}+\hbar S^{i}_{\alpha\beta} , \tag{4.5}$$

where the hat denotes an orbital operator, and where the superscript position of i has no significance except visual esthetics. The hat is omitted on S, because its components are just numbers. We conjugate this with $\hat{\mathbf{U}}$, writing the result in the form,

$$\hat{\mathbf{U}}^{\dagger}\hat{\mathbf{J}}_i\hat{\mathbf{U}}=\hat{\mathbf{U}}^{\dagger}\hat{L}_i\hat{\mathbf{U}}+\hbar\hat{\mathbf{U}}^{\dagger}\mathbf{S}_i\hat{\mathbf{U}}=\hat{L}_i\mathbf{I}-\hat{\mathbf{U}}^{\dagger}[\hat{\mathbf{U}},\hat{L}_i]+\hbar\hat{\mathbf{U}}^{\dagger}\mathbf{S}_i\hat{\mathbf{U}} , \tag{4.6}$$

where $\mathbf{I}$ is the spinor identity matrix.

To see if this is diagonal, we transcribe the three terms on the right-hand side, each of which is a matrix of orbital operators, to their corresponding matrices of Weyl symbols. The $\mu\nu$ component of the first term is

$$T^{i}_{1\mu\nu}=L_i\delta_{\mu\nu} , \tag{4.7}$$

where T_1 stands for "term 1," and where L_i is the component of the classical angular-momentum vector $\mathbf{r}\times\mathbf{p}$, in the same notation as in Secs. II and III. This term is already diagonal. In the second term on the right-hand side of Eq. (4.6) we use the Moyal formula (see Appendix A of Ref. [5]) to write

$$T^{i}_{2\mu\nu}=-i\hbar U^{*}_{a\mu}\{U_{\alpha\nu},L_i\}=-i\hbar\tau^{(\mu)*}_{\alpha}\{\tau^{(\nu)}_{\alpha},L_i\} =-i\hbar\tau^{(\mu)*}_{\alpha}\epsilon_{kji}L_k\frac{\partial\tau^{(\nu)}}{\partial L_j} , \tag{4.8}$$

where we drop terms of order $\hbar^2$, use $U_{a\mu}=\tau^{(\mu)}_{\alpha}$ as explained in Ref. [5], and finally use the fact that τ depends only on $\mathbf{L}$ to compute the Poisson bracket. Next we substitute Eq. (A22) into this and use the fact that $(\mathbf{L}\cdot\mathbf{S})\tau^{(\nu)}=\nu L\tau^{(\nu)}$ and the orthogonality relation for the eigenvectors,

$$\tau^{(\mu)*}_{\alpha}\tau^{(\nu)}_{\alpha}=\delta_{\mu\nu} , \tag{4.9}$$

to obtain

$$T^{i}_{2\mu\nu}=\hbar(\mathbf{A}^{(\mu)}\times\mathbf{L})_i\delta_{\mu\nu}+\hbar\frac{\mu L_i}{L}\delta_{\mu\nu} -\hbar(\tau^{(\mu)\dagger}S_i\tau^{(\nu)}) , \tag{4.10}$$

where $\mathbf{A}^{(\mu)}$ is Berry's vector potential on angular-momentum space as in Appendix A. Finally, the symbol matrix of the third term on the right-hand side in Eq. (4.6) is given by

$$T^{i}_{3\mu\nu}=\hbar(\tau^{(\mu)\dagger}S_i\tau^{(\nu)}) . \tag{4.11}$$

Adding these up, we find that the two terms which are not diagonal, occurring in T_2 and T_3, cancel one another, leaving a diagonal result which we write in the form $J^{(\mu)}_i\delta_{\mu\nu}$. The function $J^{(\mu)}_i$ is the symbol of the operator representing the ith component of the total angular momentum within polarization subspace μ. Reverting to three-vector notation, we have

$$\mathbf{J}^{(\mu)}=\mathbf{J}^{(\mu)}(\mathbf{r},\mathbf{p}) =\mathbf{L}\left[1+\frac{\mu\hbar}{L}\right]+\hbar\mathbf{A}^{(\mu)}\times\mathbf{L} . \tag{4.12}$$

Thus we see that the total angular momentum $\hat{\mathbf{J}}$ is diagonalized by the same $\hat{\mathbf{U}}$ as $\hat{\mathbf{D}}$, and that it does not mix polarizations; it therefore has a representative or symbol in the phase spaces of each of the polarizations, which is given by Eq. (4.12).

If we subject the orbital or spin angular momentum to the same analysis, we easily see that neither of these is diagonalized by $\hat{\mathbf{U}}$ [the result for the spin is already given in Eq. (4.11)]. Therefore neither orbital nor spin angular momentum can be represented in the subspace of a given polarization, and neither has a symbol on those subspaces. *In particular, the classical vector $\hat{\mathbf{L}}=\mathbf{r}\times\mathbf{p}$ is not the symbol of the orbital angular-momentum operator.* If we ask what function in the classical phase space represents the quantum orbital angular-momentum operator $\hat{\mathbf{L}}$, the answer is that there is no such function. The subsequent analysis of this problem cannot be understood unless this point is kept in mind; the classical vector $\mathbf{L}=\mathbf{r}\times\mathbf{p}$ must not be interpreted as the symbol of the quantum angular-momentum operator $\hat{\mathbf{L}}$.

These conclusions alleviate some of our worries of Sec. III about seeming to find a simultaneous eigenstate of $\hat{H}$ and $\hat{L}_z$ when these operators do not commute, for now we see that $L_z=\hat{\mathbf{z}}\cdot(\mathbf{r}\times\mathbf{p})$ is not the symbol of the operator representing the quantum $\hat{L}_z$ within a given polarization. But if this is so, then what operator does L_z correspond to in the original quantum system? We can answer this by reversing the symbol correspondence. We let $\hat{F}^{i}_{\alpha\beta}$ be the matrix of orbital operators corresponding to the operator whose symbol is L_i within each polarization (independent of μ). Then we have

$$\hat{F}^i_{\alpha\beta}=\sum_\mu \hat{U}_{\alpha\mu}\hat{L}_i(\hat{U}_{\beta\mu})^\dagger$$
$$=\hat{L}_i\delta_{\alpha\beta}+\sum_\mu [\hat{U}_{\alpha\mu},\hat{L}_i](\hat{U}_{\beta\mu})^\dagger . \quad (4.13)$$

This operator is more easily understood in terms of its symbol, which we compute using the same techniques as before. We find

$$F^i_{\alpha\beta}=(L_i\delta_{\alpha\beta}+\hbar S^i_{\alpha\beta})$$
$$-\hbar\frac{L_i}{L^2}(\mathbf{L}\cdot\mathbf{S})_{\alpha\beta}+\hbar\epsilon_{ijk}L_j\sum_\mu \tau^{(\mu)}_\alpha A^{(\mu)}_k\tau^{(\mu)*}_\beta . \quad (4.14)$$

The first term in this equation is the symbol of $\hat{J}^i_{\alpha\beta}$, but, overall, the operator $\hat{\mathbf{F}}^i$ (i.e., the matrix of operators with components $\hat{F}^i_{\alpha\beta}$) is not simple. This operator does commute with $\hat{\mathbf{D}}$, however, within errors of order $\hbar^2$, so at least we see that we were indeed constructing simultaneous eigenstates of commuting operators in Sec. III, even if the labeling was misleading. But the most striking thing about Eq. (4.14) is the third term, which is gauge dependent. This shows that the symbol $L_z=\hat{\mathbf{z}}\cdot(\mathbf{r}\times\mathbf{p})$, which apparently is gauge invariant, actually represents an operator which is gauge dependent. This explains why we found gauge-dependent wave functions in Sec. III, in spite of having a complete set of quantum numbers, for when one of the operators whose eigenfunctions we are computing is itself gauge dependent, then naturally the eigenfunctions are gauge dependent also.

Conversely, we have found that the gauge-invariant operator $\hat{J}_z$, when restricted to a subspace of a given polarization, is represented by a symbol which is gauge dependent, as shown in Eq. (4.12). *Thus we find that when canonical coordinates* $(\mathbf{r},\mathbf{p})$ *are used on the classical phase space, gauge-invariant operators have gauge-dependent symbols, and gauge-invariant symbols correspond to gauge-dependent operators.* The reason for this, as discussed in Ref. [5], is that the canonical coordinates $(\mathbf{r},\mathbf{p})$ are themselves, in an important sense, gauge dependent; one must use the coordinates $(\mathbf{r}',\mathbf{p}')$, which are given in Eq. (3.1) and which represent covariant derivative operations, if one wishes to avoid a gauge dependence which is hidden in the coordination themselves.

Although we have resolved many of the difficulties that arose in Sec. III when we attempted to use canonical coordinates and standard Hamilton-Jacobi methods to construct semiclassical eigenvalues and eigenfunctions, nevertheless we still have not determined the correct multiplicities, nor have we found gauge-invariant wave functions. The general difficulty has been that Berry's phase, although it does not contribute to the Hamiltonian, is still present in the problem, since Berry's 1-form on phase space, $\xi_B=i\tau^\dagger d\tau$, does not vanish. It may vanish along the Hamiltonian flow, but it does not vanish in other directions in phase space, and in particular does not vanish in all directions on the invariant torus. Therefore we now embrace the philosophy promoted in Ref. [5] of using noncanonical but gauge-invariant coordinates for the semiclassical analysis, as we might have done in the first place if the Berry's phase term in the Hamiltonian had not misled us by vanishing.

V. GAUGE-INVARIANT EIGENVALUES AND MULTIPLICITIES

The noncanonical but gauge-invariant coordinates $z'=(\mathbf{r}',\mathbf{p}')$ are given in terms of the canonical coordinates $z=(\mathbf{r},\mathbf{p})$ by Eq. (3.1), in which we can expand the Poisson bracket and express the result in terms of the vector potential $\mathbf{A}$ on angular-momentum space [defined in Eq. (A10)]. We find

$$z'_a=z_a-\hbar\mathbf{A}\cdot\{\mathbf{L},z_a\} \quad (5.1)$$

or

$$\mathbf{r}'=\mathbf{r}+\hbar\mathbf{A}\times\mathbf{r} ,$$
$$\mathbf{p}'=\mathbf{p}+\hbar\mathbf{A}\times\mathbf{p} , \quad (5.2)$$

where we have once again dropped the polarization indices. The transformation between unprimed and primed coordinates is an $O(\hbar)$ rotation which leaves magnitudes unchanged, so we can write $r'=|\mathbf{r}'|=|\mathbf{r}|=r$ and $p'=|\mathbf{p}'|=|\mathbf{p}|=p$. The small angle of rotation is gauge dependent. Furthermore, we define the vector,

$$\mathbf{L}'=\mathbf{r}'\times\mathbf{p}'=\mathbf{L}+\hbar\mathbf{A}\times\mathbf{L} , \quad (5.3)$$

which is just a convenient notation (in particular, it is to be noted that neither $\mathbf{L}$ nor $\mathbf{L}'$ is the symbol of any kind of orbital angular-momentum operator). Again, because the transformation is just a rotation, we have $L'=|\mathbf{L}'|=|\mathbf{L}|=L$.

Since the Hamiltonian of Eq. (2.11) depends only on the magnitudes r, p, and L, it has the same functional form in both the primed and unprimed coordinates. This is as it must be, since in the general case the transformation from z to z' kills the Berry's phase term in the Hamiltonian and leaves the other terms in the same functional form, and since in the present case the Berry's phase term is absent from the outset.

The total angular momentum $\hat{\mathbf{J}}$ is represented within a polarization by the symbol given in Eq. (4.12), which is a gauge-dependent expression. But when we transform to the primed coordinates, neglecting terms of order $\hbar^2$, we find

$$\mathbf{J}(\mathbf{r}',\mathbf{p}')=\mathbf{L}'\left[1+\frac{\mu\hbar}{L}\right] , \quad (5.4)$$

showing that the gauge-invariant operator $\hat{\mathbf{J}}$ is represented by a gauge-invariant symbol in the primed coordinates. Notice that $\mathbf{J}$ is parallel to $\mathbf{L}'$, but has a different magnitude.

We now construct the fundamental objects necessary for doing classical mechanics in noncanonical coordinates, beginning with the symplectic 1-form. In our primed coordinates, the symplectic 1-form is given by $\xi=\xi_c+\hbar\xi_B$, where the canonical part ξ_c is $\mathbf{p}'\cdot d\mathbf{r}'$, and where ξ_B is given by Eqs. (A8)–(A10). The total symplectic 1-form is

$$\xi=\mathbf{p}'\cdot d\mathbf{r}'+\hbar\mathbf{A}(\mathbf{L}')\cdot d\mathbf{L}' \ . \tag{5.5}$$

This is the differential form which is integrated around closed contours to compute action integrals.

From the 1-form we derive the total symplectic 2-form, $\Omega=d\xi$,

$$\Omega=\Omega_c+\hbar\Omega_B=dp_i'\wedge dr_i'-\frac{\mu\hbar}{2L^3}\epsilon_{ijk}L_i'dL_j'\wedge dL_k' \ , \tag{5.6}$$

where we use Eq. (A24) for the curl of $\mathbf{A}$. By expanding out the dL's, this can be written

$$\Omega=M_{ij}dp_i'\wedge dr_j' \ , \tag{5.7}$$

where the 3×3 symmetric matrix $\mathbf{M}$ is given by

$$M_{ij}=\delta_{ij}+\frac{\mu\hbar}{L^3}L_i'L_j' \ . \tag{5.8}$$

If we write $\Omega=\frac{1}{2}\Omega_{ab}dz_a'\wedge dz_b'$, expressing Ω in terms of its component matrix on phase space, then we have

$$\Omega_{ab}=\begin{bmatrix}0 & -\mathbf{M}\\ \mathbf{M} & 0\end{bmatrix} , \tag{5.9}$$

in the ordering $z_a=(\mathbf{r}',\mathbf{p}')$, $a=1,\ldots,6$.

From this we determine the matrix of fundamental Poisson brackets J_{ab}, which is the inverse of Ω_{ab}, as explained in Appendix B of Ref. [5]. We carry out the inversion exactly (not truncating at order $\hbar$), so that important identities such as the Jacobi identity will be exact. We have

$$J_{ab}=\begin{bmatrix}0 & \mathbf{M}^{-1}\\ -\mathbf{M}^{-1} & 0\end{bmatrix} , \tag{5.10}$$

where

$$(\mathbf{M}^{-1})_{ij}=\delta_{ij}-\frac{\mu\hbar}{L^2(L+\mu\hbar)}L_i'L_j' \ . \tag{5.11}$$

The components J_{ab} are the fundamental Poisson brackets themselves, which are otherwise expressed by

$$\{r_i',r_j'\}=\{p_i',p_j'\}=0, \quad \{r_i',p_j'\}=(\mathbf{M}^{-1})_{ij} \ , \tag{5.12}$$

or by

$$\{f,g\}=(\mathbf{M}^{-1})_{ij}\left[\frac{\partial f}{\partial r_i'}\frac{\partial g}{\partial p_j'}-\frac{\partial f}{\partial p_i'}\frac{\partial g}{\partial r_j'}\right] , \tag{5.13}$$

where f and g are any two functions of $(\mathbf{r}',\mathbf{p}')$.

We can now use Eq. (5.13) to compute Poisson brackets among various gauge-invariant expressions of interest. The components of $\mathbf{L}'$ are a good place to begin. After some algebra, we find

$$\{L_i',L_j'\}=\frac{L}{L+\mu\hbar}\epsilon_{ijk}L_k' \ . \tag{5.14}$$

This shows that the components of $\mathbf{L}'$ do not generate an SO(3) Lie algebra, and therefore their Hamiltonian flows are not rotations on the phase space of a given polarization. But the relation $\{\mathbf{L}',L^2\}=0$ follows easily from Eq. (5.14), and shows that we can multiply both sides by $(1+\mu\hbar/L)^2$ and bring the L inside the Poisson bracket. The result can be expressed in term of $\mathbf{J}$, given by Eq. (5.4). We find

$$\{J_i,J_j\}=\epsilon_{ijk}J_k \ , \tag{5.15}$$

so that it is the total angular momentum of the quantum problem, expressed in terms of a symbol on the phase space of a single polarization, which does form an SO(3) Lie algebra. Thus, it is $\mathbf{J}$, not $\mathbf{L}$ or $\mathbf{L}'$, which generates classical rotations.

The total angular momentum generates rotations in all the proper senses, as we see from the additional Poisson bracket relations,

$$\begin{aligned}\{r_i',J_j\}&=\epsilon_{ijk}r_k' \ ,\\ \{p_i',J_j\}&=\epsilon_{ijk}p_k' \ ,\\ \{L_i',J_j\}&=\epsilon_{ijk}L_k' \ .\end{aligned} \tag{5.16}$$

We now consider the problem of determining the semiclassical eigenvalues of the Hamiltonian H of Eq. (2.11), using the Liouville method in noncanonical coordinates. To begin we require three gauge-invariant observables which commute with one another and with H. Gauge-invariant observables which commute with H include $\mathbf{J}$, $\mathbf{L}'$, J^2, L^2, and H itself. We select the observables (H,J^2,J_z) for the involutive set. By the Liouville-Arnold theorem, the level sets of these observables in phase space are 3-tori, and, as in Sec. III, we determine basis contours on the tori by examining the flows generated by these observables. An important difference is that now we use the noncanonical Poisson bracket of Eq. (5.13) to compute the equations of motion.

The flow equations for J_z are

$$\begin{aligned}\frac{d\mathbf{r}'}{dt_3}&=\{\mathbf{r}',J_z\}=\hat{\mathbf{z}}\times\mathbf{r}' \ ,\\ \frac{d\mathbf{p}'}{dt_3}&=\{\mathbf{p}',J_z\}=\hat{\mathbf{z}}\times\mathbf{p}' \ .\end{aligned} \tag{5.17}$$

The orbits are rotations about $\hat{\mathbf{z}}$, exactly as in Eq. (3.4), with period $t_3=2\pi$. Now, however, we use the noncanonical expression for the symplectic 1-form, given in Eq. (5.5), to compute the action I_3. We have

$$I_3=\frac{1}{2\pi}\int_0^{2\pi}\left[\mathbf{p}'\cdot\frac{d\mathbf{r}'}{dt_3}+\hbar\mathbf{A}\cdot\frac{d\mathbf{L}'}{dt_3}\right]dt_3 \ . \tag{5.18}$$

The first term in the integrand is L_z', which can be pulled out of the integral since $\{L_z',J_z\}=0$. The second term is the loop integral of the vector potential $\mathbf{A}$ around a small circle on the sphere in angular-momentum space, as shown in Fig. 1, since we have

$$\frac{d\mathbf{L}'}{dt_3}=\{\mathbf{L}',J_z\}=\hat{\mathbf{z}}\times\mathbf{L}' \ . \tag{5.19}$$

Therefore the second term gives $-\mu\hbar$ times the solid angle of the cap containing the north pole. Altogether, we have

$$I_3=L_z'-\mu\hbar(1-\cos\theta_l)=J_z-\mu\hbar \ . \tag{5.20}$$

The flow equations for J^2 are

$$\frac{d\mathbf{r}'}{dt_2}=\{\mathbf{r}',J^2\}=2\mathbf{J}\times\mathbf{r}' ,$$
$$\frac{d\mathbf{p}'}{dt_2}=\{\mathbf{p}',J^2\}=2\mathbf{J}\times\mathbf{p}' , \tag{5.21}$$

which are rotations in the plane perpendicular to $\mathbf{J}$ with period $t_2=\pi/J$, very much as in Eq. (3.7). The second action is

$$I_2=\frac{1}{2\pi}\int_0^{\pi/J}\left[\mathbf{p}'\cdot\frac{d\mathbf{r}'}{dt_2}+\hbar\mathbf{A}\cdot\frac{d\mathbf{L}'}{dt_2}\right]dt_2 , \tag{5.22}$$

in which the second term vanishes, since $d\mathbf{L}'/dt_2=\{\mathbf{L}',J^2\}=0$. By Eq. (5.21), the first term in the integrand is $2\mathbf{J}\cdot\mathbf{L}'=2JL$, which is constant along the J^2 flow and can be taken out of the integral. Altogether we have

$$I_2=L , \tag{5.23}$$

the same answer as in Sec. III.

To find the final basis contour and action, we begin by computing the equations of motion for H itself in the primed coordinates. As noted earlier, the functional form of H is the same in both the unprimed and primed coordinates, and when we use the Poisson bracket of Eq. (5.13) to compute the equations of motion, we find that the second term of Eq. (5.11) does not contribute. Therefore the equations of motion also have the same functional form in the primed coordinates as in the unprimed coordinates, which is shown in Eq. (3.9). As before, the final basis contour on the torus is a combination of the H flow and the J^2 flow, and the final action is given by $I_1=(1/2\pi)\oint p_r dr$, exactly as in Sec. III.

We see that of the three actions, only $I_3=J_z-\mu\hbar$ differs in this calculation from what it was in Sec. III (where we had $I_3=L_z$). The two calculations give different results because they are based on different tori; the calculation of Sec. III was not wrong, but it was based on a torus which was gauge dependent (since L_z itself is gauge dependent). In this section, however, our torus is a level set of (H,J^2,J_z) and is gauge invariant. The reason there is more than one invariant torus for a given energy is that the spin-orbit problem is degenerate, both classically and quantum mechanically.

In any case, we can now quantize the actions. We assign quantum numbers (n,l,m_j) according to

$$I_1=(n-l-\tfrac{1}{2})\hbar ,$$
$$I_2=L=(l+\tfrac{1}{2})\hbar , \tag{5.24}$$
$$I_3=J_z-\mu\hbar=(m_j-\mu)\hbar .$$

The quantum numbers n and l are as in Eq. (3.11), but m_j is new. The Maslov index for the action I_3 is zero, because there are no turning points in the motion of Eq. (5.17), and the quantum number of I_3 is $m_j-\mu$, an integer. But if s is half-integral, then so will be μ and therefore also m_j. This is of course what we expect, but we notice that the half-integral quantization of J_z, when it occurs, is not due to the Maslov index.

Any function of the actions is also quantized. In particular, by Eq. (5.4) we have

$$J=L+\mu\hbar , \tag{5.25}$$

so the quantized values of J are

$$J=(j+\tfrac{1}{2})\hbar , \tag{5.26}$$

where we have "discovered" the relation $j=l+\mu$ [that is, without having to call on the exact quantum solution, as we did in writing down Eq. (2.13)]. Then, from the classical inequality $-J\le J_z\le+J$, we obtain $m_j=-j,\ldots,+j$, for a total of $2j+1$ values. Thus, the tori, when represented and counted in the noncanonical $(\mathbf{r}',\mathbf{p}')$ coordinates, give the correct multiplicities for the energy levels. There are no worries about monopole strings, since the strings are gauge dependent, and the coordinates $(\mathbf{r}',\mathbf{p}')$ are gauge invariant.

We really have $2j+1$ quantized tori for a given energy level, as is clearly shown in the gauge-invariant coordinates $(\mathbf{r}',\mathbf{p}')$. But since the transformation to the gauge-dependent coordinates $(\mathbf{r},\mathbf{p})$ always has a singularity somewhere in phase space, the representation of those tori near the singularity in terms of the coordinates $(\mathbf{r},\mathbf{p})$ cannot be trusted. From an invariant geometrical standpoint, we have to say that the phase space itself has no singularities, and that it is foliated into invariant tori exactly as the phase space in any integrable scalar WKB problem. But this fact is obscured by using the gauge-dependent coordinates $(\mathbf{r},\mathbf{p})$.

This calculation reveals an important general fact which was not pointed out in Ref. [5], namely, that the singularities associated with monopole strings only appear when canonical coordinates are used, and disappear when the gauge-invariant, noncanonical coordinates are used. This is because the monopole strings themselves are gauge dependent, and cannot therefore appear when gauge-invariant coordinates are used.

Because the radial action $I_r=I_1$ is exactly the same as in the canonical calculation of Sec. III, the energy levels determined here are also the same as there, and, in particular, they agree with a standard semiclassical treatment of the radial wave equation. Altogether, we have determined both the correct energy levels and the correct multiplicities by working in the noncanonical coordinates.

VI. SEMICLASSICAL WAVE FUNCTIONS

We will now calculate the semiclassical wave functions of the Hamiltonian of Eq. (2.1) for arbitrary values of the spin s. To do this it is advisable first to familiarize oneself with the standard calculation for the scalar case $s=0$, which is summarized in Appendix C.

The multicomponent WKB wave function has the general form

$$\psi_\alpha(\mathbf{r})=\sum_b B_b(\mathbf{r})\tau_\alpha(\mathbf{r},\mathbf{p}_b)e^{iS_b(\mathbf{r})/\hbar-i\nu_b\pi/2} , \tag{6.1}$$

which is the multicomponent generalization of Eq. (C15) and which is discussed in detail in Ref. [5]. Here

$\mathbf{p}_b=\nabla S_b(\mathbf{r})$ and the other notation is explained below Eq. (C15). We will now work out the pieces of this wave function for the problem at hand.

We work in the phase space of a given polarization μ, and generally suppress polarization indices. We will also generally suppress the quantum the quantum number j, since if l is given and μ is understood, then j follows by $j=l+\mu$. The invariant tori in the given phase space are the level sets of (H,J^2,J_z) or of $(I_1,I_2,I_3)=(I_r,L,J_z-\mu\hbar)$, which are quantized according to Eq. (5.24). To compute the wave functions, we must use the gauge-dependent coordinates $(\mathbf{r},\mathbf{p})$, in terms of which the tori have gauge-dependent representations. Actually, as we have seen, the expressions for both H and L^2 in terms of $(\mathbf{r},\mathbf{p})$ are gauge invariant, so only that for J_z is gauge dependent. To express J_z as a function of $(\mathbf{r},\mathbf{p})$, we combine Eqs. (5.3) and (5.4) and neglect terms of order $\hbar^2$ to obtain

$$J_z=L_z+\hbar\left[\mu\frac{L_z}{L}+\hat{\mathbf{z}}\cdot(\mathbf{A}\times\mathbf{L})\right], \tag{6.2}$$

where $\mathbf{A}=\mathbf{A}(\mathbf{L})$ is the vector potential for Berry's phase in angular-momentum space, as discussed in Appendix A.

The only gauges we will use are north standard gauge and south standard gauge, which we will distinguish by setting $\sigma=+1$ and $\sigma=-1$, respectively, where σ is a code to indicate the gauge. Then by Eqs. (A30) and (A33), we have

$$\mathbf{A}(\mathbf{L})=\frac{\mu(\cos\theta_l-\sigma)}{L\sin\theta_l}\hat{\boldsymbol{\phi}}_l, \tag{6.3}$$

which we cross with $\mathbf{L}=L\hat{\boldsymbol{l}}$ to obtain

$$\hat{\mathbf{z}}\cdot(\mathbf{A}\times\mathbf{L})=\mu(\sigma-\cos\theta_l). \tag{6.4}$$

Here it is important to remember that the triad $(\hat{\boldsymbol{l}},\hat{\boldsymbol{\theta}}_l,\hat{\boldsymbol{\phi}}_l)$ is attached to the tip of the vector $\mathbf{L}$, and is not the same as the triad $(\hat{\mathbf{r}},\hat{\boldsymbol{\theta}},\hat{\boldsymbol{\phi}})$ which is attached to the tip of the vector $\mathbf{r}$. Combining Eqs. (6.2) and (6.4), we have

$$J_z=L_z+\sigma\mu\hbar, \tag{6.5}$$

which is the desired expression for J_z in terms of $(\mathbf{r},\mathbf{p})$. In this equation, the gauge dependence of L_z cancels that of $\sigma\mu\hbar$, to give the gauge invariant J_z. Thus we see that L_z is invariant on any quantized torus, although its value,

$$L_z=(m_j-\sigma\mu)\hbar, \tag{6.6}$$

is gauge dependent.

In spite of this gauge dependence, the torus is still a level set of (H,L^2,L_z). Therefore if we pick one of our gauges, then we can compute the action function $S=S_r+S_\theta+S_\phi$ exactly as in Appendix C, except that we use Eq. (6.6) instead of $L_z=m\hbar$ for the quantized value of L_z. This action has the same four branches discussed in Appendix C.

Furthermore, the relation between the amplitude B and the action S is the same in multicomponent WKB theory as it is in the scalar case, so the computation of the amplitude is exactly as discussed in Appendix C. In particular, B factors into a radial and an angular part, $B=B_rB_\Omega$, as shown in Eqs. (C16)–(C18).

Next we consider the eigenvectors τ. In a general problem in multicomponent WKB theory, there are as many branches b to the eigenvector τ as there are to the action S, because $\tau(\mathbf{r},\mathbf{p})$ is evaluated at $\mathbf{p}=\nabla S_b$. In the present problem, however, the four branches of S discussed below Eq. (C4) correspond to only two branches of τ, since τ depends only on $\mathbf{L}$. That is, according to Eqs. (C3) and (C4), $\mathbf{L}$ has the same two branches as p_θ, and is independent of the branch for p_r.

The two branches of p_θ correspond to two orbits, and the two values of $\mathbf{L}$ are perpendicular to their respective orbital planes. The physical situation is illustrated in Figs. 2 and 3. The spherical angles (θ_l,ϕ_l) of either of the vectors $\mathbf{L}$ are related to the inclination κ and longitude of ascending node γ of the corresponding orbit by

$$\theta_l=\kappa,\quad \phi_l=\gamma-\pi/2, \tag{6.7}$$

as is clear geometrically from Fig. 2.

Denoting the branches of p_θ by a $\pm$ sign as in Appendix C, we write $\gamma_\pm$, $\phi_{l\pm}$, $\omega_\pm$, $\eta_\pm$, and $\tau_\pm$ for various quantities of interest (the angles ω and η are defined in Fig. 2, and discussed in Appendix C). The sign is not necessary on $\kappa=\theta_l$, because both orbits in Fig. 3 have the same inclination. By the geometry illustrated in Figs. 2 and 3, we have

$$\phi_{l-}+\phi_{l+}=2\phi, \tag{6.8}$$

where ϕ is the azimuthal angle at which the wave function $\psi(r,\theta,\phi)$ is to be evaluated, i.e., of the point P in the figures. As for the eigenvector τ, we can use Eqs. (A34) and (A35) to write

$$\tau_{\pm\alpha}=\tau_\alpha(\theta_l,\phi_{l\pm})=e^{i(\sigma\mu-\alpha)\phi_{l\pm}}d^{(s)}_{\alpha\mu}(\theta_l), \tag{6.9}$$

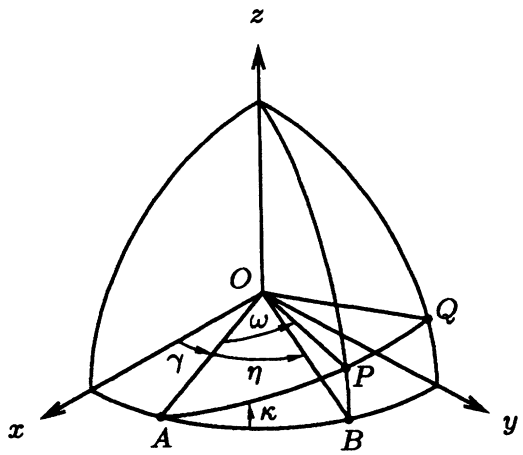

FIG. 2. Geometry of the orbit. The particle is located at P, in the plane of the orbit APQ. Point A is the ascending node, and γ is the longitude of ascending node. The inclination of the orbit is κ. The angular-momentum vector $\mathbf{L}$ (not shown) is perpendicular to the plane of the orbit, in a direction given by $(\theta_l,\phi_l)=(\kappa,\gamma-\pi/2)$.

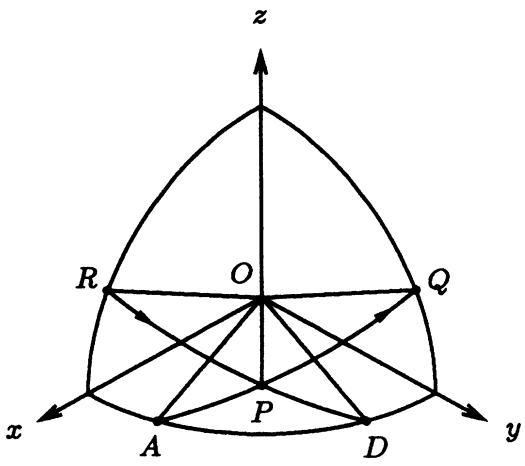

FIG. 3. For a given direction of the particle OP, i.e., for given values of (θ,ϕ) and (L,L_z), the two branches of p_θ correspond physically to two orbits. The branch $p_\theta<0$ is the orbit APQ in the figure, and the branch $p_\theta>0$ is the orbit RPD. Point A is the ascending node of the orbit $p_\theta<0$, and D is the descending node of the orbit $p_\theta>0$.

for the two branches $(\pm)$ of τ in either of the two gauges $(\sigma=\pm1)$.

We can now assemble the WKB wave function in Eq. (6.1). It separates into a radial and angular part, just as the exact wave function did in Eq. (3.12) and as the scalar wave function did in Eqs. (C16)–(C19). We write

$$\psi_\alpha^{nlm_j}(r,\theta,\phi)=\frac{1}{r}\Phi_{nl}(r)\mathcal{Y}_\alpha^{lm_j}(\theta,\phi) \tag{6.10}$$

to indicate this separation, and we concentrate on the angular part $\mathcal{Y}$, which carries the spinor index, and which alone can be calculated explicitly without knowledge of the functional form of the potential.

The WKB formula for $\mathcal{Y}$ is

$$\mathcal{Y}_\alpha^{lm_j}(\theta,\phi)=B_\Omega e^{iL_z\phi/\hbar}(\tau_{-\alpha}e^{iS_{\theta-}/\hbar}+\tau_{+\alpha}e^{iS_{\theta+}/\hbar-i\pi/2}) , \tag{6.11}$$

which is a generalization of the first line of Eq. (C19). We substitute into this formula the quantized values of L and L_z given in Eqs. (5.24) and (6.6), and we use Eqs. (6.8), (6.9), and (C14) to express everything in terms of the $-$ branch $(p_\theta<0)$. We find

$$\mathcal{Y}_\alpha^{lm_j}(\theta,\phi)=B_\Omega e^{i(m_j-\alpha)\phi}d_{\alpha\mu}^{(s)}(\theta_l) \times\{e^{i[x]}+(-1)^{l-m_j+\sigma\mu}e^{-i[x]}\} , \tag{6.12}$$

where

$$[x]=(\sigma\mu-\alpha)(\phi_l-\phi)+(l+\tfrac{1}{2})\omega-(m_j-\sigma\mu)\eta . \tag{6.13}$$

In these equations and below we suppress the branch index $\pm$ on ϕ_l,ω,η, etc., it being understood that we are referring to the $-$ branch. Next we use Eq. (6.7) and the fact that $\phi=\gamma+\eta$, evident from Fig. 2, to write

$$\phi_l-\phi=-\eta-\pi/2 , \tag{6.14}$$

which allows us to rewrite the wave function in the form

$$\mathcal{Y}_\alpha^{lm_j}(\theta,\phi)=B_\Omega e^{i(m_j-\alpha)\phi+i(\alpha-\sigma\mu)\pi/2}d_{\alpha\mu}^{(s)}(\theta_l) \times\{e^{i[x']}+(-1)^{l-m_j+\alpha}e^{-i[x']}\} , \tag{6.15}$$

where now

$$[x']=(l+\tfrac{1}{2})\omega-(m_j-\alpha)\eta . \tag{6.16}$$

In these manipulations we are seeing the gradual disappearance of the gauge-dependent terms (those depending on σ), and the appearance of the phase of the asymptotic form for $Y_{lm}(\theta,\phi)$, shown in Eq. (C19), with $m=m_j-\alpha$. We must remember, however, that ω and η are functions of $L=(l+\frac{1}{2})\hbar$ and $L_z=(m_j-\sigma\mu)\hbar$, so that the value of L_z is not the right one for the asymptotic form of Y_{lm} with $m=m_j-\alpha$. If, however, ω and η were evaluated at $\tilde{L}_z=(m_j-\alpha)\hbar$, then we would have the asymptotic form of Y_{lm} which otherwise seems to be appearing. Since the difference $\Delta L_z=\tilde{L}_z-L_z=(\sigma\mu-\alpha)\hbar$ is small, i.e., of order $\hbar$, we can expand the phase in ΔL_z to convert the given phase into the desired one. We must retain terms of first order in ΔL_z, i.e., first order in $\hbar$, because we are expanding the action in the exponent of a WKB expression. But by using homogeneity arguments as in Eq. (C13), it is easy to show that the first-order terms vanish, i.e., that

$$L\omega(L,\tilde{L}_z)-L_z\eta(L,\tilde{L}_z)=L\omega(L,L_z)-L_z\eta(L,L_z) +O(\Delta L_z^2) . \tag{6.17}$$

A similar but easier argument applies to the amplitude B_Ω, which can be evaluated at either $\tilde{L}_z$ or L_z, because the amplitude is only needed to lowest order in $\hbar$.

Thus we are able to introduce the asymptotic form for Y_{lm} with $m=m_j-\alpha$. In doing this, we ignore real and positive multiplicative constants, but keep the conventional phases indicated in Eq. (C20). This gives

$$\mathcal{Y}_\alpha^{lm_j}(\theta,\phi)=e^{i(l+m_j-\sigma\mu)\pi/2}d_{\alpha\mu}^{(s)}(\theta_l)Y_{l,m_j-\alpha}(\theta,\phi) . \tag{6.18}$$

Finally, we introduce the asymptotic form for the Clebsch-Gordan coefficient,

$$\langle l,m_j-\alpha,s,\alpha|j,m_j\rangle=(-1)^{s+\mu}d_{\alpha\mu}^{(s)}(\theta_l) , \tag{6.19}$$

with $j=l+\mu$. This asymptotic form is valid when j and l are large and s is small, exactly as we require in the present calculation. It is important that the phase conventions used in the Clebsch-Gordan coefficient be coordinated with those used in the Y_{lm}; here we follow the phase conventions of Edmonds [29] in both cases. [However, Edmonds interprets his rotation matrices in a passive sense, whereas we are taking the active point of view; this means that the indices (α,μ) on the d matrix should be reversed when comparing to Edmond's formulas.] Combining Eqs. (6.18) and (6.19), we obtain the correct asymptotic form of the exact wave function shown in Eq. (3.12), to within an overall phase. The overall phase de-

pends on the quantum numbers and on gauge code σ, as it may, but not on the spinor index α, as it must not.

Thus we see that the asymptotic theory of vector-wave functions developed in Ref. [5], when applied to the angular part of three-dimensional wave functions, reproduces the asymptotic forms not only of the spherical harmonics, but also of the Clebsch-Gordan coefficients.

VII. CONCLUSIONS

In conclusion, we have shown by an explicit example how Bohr-Sommerfeld vector wave quantization works, and how Berry's phase, noncanonical coordinates, gauge structures, and monopolelike singularities are used in a practical calculation of eigenvalues and eigenfunctions. We have also obtained new insights into the meaning of invariant tori in the presence of gauge fields, and showed how symmetries, conservation laws, and conserved quantities express themselves in vector wave systems. In the future we will report on calculations involving potentials with only axial symmetry, which are not integrable and which are of greater interest in nuclear applications than the potentials studied in this paper.

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APPENDIX A: EIGENVALUES AND EIGENVECTORS OF L·S

In this appendix $\mathbf{L}\cdot\mathbf{S}$ is regarded as a $(2s+1)\times(2s+1)$ matrix, with components which are functions of the classical vector $\mathbf{L}$.

Since the eigenvalues of any component of $\mathbf{S}$ are just $\mu=-s,\ldots,+s$, the eigenvalues of $\mathbf{L}\cdot\mathbf{S}$ are μL, where μ is the polarization index and $L=|\mathbf{L}|$. We will assume that $L\neq 0$, i.e., we will stay away from those regions of phase space where $L=0$, so that the eigenvalues can be assumed to be nondegenerate.

If R is some 3×3 proper rotation matrix, then we write $U(R)$ for the corresponding spinor rotation, i.e., the $(2s+1)$-dimensional unitary representative of R if s is integral, or one of the two representatives, appropriately chosen, if s is half-integral. In terms of $U(R)$, the formula expressing the adjoint action of the rotation group is

$$U(R)^{\dagger}(\mathbf{a}\cdot\mathbf{S})U(R)=\mathbf{a}\cdot(R\mathbf{S})=(R^{-1}\mathbf{a})\cdot\mathbf{S}\ , \tag{A1}$$

where $\mathbf{a}$ is any three-vector. The exponentiated version of this equation is

$$U(R)^{\dagger}U(\hat{\mathbf{n}},\gamma)U(R)=U(R^{-1}\hat{\mathbf{n}},\gamma)\ , \tag{A2}$$

where a rotation matrix in axis angle form is conjugated by another, and where γ is any angle.

If $\mathbf{L}\neq 0$, we will write the direction of $\mathbf{L}$ as $\hat{l}$, and denote the spherical angles of $\hat{l}$ by (θ_l,ϕ_l). The subscripts on these angles are to distinguish them from the angles (θ,ϕ) which elsewhere in the paper are used to denote the spherical angles of the particle position, i.e., the vector $\mathbf{r}$. A particular rotation R of interest is one which rotates the $\hat{\mathbf{z}}$ axis into $\hat{l}$,

$$R\hat{\mathbf{z}}=\hat{l}\ . \tag{A3}$$

Since this R is parametrized by $\mathbf{L}$, we will write $R(\mathbf{L})$, $R(\hat{l})$, or $R(\theta_l,\phi_l)$ for it, and $U(\mathbf{L})$, $U(\hat{l})$, or $U(\theta_l,\phi_l)$ for the corresponding spinor rotation.

We denote the orthonormal eigenvectors of S_z by $\tau_z^{(\mu)}$, so that

$$S_z\tau_z^{(\mu)}=\mu\tau_z^{(\mu)}\ . \tag{A4}$$

If the standard representations for the matrices $\mathbf{S}$ are used, in which S_z is diagonal, then $\tau_{z\alpha}^{(\mu)}=\delta_{\alpha\mu}$. In terms of the eigenvectors of S_z, we define

$$\tau^{(\mu)}=U(\mathbf{L})\tau_z^{(\mu)}\ , \tag{A5}$$

which, as one can show by using Eqs. (A1)–(A4), are eigenvectors of $\mathbf{L}\cdot\mathbf{S}$,

$$(\mathbf{L}\cdot\mathbf{S})\tau^{(\mu)}=\mu L\tau^{(\mu)}\ . \tag{A6}$$

In the standard representations for the matrices S, the eigenvectors $\tau^{(\mu)}$ are the columns of $U(\mathbf{L})$.

We will sometimes write $\tau^{(\mu)}(\mathbf{L})$ or $\tau^{(\mu)}(\hat{l})$ or $\tau^{(\mu)}(\theta_l,\phi_l)$ for the eigenvectors, to show that they, like R and U, are functions of $\mathbf{L}$ or of its direction. We choose phase conventions so that the eigenvector $\tau^{(\mu)}$ actually depends only on $\hat{l}$ and not on the magnitude of $\mathbf{L}$; thus, $\tau^{(\mu)}$ can be regarded primarily as a spinor field over the unit sphere in angular-momentum space, and becomes a function of $\mathbf{L}$ only by lifting, i.e., by writing $\tau^{(\mu)}(\mathbf{L})=\tau^{(\mu)}(\hat{l}(\mathbf{L}))$. Similarly, we will regard R and U as fields of matrices over the unit $\hat{l}$ sphere, which can be lifted into the full angular-momentum space in the same way. The collection of eigenvectors $\tau^{(\mu)}$ for all μ forms a field of orthonormal spinor frames over the unit $\hat{l}$ sphere, which can be lifted along with the individual eigenvectors themselves. All these fields, R, U, $\tau^{(\mu)}$, and the orthonormal frames, can be lifted a second time from angular-momentum space to the full phase by writing, for example, $R(\mathbf{r},\mathbf{p})=R(\mathbf{L}(\mathbf{r},\mathbf{p}))$, where $\mathbf{L}(\mathbf{r},\mathbf{p})=\mathbf{r}\times\mathbf{p}$.

Changes in phase conventions for the eigenvectors $\tau^{(\mu)}$ are the gauge transformations in the theory of Berry's phase [21]. In order to preserve the interpretation of the eigenvectors as fields over the unit $\hat{l}$ sphere, we require that the gauge scalar g also be such a field, i.e., a function of $\hat{l}$, or else the lift of such a function into the full angular-momentum space or phase space. The gauge transformation itself has the form,

$$\tau^{(\mu)}\rightarrow e^{ig^{(\mu)}}\tau^{(\mu)}\ ; \tag{A7}$$

notice that g, like τ, depends on the polarization μ (different polarizations can be subjected to different gauge

transformations).

The rotation matrices R that satisfy Eq. (A3) are not uniquely determined by that equation, since an R that satisfies Eq. (A3) can be multiplied on the right by any rotation about the $\hat{\mathbf{z}}$ axis, or on the left by any rotation about the $\hat{\boldsymbol{l}}$ axis, and the new R will also satisfy Eq. (A3). Thus, there is a convention involved in the selection of R and therefore of U as fields over the unit $\hat{\boldsymbol{l}}$ sphere. If $\mu \neq 0$, then redefining R in this way is equivalent to performing a gauge transformation on $\tau^{(\mu)}$, so the conventions for R, U, and $\tau^{(\mu)}$ are all closely related.

Given a convention for $\tau^{(\mu)}$, we define Berry's 1-form by

$$\xi_B^{(\mu)} = i(\tau^{(\mu)})^\dagger d\tau^{(\mu)} , \tag{A8}$$

where B stands for "Berry." This may be regarded primarily as a 1-form over the unit $\hat{\boldsymbol{l}}$ sphere, which can be progressively lifted into $\mathbf{L}$ space and then into the full phase space. When $\xi_B^{(\mu)}$ is regarded as a 1-form over $\mathbf{L}$ space, we will use the alternative notation,

$$\xi_B^{(\mu)} = \mathbf{A}^{(\mu)}(\mathbf{L})\cdot d\mathbf{L} , \tag{A9}$$

where $\mathbf{A}^{(\mu)}(\mathbf{L})$ is a "vector potential" in angular-momentum space. Thus, we have

$$\mathbf{A}^{(\mu)}(\mathbf{L}) = i(\tau^{(\mu)})^\dagger \frac{\partial \tau^{(\mu)}}{\partial \mathbf{L}} . \tag{A10}$$

Under the gauge transformation of Eq. (A7), we have the transformation laws,

$$\xi_B^{(\mu)} \rightarrow \xi_B^{(\mu)} - dg^{(\mu)} , \tag{A11}$$

$$\mathbf{A}^{(\mu)} \rightarrow \mathbf{A}^{(\mu)} - \frac{\partial g^{(\mu)}}{\partial \mathbf{L}} . \tag{A12}$$

For the remainder of this appendix, we will drop the polarization index (μ), it being henceforth understood that we are working with a definite polarization, and that all the quantities, τ, g, ξ_B, and $\mathbf{A}$, depend implicitly on μ.

We now consider the parallel transport of an eigenvector τ along a curve. Let some phase convention for $\tau(\mathbf{L})$ be chosen, and let $\mathbf{L}_0$ be some value of angular momentum through which a curve $\mathbf{L}(s)$ passes, with $\mathbf{L}(0)=\mathbf{L}_0$. Let $\bar{\tau}(s)$ be the parallel transported eigenvector along the curve, subject to the initial condition $\bar{\tau}(0)=\tau(\mathbf{L}_0)$. Then $\bar{\tau}(s)$ is equal to $\tau(\mathbf{L}(s))$ to within a phase, and satisfies the differential equation [21]

$$i\bar{\tau}^\dagger \frac{d\bar{\tau}}{ds} = 0 . \tag{A13}$$

The phase factor relating the transported eigenvector $\bar{\tau}(s)$ and the conventional eigenvector $\tau(\mathbf{L}(s))$ along the curve can be worked out by using Eqs. (A10) and (A13). The result is

$$\bar{\tau}(s) = \exp\left[i\int_0^s \mathbf{A}\cdot\frac{d\mathbf{L}}{ds} ds \right] \tau(\mathbf{L}(s)) . \tag{A14}$$

In particular, if the curve is a closed loop, then we have

$$\bar{\tau}_{\text{final}} = \exp\left[\oint \mathbf{A}\cdot d\mathbf{L} \right] \tau_{\text{initial}} . \tag{A15}$$

Now suppose the curve $\mathbf{L}(s)$, when projected onto the unit $\hat{\boldsymbol{l}}$ sphere, is a great circle, and that the parameter $s=\alpha$ is the angle along the great circle. Then the parallel transported vector can be expressed in terms of a rotation taking place in the plane of the great circle,

$$\bar{\tau}(\alpha) = U(\hat{\mathbf{m}},\alpha)\tau(\mathbf{L}_0) , \tag{A16}$$

where $\hat{\mathbf{m}}$ is a unit vector perpendicular to the plane of the great circle, and $U(\hat{\mathbf{m}},\alpha)$ denotes a rotation about $\hat{\mathbf{m}}$ by angle α, i.e.,

$$U(\hat{\mathbf{m}},\alpha) = e^{-i\alpha\hat{\mathbf{m}}\cdot\mathbf{S}} . \tag{A17}$$

To prove Eq. (A16), first we note that $\bar{\tau}(\alpha)$ is indeed an eigenvector of $\mathbf{L}(\alpha)\cdot\mathbf{S}$, as follows from Eq. (A1). Next, we use Eq. (A16) to compute the left-hand side of Eq. (A13), to get

$$i\bar{\tau}^\dagger \frac{d\bar{\tau}}{d\alpha} = \bar{\tau}^\dagger(\hat{\mathbf{m}}\cdot\mathbf{S})\bar{\tau} . \tag{A18}$$

We have here the expectation value of $\hat{\mathbf{m}}\cdot\mathbf{S}$ with respect to an eigenvector of a component of $\mathbf{S}$, namely, $\hat{\boldsymbol{l}}\cdot\mathbf{S}$, which is in a direction perpendicular to $\hat{\mathbf{m}}$. This must vanish, as one can see by taking expectation values of the commutation relations of the $\mathbf{S}$ matrices. This proves Eq. (A16).

Next we consider two neighboring points $\mathbf{L}$ and $\mathbf{L}+\Delta\mathbf{L}$ of angular-momentum space, assuming again that definite phase conventions for $\tau(\mathbf{L})$ have been chosen. We parallel transport $\tau(\mathbf{L})$ over to $\mathbf{L}+\Delta\mathbf{L}$, and compute the result $\bar{\tau}(\mathbf{L}+\Delta\mathbf{L})$ in two different ways. In the first computation, we use Eq. (A14), which we write in the form

$$\bar{\tau}(\mathbf{L}+\Delta\mathbf{L}) = (1+i\,\mathbf{A}\cdot\Delta\mathbf{L})\tau(\mathbf{L}+\Delta\mathbf{L}) , \tag{A19}$$

since the path is infinitesimal. In the second calculation, we rotate by an infinitesimal angle $\Delta\alpha$ in the plane spanned by $\mathbf{L}$ and $\mathbf{L}+\Delta\mathbf{L}$, i.e., we use Eq. (A16), setting

$$\hat{\mathbf{m}}\Delta\alpha = \frac{\mathbf{L}\times\Delta\mathbf{L}}{L^2} . \tag{A20}$$

Then we have

$$\bar{\tau}(\mathbf{L}+\Delta\mathbf{L}) = \left[1 - \frac{i}{L^2}(\mathbf{L}\times\Delta\mathbf{L})\cdot\mathbf{S} \right] \tau(\mathbf{L}) . \tag{A21}$$

Equating these two results and setting $\tau(\mathbf{L}+\Delta\mathbf{L})=\tau(\mathbf{L})+\Delta\tau$, we obtain the useful result,

$$\frac{\partial\tau}{\partial\mathbf{L}} = i\left[-\mathbf{A} + \frac{\mathbf{L}\times\mathbf{S}}{L^2} \right]\tau . \tag{A22}$$

This result is consistent with Eq. (A10) because, when we multiply by $\tau^\dagger$, the second term on the right-hand side vanishes, for the same reason as the right-hand side of Eq. (A18).

Rotations can also be used to parallel transport vectors along arbitrary curves in $\mathbf{L}$ space, not just those which project onto great circles on the unit $\hat{\boldsymbol{l}}$ sphere. We simply break the curve into a large number of small segments, each of which is the small arc of a great circle, and apply

Eqs. (A20) and (A21) to each of them. The result is the parallel transport equation,

$$\frac{d\bar{\tau}}{ds}=\frac{i}{L^2}\left[\left[\frac{d\mathbf{L}}{ds}\times\mathbf{L}\right]\cdot\mathbf{S}\right]\bar{\tau}=i\left[\left[\frac{d\hat{\mathbf{l}}}{ds}\times\hat{\mathbf{l}}\right]\cdot\mathbf{S}\right]\bar{\tau}\ . \quad \text{(A23)}$$

By using this to transport a vector around a small closed loop on the unit circle and comparing the result with Eq. (A15), we obtain

$$\nabla\times\mathbf{A}=-\frac{\mu\hat{\mathbf{l}}}{L^2}\ , \quad \text{(A24)}$$

where $\nabla=\partial/\partial\mathbf{L}$, or,

$$\oint\mathbf{A}\cdot d\mathbf{L}=-\mu\Omega\ , \quad \text{(A25)}$$

where Ω is the solid angle subtended by the loop. This is the usual result in the theory of Berry's phase [21], here obtained without committing ourselves to any specific gauge.

Now we introduce two gauges. The first, which we call "north standard gauge," is obtained by rotating the eigenstates of S_z away from the north pole along great circles of constant longitude. That is, we set

$$U(\theta_l,\phi_l)=U(\hat{\boldsymbol{\phi}}_l,\theta_l)=U(\hat{\mathbf{z}},\phi_l)U(\hat{\mathbf{y}},\theta_l)U(\hat{\mathbf{z}},-\phi_l)\ , \quad \text{(A26)}$$

where in the middle expression we use an axis-angle notation for the rotation, where we have used Eq. (A2) to factor the operator, and where

$$\hat{\boldsymbol{\phi}}_l=-\hat{\mathbf{x}}\sin\phi_l+\hat{\mathbf{y}}\cos\phi_l \quad \text{(A27)}$$

is the usual unit vector in spherical coordinates.

The vector potential $\mathbf{A}$ can be determined in this gauge by using the geometrical construction illustrated in Fig. 4. Once again we consider two neighboring points $\mathbf{L}$ and $\mathbf{L}+\Delta\mathbf{L}$, and we parallel transport τ from $\mathbf{L}$ to $\mathbf{L}+\Delta\mathbf{L}$, calling the result $\bar{\tau}(\mathbf{L}+\Delta\mathbf{L})$. We also write U_1,U_2,U_3 for the three spinor rotations which parallel transport eigenvectors along the arcs of great circles shown in the figure. Then we have

$$\begin{aligned}\bar{\tau}(\mathbf{L}+\Delta\mathbf{L})&=U_3\tau(\mathbf{L})\\&=U_3U_2\tau_z\\&=U_3U_2U_1\tau(\mathbf{L}+\Delta\mathbf{L})\\&=e^{i\mathbf{A}(\mathbf{L})\cdot\Delta\mathbf{L}}\tau(\mathbf{L}+\Delta\mathbf{L})=e^{-i\mu\Omega}\tau(\mathbf{L}+\Delta\mathbf{L})\ ,\end{aligned} \quad \text{(A28)}$$

where the fourth equality follows from Eq. (A14) and the last from Eq. (A15), and where Ω is the solid angle subtended by the path 123 on the sphere. By simple geometry we have $\Omega=(1-\cos\theta_l)\Delta\phi_l$, so the equality of the final two expressions in Eq. (A28) gives

$$\mathbf{A}(\mathbf{L})\cdot d\mathbf{L}=-\mu(1-\cos\theta_l)d\phi_l\ , \quad \text{(A29)}$$

or

$$\mathbf{A}(\mathbf{L})=-\frac{\mu(1-\cos\theta_l)}{L\sin\theta_l}\hat{\boldsymbol{\phi}}_l\ . \quad \text{(A30)}$$

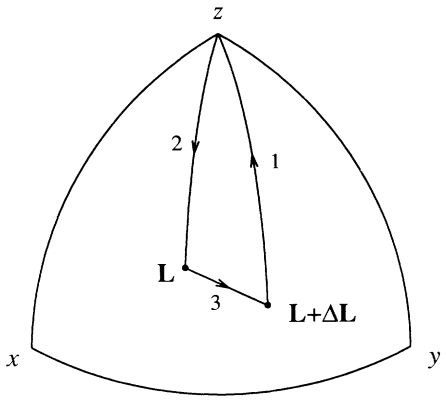

FIG. 4. The positive octant of the unit sphere in angular-momentum space, on which the projections of two points $\mathbf{L}$ and $\mathbf{L}+\Delta\mathbf{L}$ are shown. The spherical triangle 123 subtends solid angle $(1-\cos\theta_l)\Delta\phi_l$, where $\Delta\phi_l$ is the increment corresponding to $\Delta\mathbf{L}$. This fact can be used to find the vector potential $\mathbf{A}$ in north standard gauge.

North standard gauge is so called because it is nonsingular in the northern hemisphere, becoming singular only at the south pole.

In a similar manner we define south standard gauge, by setting

$$\begin{aligned}U(\theta_l,\phi_l)&=U(\hat{\boldsymbol{\phi}}_l,\theta_l-\pi)U(\hat{\mathbf{y}},\pi)\\&=U(\hat{\mathbf{z}},\phi_l)U(\hat{\mathbf{y}},\theta_l)U(\hat{\mathbf{z}},\phi_l)\ ,\end{aligned} \quad \text{(A31)}$$

which in the first form first rotates the eigenvectors from the north pole to the south pole with $U(\hat{\mathbf{y}},\pi)$, and then along great circles to their final destinations. The second form is obtained from the first by application of Eq. (A2). In south standard gauge we have

$$\mathbf{A}(\mathbf{L})\cdot d\mathbf{L}=\mu(1+\cos\theta_l)d\phi_l\ , \quad \text{(A32)}$$

or

$$\mathbf{A}(\mathbf{L})=\frac{\mu(1+\cos\theta_l)}{L\sin\theta_l}\hat{\boldsymbol{\phi}}_l\ . \quad \text{(A33)}$$

South standard gauge is nonsingular over the entire southern hemisphere, becoming singular only at the north pole.

Finally, we quote the eigenvectors themselves in the two gauges. In north standard gauge, we have

$$\tau_\alpha^{(\mu)}(\theta_l,\phi_l)=e^{i(\mu-\alpha)\phi_l}d_{\alpha\mu}^{(s)}(\theta_l)\ , \quad \text{(A34)}$$

and in south standard gauge,

$$\tau_\alpha^{(\mu)}(\theta_l,\phi_l)=e^{-i(\alpha+\mu)\phi_l}d_{\alpha\mu}^{(s)}(\theta_l)\ , \quad \text{(A35)}$$

where there is no sum on α and where $d^{(s)}$ is the reduced rotation matrix, i.e., it is the same as our $U(\hat{\mathbf{y}},\theta_l)$. For the special case of a spin-$\frac{1}{2}$ particle, we have

$$\tau^{(1/2)}=\begin{bmatrix}\cos\theta_l/2\\ e^{i\phi_l}\sin\theta_l/2\end{bmatrix},\qquad \tau^{(-1/2)}=\begin{bmatrix}-e^{-i\phi_l}\sin\theta_l/2\\ \cos\theta_l/2\end{bmatrix} \tag{A36}$$

in north standard gauge, while in south standard gauge we have

$$\tau^{(1/2)}=\begin{bmatrix}e^{-i\phi_l}\cos\theta_l/2\\ \sin\theta_l/2\end{bmatrix},\qquad \tau^{(-1/2)}=\begin{bmatrix}-\sin\theta_l/2\\ e^{i\phi_l}\cos\theta_l/2\end{bmatrix}. \tag{A37}$$

APPENDIX B: THE CALCULATION OF λ_{12}

The calculation of λ_{12}, yielding the result in Eq. (2.10), is straightforward, but involves some algebra. In this appendix we summarize the principal steps.

We begin by computing $\{\tau_\alpha^*,\tau_\beta\}$ by using Eq. (2.9), into which we substitute Eq. (A22) for the derivatives of τ with respect to $\mathbf{L}$. There is one term involving two factors of $\mathbf{A}$, two cross terms involving one factor of $\mathbf{A}$, and a gauge-invariant term involving no $\mathbf{A}$ at all. The term involving two factors of $\mathbf{A}$ is easily seen to vanish. The two cross terms involve two Levi-Civita symbols, which are easily expanded out. Some simplification comes from Eq. (A6). The final form of the sum of the two cross terms is

$$[(\mathbf{A}\cdot\mathbf{S})\tau]_\alpha^*\tau_\beta-\tau_\alpha^*[(\mathbf{A}\cdot\mathbf{S})\tau]_\beta . \tag{B1}$$

This vanishes when contracted with either $\delta_{\alpha\beta}$ or $D_{\alpha\beta}$, in the latter case because of Eq. (2.5). Therefore all terms involving the gauge-dependent vector potential $\mathbf{A}$ vanish in the computation of λ_{12}, as expected.

Only the gauge-invariant term remains, which involves three Levi-Civita symbols. We expand two of these and write the result in the form,

$$\frac{1}{L^2}\epsilon_{ijk}L_i(S_j\tau)_\alpha^*(S_k\tau)_\beta . \tag{B2}$$

We wish to contract this with

$$-(i/2)(D_{\alpha\beta}-\lambda_0\delta_{\alpha\beta})=(i/2)f(r)[\mu L\delta_{\alpha\beta}-(\mathbf{L}\cdot\mathbf{S})_{\alpha\beta}] , \tag{B3}$$

to obtain λ_{12}. Contracting Eq. (B2) with $\delta_{\alpha\beta}$ gives

$$\frac{1}{L^2}\epsilon_{ijk}L_i(\tau^\dagger S_jS_k\tau)=\frac{1}{2L^2}\epsilon_{ijk}L_i(\tau^\dagger[S_j,S_k]\tau)=\frac{i}{L^2}[\tau^\dagger(\mathbf{L}\cdot\mathbf{S})\tau]=\frac{i\mu}{L} . \tag{B4}$$

Similarly contracting Eq. (B2) with $(\mathbf{L}\cdot\mathbf{S})_{\alpha\beta}$ gives

$$\begin{aligned}\frac{1}{L^2}\epsilon_{ijk}L_i[\tau^\dagger S_j(\mathbf{L}\cdot\mathbf{S})S_k\tau]&=\frac{1}{L^2}\epsilon_{ijk}L_i[\tau^\dagger S_jS_k(\mathbf{L}\cdot\mathbf{S})\tau]-\frac{i}{L^2}[\tau^\dagger(\mathbf{L}\times\mathbf{S})^2\tau]\\ &=\frac{\mu}{2L}\epsilon_{ijk}L_i(\tau^\dagger[S_j,S_k]\tau)-\frac{i}{L^2}\{\tau^\dagger[L^2S^2-(\mathbf{L}\cdot\mathbf{S})^2]\tau\}\\ &=i[2\mu^2-s(s+1)] .\end{aligned} \tag{B5}$$

Combining these results, we obtain Eq. (2.10).

We suspect there is an easier way of doing this calculation, since if the entire result is gauge invariant, then it must be possible to construct it out of manifestly gauge-invariant objects. Indeed, this can be done in the case of the term involving $\delta_{\alpha\beta}$, which is the total contraction of the canonical symplectic Poisson tensor with Berry's 2-form on phase space. But we have not been able to express the part involving $D_{\alpha\beta}$ similarly, so what we have presented in this appendix is simply a brute-force calculation.

APPENDIX C: SEMICLASSICAL EIGENFUNCTIONS FOR SCALAR PARTICLES

The problem of determining the semiclassical eigenfunctions of a scalar Hamiltonian of the form

$$H(\mathbf{r},\mathbf{p})=\frac{|\mathbf{p}|^2}{2m}+V(r) \tag{C1}$$

should be a standard one in WKB theory, just as the determination of the eigenvalues is standard. In fact, the calculation of the semiclassical eigenfunctions, which includes asymptotic forms for the spherical harmonics Y_{lm}, is somewhat difficult to find in the literature. Surprisingly, the asymptotic forms for the Y_{lm} cannot be found in any of the standard references on special functions or on the theory of angular momentum, except for the case $m=0$. References of which we are aware which do treat this problem or related problems include Brussard and Tolhoek [30] and recent work by More and Warren [31]. The classical mechanics involved in the following calculation is essentially that of finding Delaunay's canonical transformation [32].

Our purpose in this appendix is to summarize the semiclassical calculation of the eigenfunctions of the Hamiltonian of Eq. (C1) in such a manner as will be useful for the generalization to vector particles given in Sec. VI. Our approach is essentially standard for multidimensional WKB theory, except that we pay more attention than is common to the invariant torus in phase space, and less to the separation of the Hamilton-Jacobi equation.

We begin with the three commuting classical observables (H,L^2,L_z), whose level set in phase space is a 3-

torus. As in Sec. III, we compute the three actions (I_r,I_θ,I_ϕ) or $(I_1,I_2,I_3)=(I_r,L,L_z)$, which are related to one another and quantized in Eq. (3.11).

Next we find an expression for the momentum field $\mathbf{p}=\mathbf{p}(\mathbf{r},\mathbf{I})=\nabla S(\mathbf{r},\mathbf{I})$ by holding (H,L^2,L_z) constant and solving for $\mathbf{p}$. We write $\mathbf{p}$ in spherical coordinates,

$$\mathbf{p}=p_r\hat{\mathbf{r}}+\frac{p_\theta}{r}\hat{\boldsymbol{\theta}}+\frac{p_\phi}{r\sin\theta}\hat{\boldsymbol{\phi}}\ , \tag{C2}$$

where (p_r,p_θ,p_ϕ) are the covariant components of the momentum, i.e., the momenta conjugate to (r,θ,ϕ), not the components of the momentum projected onto $(\hat{\mathbf{r}},\hat{\boldsymbol{\theta}},\hat{\boldsymbol{\phi}})$. Crossing with $\mathbf{r}$, we find

$$\mathbf{L}=\mathbf{r}\times\mathbf{p}=p_\theta\hat{\boldsymbol{\phi}}-\frac{p_\phi}{\sin\theta}\hat{\boldsymbol{\theta}}\ , \tag{C3}$$

which can be combined with the relations above to solve for the three components of the momentum,

$$p_\phi=L_z\ , \tag{C4a}$$

$$p_\theta=\pm\left[L^2-\frac{L_z^2}{\sin^2\theta}\right]^{1/2}\ , \tag{C4b}$$

$$p_r=\pm\left[2m\left[E-\frac{L^2}{2mr^2}-V(r)\right]\right]^{1/2}\ . \tag{C4c}$$

In these equations, E is understood as the function $E(I_r,L)$.

The momentum field $\mathbf{p}(\mathbf{r},\mathbf{I})$ has four branches, corresponding to the signs of p_r and p_θ. All four branches are defined (i.e., as a real vector field) over the same region of configuration space, which is the projection of the 3-torus in the six-dimensional phase space onto configuration space. The region is a solid of revolution, defined by $r_1\le r\le r_2$, $\theta_1\le\theta\le\theta_2$, where $r_{1,2}$ and $\theta_{1,2}$ are the turning points. Its cross section in the x-z plane is illustrated in Fig. 5.

Because central-force motion is classically degenerate (the frequencies in the θ and ϕ directions are equal for all initial conditions), the 3-torus in phase space is not explored by a single orbit. Here we can distinguish typical and atypical cases of central-force motion. The atypical case consists of either the Coulomb or harmonic-oscillator potential, $V(r)=-k/r$ or $V(r)=kr^2/2$. These potentials are atypical because they give rise to another degeneracy, since the radial frequency is commensurable with the θ and ϕ frequencies for all initial conditions. The typical case, for which the potential $V(r)$ is anything except the Coulomb or harmonic-oscillator potential, is easier to think about, and we shall mainly have it in mind in the following discussion.

In the typical case, a single orbit only fills in a 2-torus in phase space, whose projection onto configuration space lies on an annular region in the plane of the orbit between the two radial turning points. By rotating about the z axis, such an orbit is converted into a one-parameter family of orbits which does fill up the 3-torus in phase space, and which has a projection onto configuration space which is the solid of revolution illustrated in Fig. 5. The rotation causes the angular-momentum vector $\mathbf{L}$, which

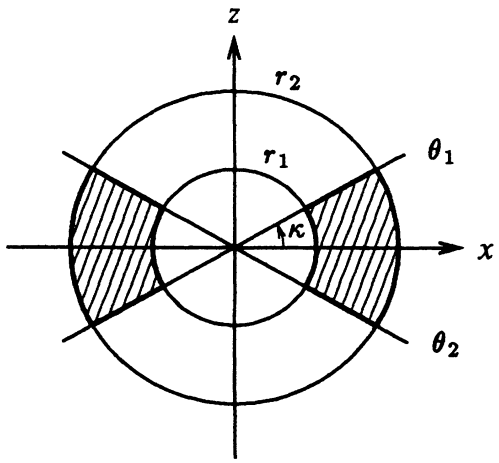

FIG. 5. The 3-torus in phase space which is the level set of (H,L^2,L_z) projects onto configuration space as a three-dimensional region which is a solid of revolution about the z axis, bounded by the r and θ turning points. The region is filled by a family of orbits, all of which have the same inclination κ to the x-y plane.

is perpendicular to the plane of the orbit, to sweep out a cone as in Fig. 1, without affecting the inclination κ of the orbit to the x-y plane. Thus, for all orbits in the family, we have

$$L_z=L\cos\kappa\ , \tag{C5}$$

so that κ, regarded as a function of $(\mathbf{r},\mathbf{p})$, is constant on the 3-torus. This is evident in any case, since the torus is a level set of both L and L_z, but it is important to visualize the appearance in configuration space of the orbits which lie on a give torus. These orbits all have the same r and θ turning points and the same inclination κ, but differ from one another in their values of γ, the longitude of ascending node, as illustrated in Fig. 2.

The action $S(\mathbf{r},\mathbf{I})$ is obtained by writing $\mathbf{p}=\nabla S$ in spherical coordinates and comparing to Eq. (C4). This shows that S separates, i.e., has the form

$$S(\mathbf{r},\mathbf{I})=S_r(r,L,E)+S_\theta(\theta,L,L_z)+S_\phi(\phi,L_z)\ , \tag{C6}$$

where $p_r=\partial S/\partial r$, $p_\theta=\partial S/\partial\theta$, $p_\phi=\partial S/\partial\phi$, and where $E=E(I_r,L)$. The term S_r cannot be calculated explicitly without the knowledge of the form of $V(r)$, so we will henceforth concentrate on the terms S_θ and S_ϕ.

Of these, $S_\phi=L_z\phi$ is trivial. As for S_θ, it has two branches $S_{\theta\pm}$, corresponding to the sign of p_θ in Eq. (C4b) and to the upper and lower branches of the $\theta-p_\theta$ orbit illustrated in Fig. 6. The turning points θ_1,θ_2 are given by

$$\theta_1=\begin{cases}\pi/2-\kappa & \text{if } 0<\kappa<\pi/2\\ \kappa-\pi/2 & \text{if } \pi/2<\kappa<\pi\ ,\end{cases}$$
$$\theta_2=\begin{cases}\pi/2+\kappa & \text{if } 0<\kappa<\pi/2\\ 3\pi/2-\kappa & \text{if } \pi/2<\kappa<\pi\ .\end{cases} \tag{C7}$$

The upper and lower cases correspond to forward motion $(L_z>0)$ and retrograde motion $(L_z<0)$, respectively.

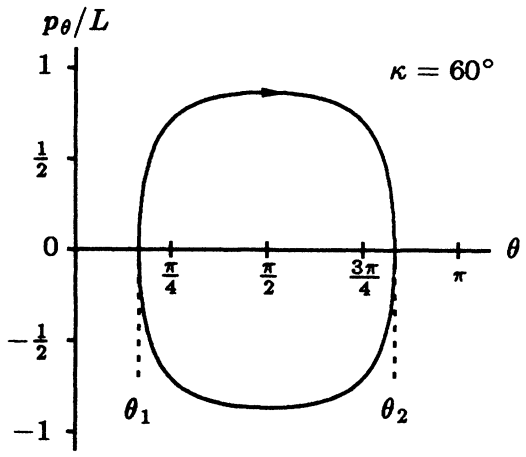

FIG. 6. The orbit as seen in the θ-p_θ plane. The lower branch ($p_\theta < 0$) is regarded as the primary branch. The ascending node occurs at $\theta = \pi/2$ on the lower branch.

We will regard the branch $p_\theta < 0$ as the primary one, since it is on this branch that the particle crosses the ascending node, at $\theta = \pi/2$. Taking the action $S_{\theta-}$ to vanish at the ascending node, we have

$$S_{\theta-}(\theta,L,L_z) = -\int_{\pi/2}^{\theta} \left[L^2 - \frac{L_z^2}{\sin^2\theta} \right]^{1/2} d\theta \ ,$$
$$S_{\theta+}(\theta,L,L_z) = -\int_{\pi/2}^{\theta_1} \left[L^2 - \frac{L_z^2}{\sin^2\theta} \right]^{1/2} d\theta - S_{\theta-} \ . \tag{C8}$$

We denote the angles conjugate to $(I_1,I_2,I_3) = (I_r,L,_z)$ by $(\zeta_1,\zeta_2,\zeta_3)$. In view of the dependencies shown in Eq. (C6), we have

$$\zeta_1 = \frac{\partial S_r}{\partial I_r}, \quad \zeta_2 = \frac{\partial S_r}{\partial L} + \frac{\partial S_\theta}{\partial L}, \quad \zeta_3 = \frac{\partial S_\theta}{\partial L_z} + \frac{\partial S_\phi}{\partial L_z} \ . \tag{C9}$$

Concentrating on the angular parts, we abbreviate,

$$\omega = \frac{\partial S_\theta}{\partial L}, \quad \eta = -\frac{\partial S_\theta}{\partial L_z} \ , \tag{C10}$$

so that $\zeta_3 = \phi - \eta$. Differentiating Eqs. (C8) with respect to L and L_z, we obtain integrals for ω and η which are easily evaluated (respectively by substitutions $x = \cos\theta$, $x = \cot\theta$), giving

$$\omega_- = \sin^{-1}\left[\frac{\cos\theta}{\sin\kappa} \right], \quad \omega_+ = \pi - \omega_- \tag{C11}$$

and

$$\eta_- = \sin^{-1}(\cot\kappa \cot\theta), \quad \eta_+ = \pi \,\mathrm{sgn}(L_z) - \eta_- \ , \tag{C12}$$

where again the $\pm$ refers to the branches of p_θ, S_θ, etc.

The geometrical significance of the angles ω_- and η_- is easily deduced from some spherical trigonometry, and is illustrated in Fig. 2. (The subscript is suppressed in the figure, it being understood that the principle branch $p_\theta < 0$ is referred to.) In particular, ω is the angle in the plane of the orbit between the ascending node and the particle, i.e., angle AOP in the figure, and η is the angle AOB in the figure, measured in the x-y plane. Evidently we have $\phi = \gamma_- + \eta_-$, or $\zeta_{3\pm} = \gamma_\pm$, so that it is the longitude of ascending node which is the angle conjugate to L_z.

The angles ω_+ and η_+, corresponding to the other branch $p_\theta > 0$, have the same geometrical significance in terms of an orbit as ω_- and η_-, but it is a different orbit. The two orbits $p_\theta < 0$ and $p_\theta > 0$, each of which contributes a term to the asymptotic form of the Y_{lm}, are illustrated in Fig. 3.

The action itself is easily computed by noting from Eq. (C8) that S_θ is homogeneous in L and L_z of degree 1, so that

$$S_{\theta\pm} = L\frac{\partial S_{\theta\pm}}{\partial L} + L_z\frac{\partial S_{\theta\pm}}{\partial L_z} = L\omega_\pm - L_z\eta_\pm \ , \tag{C13}$$

or

$$S_{\theta-} = L\sin^{-1}\left[\frac{\cos\theta}{\sin\kappa} \right] - L_z\sin^{-1}(\cot\theta\cot\kappa) \ ,$$
$$S_{\theta+} = (L - |L_z|)\pi - S_{\theta-} \ . \tag{C14}$$

The total WKB wave function is

$$\psi = \sum_b B_b e^{iS_b/\hbar - i\nu_b\pi/2} \ , \tag{C15}$$

where b is the branch index, B is the amplitude, and ν is the Maslov index. The amplitude is given by

$$B^2 = \left| \det\frac{\partial^2 S}{\partial \mathbf{r}\partial \mathbf{I}} \right| = \frac{1}{r^2\sin\theta}\left| \det\frac{\partial^2 S}{\partial(r,\theta,\phi)\partial(I_r,L,L_z)} \right| \ . \tag{C16}$$

It is the same for all four branches of S. By Eq. (C6), the final determinant in this equation is upper triangular, and factors into a radial and angular part, so that $B^2 = B_r^2 B_\Omega^2$, where

$$B_r^2 = \frac{1}{r^2}\left| \frac{\partial^2 S_r}{\partial r \partial I_r} \right| \tag{C17}$$

and

$$B_\Omega^2 = \frac{1}{\sin\theta}\left| \frac{\partial^2 S_\theta}{\partial\theta\partial L} \right| = \frac{1}{(\sin^2\kappa - \cos^2\theta)^{1/2}} \ . \tag{C18}$$

Corresponding to the exact representation of the wave function $\psi(r,\theta,\phi) = (1/r)\Phi(r)Y_{lm}(\theta,\phi)$, we have radial and angular parts of the WKB approximation. The angular part gives us an asymptotic formula for Y_{lm},

$$Y_{lm}(\theta,\phi)=\frac{c}{2\pi}B_\Omega e^{iL_z\phi/\hbar}\left[e^{iS_-/\hbar}+e^{iS_+/\hbar-i\pi/2}\right]$$
$$=\frac{ce^{im\phi}}{\pi(\sin^2\kappa-\cos^2\theta)^{1/4}}\begin{bmatrix}\cos\\ i\sin\end{bmatrix}$$
$$\times\left[(l+\tfrac{1}{2})\sin^{-1}\left[\frac{\cos\theta}{\sin\kappa}\right]\right.$$
$$\left.-m\sin^{-1}(\cot\kappa\cot\theta)\right], \qquad \text{(C19)}$$

where c is a constant, where we have used the quantized values $L=(l+\frac{1}{2})\hbar$ and $L_z=m\hbar$ according to Eq. (3.11), where κ is given by

$$\cos\kappa=\frac{L_z}{L}=\frac{m}{l+\frac{1}{2}}, \qquad \text{(C20)}$$

and where the choice of cosine is made when $l+m$ is even, and i sin when $l+m$ is odd. If c is chosen to be a phase factor, then Eq. (C19) for Y_{lm} is normalized in the stationary-phase sense. In this paper, we follow the phase conventions of Edmonds [29], which are realized if we take

$$c=e^{-i(l+m)\pi/2}. \qquad \text{(C21)}$$

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