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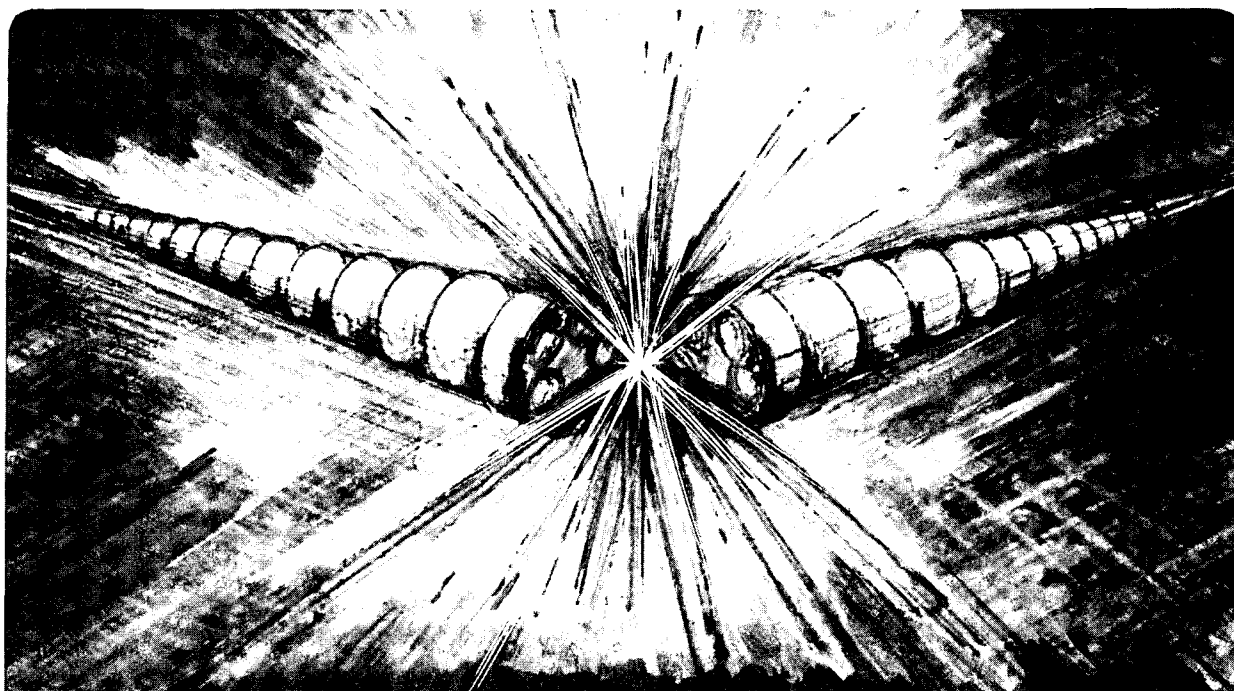
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A New Way to Compute Maslov Indices*

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A New Way to Compute Maslov Indices

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Abstract

A new formula is presented for computing Maslov indices in integrable and near-integrable Hamiltonian systems. For several kinds of applications the new formula is particularly easy to use. It does not rely on counting caustics or other kinds of discontinuities. Its theoretical justification calls on wave packet concepts and the topological properties of the group of symplectic matrices. Techniques are also presented for manipulating the Maslov index in analytical expressions.

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1. Introduction

The main purpose of this paper is to present and prove, in as nontechnical a manner as possible, a new formula for computing the Maslov indices, as well as to provide examples of algebraic techniques for working with them. The Maslov indices to which we refer are the even integers μ_k which occur in the Einstein-Brillouin-Keller (EBK) semiclassical quantization conditions.¹⁻⁴ As is well known, these conditions apply to integrable and near-integrable Hamiltonian systems, and are represented by the formula

$$J_k = \left(n_k + \frac{\mu_k}{4}\right)\hbar, \quad (1)$$

where J_k is the k -th action and n_k is the corresponding quantum number. We shall not discuss the other principal version of the Maslov index (which may be even or odd), which occurs in the phase shifts of WKB wave functions:

We believe our formula is easier to use in certain kinds of calculations than are traditional methods for determining the Maslov index, which are based on counting caustics. This is especially true when more than two degrees of freedom are considered, or when resonances complicate the caustic structure. (We have dealt with the Maslov indices of resonant tori as a separate issue in another publication.⁵) Even for simple problems, however, our method is probably easier to automate than traditional methods, and it is free of worries about exceptional cases (such as caustics of higher order than the first, or curves which do not cross a caustic transversally, etc.) Furthermore, completely apart from any consideration of numerical calculation, our formula can be used in an analytical way, for deriving relations and proving theorems about the Maslov index. Some examples of this are given in this paper, and some in Ref. 5.

Since it is easy to state our result and explain how to use it, we will do this first, in Sec. 2. Although the theory behind our formula is based on wave packet concepts, it can nevertheless be used in a practical way without any explicit need for wave packets. However, an excursion into wave packet theory is needed to prove our formula, which we undertake in Sec. 3. We begin by reviewing the essentials of the semiclassical evolution of wave packets, as well as some recent ideas which provide

a general relationship between wave packet evolution and EBK quantization. We also show how the spreading of wave packets in quasiperiodic systems can be decomposed into two parts, one of which itself is quasiperiodic, and the other of which is unbounded in time. The latter kind of behavior is inimical to quantization, since it is aperiodic, and it is dispensed with by shifting attention to the action variables as evolution operators. This leads to the EBK rules and a formula for the Maslov index, Eq. (26). This formula suffers from certain drawbacks in a practical sense, so in Sec. 4 we invoke topological methods to show its equivalence to a more useful formula, Eq. (7), which is our principal result. We also show that our formula for the Maslov index is invariant under canonical transformations. Section 4 contains in addition a number of useful relations for manipulating the Maslov index. We expect our results to be mainly of value in applications to physical problems, and we make no claim for new mathematics.

2. The Result and How to Use It

The most common application for the Maslov index is in connection with the invariant tori of integrable and near-integrable systems. Therefore we shall explain our result in this context, although, as will become apparent in Sec. 4, the result is actually more general than this.

We consider a system of any number N of degrees of freedom, in which there exist invariant tori in some region of phase space. Although the action-angle variables (θ, \mathbf{J}) corresponding to these tori may not be known explicitly, we will assume that they exist in principle, and we shall refer to them as need be. In order to use our formula for the Maslov indices, it is required that the rectangular canonical coordinates (q, p) be known on at least one torus as functions of θ . As a practical matter, such information can be obtained either by classical perturbation theory,^{6,7} variational principles,^{3,8} Fourier transforms of numerical orbit integrations,⁹⁻¹¹ solution of the Hamilton-Jacobi equation,¹² or other means. Indeed, getting this information is the hard part in the use of our formula; fortunately, considerable work has been done on this problem, and several methods are known. We do not

require that (q, p) be known as functions of the actions \mathbf{J} . This is important, because often the \mathbf{J} -dependence is more difficult to obtain than the θ -dependence. Usually the θ -dependence is expressed as a Fourier series,

$$q(\theta) = \sum_{\mathbf{n}} q(\mathbf{n}) \exp(i\mathbf{n} \cdot \theta), \quad p(\theta) = \sum_{\mathbf{n}} p(\mathbf{n}) \exp(i\mathbf{n} \cdot \theta), \quad (2)$$

where \mathbf{n} runs over all integer N -vectors. We write $q(\mathbf{n})$, $p(\mathbf{n})$ for the Fourier coefficients of $q(\theta)$, $p(\theta)$; these are also functions of the actions \mathbf{J} , but we suppress this dependency. Various algorithms or numerical schemes produce the coefficients $q(\mathbf{n})$, $p(\mathbf{n})$ as tables of numbers; given this information, the rest of the calculation we propose is straightforward.

The Maslov indices in Eq. (1) are specified by means of the basis contours on the torus which correspond to the different actions. The k -th contour, which we shall denote by Γ_k , is formed by letting the angle θ_k vary between 0 and 2π , while holding all the other θ 's and all the J 's fixed. It is also the orbit generated by J_k , in the sense of the trajectory in phase space which results by treating J_k as a Hamiltonian. We prefer to reserve the symbols θ_k for coordinates in phase space, and not to use them in the role of parameters for these contours. Instead, we use the symbol λ for the latter purpose, as in the following specification of the k -th contour $\Gamma_k(\lambda)$:

$$\begin{aligned} \theta_l &= \theta_{l0}, & l &\neq k; \\ \theta_k &= \theta_{k0} + \lambda; \\ J_l &= J_{l0}, & \text{all } l. \end{aligned} \quad (3)$$

Here (θ_0, \mathbf{J}_0) are the coordinates of any point on the contour. Clearly, this contour is the solution of Hamilton's equations,

$$\begin{aligned} \frac{d\theta_l}{d\lambda} &= \frac{\partial H}{\partial J_l}, \\ \frac{dJ_l}{d\lambda} &= -\frac{\partial H}{\partial \theta_l}, \end{aligned} \quad (4)$$

in which we set $H = J_k$ and take (θ_0, \mathbf{J}_0) as initial conditions. The contour has period 2π in the parameter λ .

Our prescription for computing the k -th Maslov index is the following. First we compute the $N \times N$ complex matrix \mathbf{M} as a function of λ along the contour Γ_k , according to the formula

$$M_{kl}(\lambda) = \frac{\partial q_k}{\partial \theta_l}(\lambda) - i \frac{\partial p_k}{\partial \theta_l}(\lambda). \quad (5)$$

Since \mathbf{q} and \mathbf{p} are periodic in λ , so is \mathbf{M} . If \mathbf{q} and \mathbf{p} are expressed in terms of Fourier series, as in Eq. (2), then we have

$$M_{kl}(\lambda) = \sum_{\mathbf{n}} i n_l [q_k(\mathbf{n}) - i p_k(\mathbf{n})] \exp[i\mathbf{n} \cdot \boldsymbol{\theta}(\lambda)], \quad (6)$$

where $\boldsymbol{\theta}(\lambda)$ is given by Eq. (3). As will be shown below, the matrix $\mathbf{M}(\lambda)$ can never be singular, so long as (\mathbf{q}, \mathbf{p}) and $(\boldsymbol{\theta}, \mathbf{J})$ are two sets of canonical variables. Therefore $\det \mathbf{M}(\lambda)$ is a nonzero complex number, which, like \mathbf{M} itself, is periodic in λ with period 2π . As λ varies from 0 to 2π , this complex number executes a closed curve in the complex plane, which never passes through the origin. Therefore this curve has a well defined winding number, representing the number of circuits it makes in a positive (counterclockwise) sense about the origin. As will be shown below, it turns out that the Maslov index μ_k is simply twice this winding number. We designate this relation by writing

$$\mu_k = 2 \text{wn}(\det \mathbf{M}(\lambda)), \quad (7)$$

which is our principal result.

As a practical matter, one could use Eq. (7) by plotting $\det \mathbf{M}(\lambda)$ in the complex plane, and simply viewing the curve which results. Alternatively, one could automate the process by accumulating the phase of $\det \mathbf{M}(\lambda)$. One way of doing this is to use the Cauchy formula,

$$\text{wn} \det \mathbf{M}(\lambda) = \frac{1}{2\pi i} \oint \frac{d}{d\lambda} \ln \det \mathbf{M}(\lambda) d\lambda. \quad (8)$$

Since the answer must be an integer, high precision is not required in evaluating this integral; usually one or two significant digits will suffice.

An obvious objection to Eq. (7) is that it is not dimensionally correct, since q and p may have different physical dimensions. Amazingly enough, however, this does not make any difference, for the following reason. As will be shown below, Eq. (7) is invariant under canonical transformations of the form $(q, p) \rightarrow (q', p')$, including nonlinear ones, so long as the transformation is smooth and well defined over a simply connected region of phase space surrounding the contours in question. For example, one can set $q' = cq$, $p' = p/c$, for some nonzero constant c ; such a scaling transformation can always be used to convert q and p into a form in which they have the same physical dimensions. One can, if one likes, precede the use of Eq. (7) by such a transformation, in order to deal exclusively with quantities which make sense dimensionally. But in view of the invariance of Eq. (7) under canonical transformations, the results will be the same even if one does not do so.

In a sense, the reason for this peculiar property is that the Maslov index represents only a very small piece of the information which is contained in the periodic matrix function $M(\lambda)$. Therefore $M(\lambda)$ can be subjected to many kinds of modifications without affecting the Maslov index. This observation suggests that it might be possible to compute the winding number of $M(\lambda)$ with even less work than that outlined above, but, so far, we have not been able to find any such improved method.

The justification of Eq. (7) and the other statements we have made involves wave packets, to which we now turn.

3. The Connection with Wave Packet Evolution

A multiplicative factor similar to $\det M(\lambda)$ occurs in the semiclassical evolution of wave packets, and it is not hard to see, in simple examples like the harmonic oscillator, that it is responsible for the Maslov phase shifts. This is the factor $\det(A + iB)$, seen in Eq. (17) below. There are, however, several subtleties in establishing the precise connection between this factor and the results given above,

which call for some discussion. For the sake of concreteness, we will work with Gaussian wave packets, although in fact our results can be justified without reference to Gaussians. The semiclassical evolution of Gaussian wave packets was first developed with a degree of thoroughness by Heller, as seen especially in Refs. 13 and 14. Several of our formulas below are reproductions of Heller's results, although in a different notation. In addition, one of us (R.G.L.) has given a group theoretical analysis of wave packet evolution in Ref. 15, which explains many details not covered in this paper, such as the reason why Gaussians are not really essential to our results, and which also develops much of the basic group theory of the symplectic matrices and their unitary representations.

We begin by reviewing some of the essential features of wave packet evolution. It is convenient to establish a standard or reference Gaussian wave packet, which we take to be

$$\psi_0(\mathbf{x}) = \langle \mathbf{x} | 0 \rangle = \frac{1}{(\pi \hbar)^{N/4}} \exp\left(-\frac{|\mathbf{x}|^2}{2\hbar}\right). \quad (9)$$

Here \mathbf{x} is a scaled configuration space variable, with dimensions of $\hbar^{1/2}$. Following Klauder,¹⁶ we call $|0\rangle$ the "fiducial" state. The fiducial state is not generally suitable as an initial state in studies of wave packet evolution, because its expectation values of both \hat{q} and \hat{p} vanish. (The hats denote quantum operators, as distinct from the classical phase space coordinates (\mathbf{q}, \mathbf{p})). If instead an initial state centered at location $(\mathbf{q}_0, \mathbf{p}_0)$ in phase space is desired, i.e. one for which $\langle \hat{q} \rangle = \mathbf{q}_0$, $\langle \hat{p} \rangle = \mathbf{p}_0$, then it can be obtained by applying the Heisenberg operator $T(\mathbf{q}_0, \mathbf{p}_0)$ to the fiducial state, as is well known in the theory of coherent states.¹⁷ The Heisenberg operators are defined by

$$T(\mathbf{q}_0, \mathbf{p}_0) = \exp\left[\frac{i}{\hbar}(\mathbf{p}_0 \cdot \hat{q} - \mathbf{q}_0 \cdot \hat{p})\right], \quad (10)$$

and act as displacement operators in phase space. We apply this Heisenberg operator to $|0\rangle$, to obtain a state which we denote by

$$|\mathbf{q}_0, \mathbf{p}_0\rangle = T(\mathbf{q}_0, \mathbf{p}_0)|0\rangle, \quad (11)$$

which has the wave function

$$\langle \mathbf{x} | \mathbf{q}_0, \mathbf{p}_0 \rangle = \frac{1}{(\pi \hbar)^{N/4}} \exp\left[\frac{1}{\hbar} \left(-\frac{1}{2}|\mathbf{x} - \mathbf{q}_0|^2 + i\mathbf{p}_0 \cdot \mathbf{x} - \frac{i}{2}\mathbf{p}_0 \cdot \mathbf{q}_0\right)\right]. \quad (12)$$

This state is simply a coherent state in the usual sense, which is characterized by its expectation values of \hat{q} and \hat{p} . It may still not be suitable as an initial state, because it has rather special values for the second moments of \hat{q} and \hat{p} . We shall return to this question in Sec. 4; for now we will simply proceed to use it as an initial state.

The state $|q_0, p_0\rangle$ may be propagated forward in time under the quantum Hamiltonian $H(\hat{q}, \hat{p})$ by using the quadratic approximation of Heller.¹³ The expectation values of \hat{q} , \hat{p} obey the Ehrenfest relations, i.e. $\langle \hat{q} \rangle(t) = q(t)$, $\langle \hat{p} \rangle(t) = p(t)$, where $q(t)$, $p(t)$ are the solutions of Hamilton's equations under the classical Hamiltonian $H(q, p)$, with initial conditions (q_0, p_0) . In addition, the wave packet spreads. As apparently first observed by Heller,¹⁴ the spreading can be described in terms of the $2N \times 2N$ matrix S , given by

$$S = \frac{\partial(q, p)}{\partial(q_0, p_0)} = \begin{pmatrix} \frac{\partial q}{\partial q_0} & \frac{\partial q}{\partial p_0} \\ \frac{\partial p}{\partial q_0} & \frac{\partial p}{\partial p_0} \end{pmatrix}, \quad (13)$$

where q, p represent $q(t), p(t)$. (In formulas of this type, we shall always let the row index be determined by the numerator of the partial derivatives shown, and the column index by the denominator.)

This was a most important observation, because such a matrix is a symplectic matrix, and it turns out that the entire structure of semiclassical wave packet evolution is founded on the symplectic matrices. The special properties of these matrices arise in the following way. By a general property of the solutions to Hamilton's equations, the transformation $(q_0, p_0) \rightarrow (q, p)$ is canonical, so $S(t)$ is the Jacobian matrix of a canonical transformation. Therefore the Poisson brackets of $(q(t), p(t))$ among themselves, computed with respect to (q_0, p_0) , must take on their standard forms of 1's and 0's. These can be summarized by writing

$$S\tilde{J}S = J, \quad (14)$$

where the tilde represents the transpose, and where J is the $2N \times 2N$ antisymmetric matrix,

$$J = \begin{pmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 0 \end{pmatrix}. \quad (15)$$

Equation (14) is the defining relation for the symplectic matrices, so that this matrix \mathbf{S} , and, more generally, the Jacobian matrix of any canonical transformation, is a symplectic matrix. Many of the properties of the symplectic matrices are summarized in Appendix A of Ref. 15; the main ones for our present purposes are that the symplectic matrices form a group, and that every symplectic matrix has the determinant +1. For any symplectic matrix (not just the one in Eq. (13)) we shall adopt the decomposition,

$$\mathbf{S} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix}, \quad (16)$$

where \mathbf{A} , \mathbf{B} , \mathbf{C} , \mathbf{D} are four $N \times N$ real matrices.

To return to the wave packet evolution in the quadratic approximation, it turns out that the final wave packet at time t can be written

$$\begin{aligned} \psi(\mathbf{x}, t) = & \frac{1}{(\pi\hbar)^{N/4}} \frac{1}{\sqrt{\det(\mathbf{A} + i\mathbf{B})}} \\ & \times \exp \left\{ \frac{1}{\hbar} \left[i\alpha + i\mathbf{p} \cdot (\mathbf{x} - \mathbf{q}) \right. \right. \\ & \left. \left. - \frac{1}{2}(\mathbf{x} - \mathbf{q}) \cdot (\mathbf{D} - i\mathbf{C})(\mathbf{A} + i\mathbf{B})^{-1} \cdot (\mathbf{x} - \mathbf{q}) \right] \right\}, \quad (17) \end{aligned}$$

where \mathbf{A} , \mathbf{B} , \mathbf{C} , \mathbf{D} are obtained by identifying the matrices of Eqs. (13) and (16), and where α is a Bohr-Sommerfeld phase, obtained by integrating along the orbit,

$$\alpha = \int_{(\mathbf{q}_0, \mathbf{p}_0)}^{(\mathbf{q}, \mathbf{p})} \mathbf{p} \cdot d\mathbf{q} - Et. \quad (18)$$

Here E is the (conserved) energy of the classical orbit. The factor under the square root in Eq. (17) is responsible for the Maslov phase shifts; the choice of branch of the square root is determined by continuity, giving a complex number which may pass back and forth between the two Riemann sheets. [It may help the reader in making a detailed comparison of this formula with the results of Ref. 14 to note that the symbols \mathbf{q} , \mathbf{q}_t , \mathbf{p}_t , \mathbf{Z} , \mathbf{P}_z , and \mathbf{A} of Ref. 14 correspond respectively to \mathbf{x} , \mathbf{q} , \mathbf{p} , $\mathbf{A} + i\mathbf{B}$, $\mathbf{C} + i\mathbf{D}$, and $\frac{1}{2}(\mathbf{C} + i\mathbf{D})(\mathbf{A} + i\mathbf{B})^{-1}$ of this paper.]

The matrix $\mathbf{A} + i\mathbf{B}$, which is of special concern to us, can never be singular. If it were, the wave function $\psi(\mathbf{x}, t)$ would diverge, and we do not expect this. (Of course, wave functions do diverge in WKB theory.) Nevertheless, it is not immediately apparent why Hamilton's equations should forbid such a singularity. Furthermore, this nonsingularity is important in making our formula for the Maslov indices, Eq. (7), well defined. Since the proof of this fact was incorrectly stated in Ref. 15, we will provide a correct proof here.

If Eq. (16) is substituted into Eq. (14), we find that the submatrices satisfy $\mathbf{A}\tilde{\mathbf{B}} = \mathbf{B}\tilde{\mathbf{A}}$ and $\mathbf{D}\tilde{\mathbf{A}} - \mathbf{C}\tilde{\mathbf{B}} = \mathbf{I}$. Now suppose that $\mathbf{A} + i\mathbf{B}$ were singular. Then its Hermitian conjugate $\tilde{\mathbf{A}} - i\tilde{\mathbf{B}}$ must also be singular. Multiplying these together gives the real singular matrix, $\mathbf{A}\tilde{\mathbf{A}} + \mathbf{B}\tilde{\mathbf{B}}$ (the imaginary part vanishes on account of $\mathbf{A}\tilde{\mathbf{B}} = \mathbf{B}\tilde{\mathbf{A}}$.) This matrix must possess a real, nonzero eigenvector \mathbf{u} with eigenvalue zero. Hence

$$\tilde{\mathbf{u}} \cdot (\mathbf{A}\tilde{\mathbf{A}} + \mathbf{B}\tilde{\mathbf{B}}) \cdot \mathbf{u} = (\tilde{\mathbf{A}}\mathbf{u})^2 + (\tilde{\mathbf{B}}\mathbf{u})^2 = 0, \quad (19)$$

implying $\tilde{\mathbf{A}}\mathbf{u} = \tilde{\mathbf{B}}\mathbf{u} = 0$. But this yields the contradiction $\mathbf{u} = \mathbf{I}\mathbf{u} = \mathbf{D}\tilde{\mathbf{A}}\mathbf{u} - \mathbf{C}\tilde{\mathbf{B}}\mathbf{u} = 0$. Therefore $\mathbf{A} + i\mathbf{B}$ is nonsingular. (The proof of Ref. 15 was incorrect because it worked with complex matrices, and ignored the possibility of complex eigenvectors.)

Let us now consider the relationship between wave packet evolution and the EBK quantization rules, in which the Maslov indices are contained. We begin with the matrix $\mathbf{A} + i\mathbf{B}$, which is given explicitly as a function of time by

$$\mathbf{A} + i\mathbf{B} = \frac{\partial \mathbf{q}(t)}{\partial \mathbf{q}_0} + i \frac{\partial \mathbf{q}(t)}{\partial \mathbf{p}_0}. \quad (20)$$

As mentioned previously, experimentation with the one-dimensional harmonic oscillator shows that the square root of the determinant of this matrix (in this case only a scalar), by passing onto the second Riemann sheet, gives the $\frac{1}{2}$ in the quantization of this system. Therefore we have the strong suggestion that this matrix is related to the Maslov index. Unfortunately, it is hard to pursue this idea for other Hamiltonians, even in one dimension. The most immediate problem is that for nonlinear Hamiltonians, $\mathbf{A} + i\mathbf{B}$ is not periodic in time, even when the orbit itself, given by $\mathbf{q}(t)$, $\mathbf{p}(t)$, is. That is, the time evolution of wave packets in the quadratic approximation is not generally periodic, and does not give rise to quantization conditions (either the EBK rules or any other).

The resolution of this problem is given in detail in Ref. 18. Briefly, the main idea is to propagate the wave packet, not with the physical Hamiltonian as the evolution operator, but rather to use the actions J_k , $k = 1, \dots, N$, as a set of evolution operators. Now the parameter describing the orbits is no longer physical time; we may call it λ instead. There is no difficulty in propagating a wave packet with one of the actions, say J_k , as an evolution operator. We merely use Eq. (17), as before, for the evolution of the wave packet along the orbit, writing $\psi(\mathbf{x}, \lambda)$ instead of $\psi(\mathbf{x}, t)$. Now, however, \mathbf{q} and \mathbf{p} represent, not $\mathbf{q}(t)$ and $\mathbf{p}(t)$, but rather $\mathbf{q}(\lambda)$ and $\mathbf{p}(\lambda)$, obtained by solving Hamilton's equations,

$$\begin{aligned} \frac{d\mathbf{q}}{d\lambda} &= \frac{\partial J_k(\mathbf{q}, \mathbf{p})}{\partial \mathbf{p}}, \\ \frac{d\mathbf{p}}{d\lambda} &= -\frac{\partial J_k(\mathbf{q}, \mathbf{p})}{\partial \mathbf{q}}, \end{aligned} \quad (21)$$

where the initial conditions are still the same $(\mathbf{q}_0, \mathbf{p}_0)$ which appear in the initial wave packet. Here Hamilton's equations have been written with J_k expressed as a function of (\mathbf{q}, \mathbf{p}) , but, since Hamilton's equations can be transformed to any set of canonical coordinates, we could just as well use the action-angle variables $(\boldsymbol{\theta}, \mathbf{J})$ themselves as phase space coordinates. Doing so, we obtain Eq. (4) above, whose solution is given by Eq. (3). Thus we see that the orbit $\mathbf{q}(\lambda)$, $\mathbf{p}(\lambda)$ is nothing but the contour Γ_k , expressed in terms of the variables \mathbf{q}, \mathbf{p} .

As for the matrices \mathbf{A} , \mathbf{B} , \mathbf{C} , \mathbf{D} (or collectively, \mathbf{S}), which occur in Eq. (17), they are still defined by Eqs. (13) and (16), except, again, \mathbf{q} and \mathbf{p} stand for $\mathbf{q}(\lambda)$ and $\mathbf{p}(\lambda)$. Now, however, these matrices are periodic in the independent variable λ . This is a crucial fact, which is worth elaboration. To see why the matrix \mathbf{S} is periodic (in λ) when J_k is used as an evolution operator and not (in t) when H is so used, it is convenient to use the chain rule to rewrite Eq. (13), in order to represent a shift from (\mathbf{q}, \mathbf{p}) to action-angle variables and back again:

$$\mathbf{S} = \frac{\partial(\mathbf{q}, \mathbf{p})}{\partial(\mathbf{q}_0, \mathbf{p}_0)} = \frac{\partial(\mathbf{q}, \mathbf{p})}{\partial(\boldsymbol{\theta}, \mathbf{J})} \cdot \frac{\partial(\boldsymbol{\theta}, \mathbf{J})}{\partial(\boldsymbol{\theta}_0, \mathbf{J}_0)} \cdot \frac{\partial(\boldsymbol{\theta}_0, \mathbf{J}_0)}{\partial(\mathbf{q}_0, \mathbf{p}_0)}. \quad (22)$$

All three of these matrices on the right are Jacobian matrices of canonical transformations, and are, therefore, symplectic. This formula can be used in both cases, when \mathbf{q}, \mathbf{p} stand for $\mathbf{q}(t), \mathbf{p}(t)$, or for $\mathbf{q}(\lambda), \mathbf{p}(\lambda)$.

In both cases, the first of these matrices is periodic in the angles θ . Thus, under the H -evolution, this matrix is quasiperiodic in t , while under the J_k -evolution, it is strictly periodic in λ . The third matrix, in both cases, is constant. It is the middle matrix, which represents the transformation from initial to final conditions under the H - or J_k -evolution, as expressed in action-angle variables, which really distinguishes the two cases. For the H -evolution, the solution of Hamilton's equations can be written

$$\begin{aligned}\theta(t) &= \theta_0 + \omega(\mathbf{J}_0)t, \\ \mathbf{J}(t) &= \mathbf{J}_0,\end{aligned}\tag{23}$$

so that

$$\frac{\partial(\theta, \mathbf{J})}{\partial(\theta_0, \mathbf{J}_0)} = \begin{pmatrix} \mathbf{I} & \frac{\partial^2 H}{\partial \mathbf{J} \partial \mathbf{J}^t} t \\ 0 & \mathbf{I} \end{pmatrix}.\tag{24}$$

It is the matrix in the upper right corner of Eq. (24) which is responsible for the lack of periodicity (or even quasiperiodicity) of the wave packet under the evolution governed by the Hamiltonian. This matrix causes an unbounded spreading of the wave packet, a phenomenon which is always present when H is used as the evolution operator, and which prevents $\mathbf{S}(t)$ from being periodic. (The only exception is when H is linear in the actions, as in the harmonic oscillator.) On the other hand, when J_k is used as an evolution operator, then, by differentiating Eq. (3) with respect to initial conditions, the middle matrix is seen to be simply the $2N \times 2N$ identity matrix, which is constant. Altogether, this shows that $\mathbf{S}(\lambda)$ is periodic in λ .

A more pictorial way of seeing the same thing is to note that the matrix \mathbf{S} , which represents the changes in final conditions due to small changes in initial conditions along some orbit, must be periodic under the J_k -evolution, because the J_k orbits all have the same period (namely, 2π), independent of initial conditions. That is, a localized ensemble of particles, propagated with J_k as an evolution operator, will exactly return to its initial state when $\lambda = 2\pi$. Under the Hamiltonian evolution, however, even when orbits are periodic, different orbits generally have different periods, so even if one particle in a localized ensemble has returned to its

initial conditions in some time T , the other particles generally will not have done so.

Since $\mathbf{q}(\lambda)$, $\mathbf{p}(\lambda)$, and $\mathbf{S}(\lambda)$ are all periodic under the J_k -evolution, the wave packet $\psi(\mathbf{x}, \lambda)$ returns at $\lambda = 2\pi$ to its original condition $\psi_0(\mathbf{x})$, to within an overall phase. The Bohr-Sommerfeld phase α , with $-Et$ replaced by $-J_k\lambda$, vanishes at $\lambda = 2\pi$, since

$$\oint \mathbf{p} \cdot d\mathbf{q} = 2\pi J_k. \quad (25)$$

The only remaining phase is that due to the crossing of $\sqrt{\det(\mathbf{A} + i\mathbf{B})}$ onto successive Riemann sheets of the square root function. We write this phase in the form $\exp(-i\mu_k\pi/2)$, where μ_k is the Maslov index and is an even integer. Effectively, $\mu_k/2$ represents the number of Riemann sheet crossings of the square root function, and it can therefore be represented by

$$\frac{\mu_k}{2} = \text{wn det}(\mathbf{A} + i\mathbf{B}) = \text{wn det} \left(\frac{\partial \mathbf{q}(\lambda)}{\partial \mathbf{q}_0} + i \frac{\partial \mathbf{q}(\lambda)}{\partial \mathbf{p}_0} \right). \quad (26)$$

This formula represents the manner in which the Maslov index emerges from wave packet evolution.

The rest of the EBK quantization conditions, including the integer n_k shown in Eq. (1), emerge by considering the spectrum of the λ -evolution of the wave packet, as discussed in more detail in Ref. 18. The same reference also explains how wave functions, as well as energy eigenvalues, can be obtained from the action propagation. Since we are mainly interested in the Maslov index here, we will not pursue these issues.

For the purposes of this paper, we are now done with wave packets, since Eq. (26) is the result for which we needed them. Note that Eq. (26), while similar in appearance to Eq. (7), is actually distinct in several respects. In particular, Eq. (26) would be less convenient to use in a practical calculation than Eq. (7), since often \mathbf{q} is not known as a function of both \mathbf{q}_0 , \mathbf{p}_0 along an action trajectory. (That is, the differentiations indicated effectively involve the consideration of nearby trajectories, including those which are not on the same torus as the initial conditions \mathbf{q}_0 , \mathbf{p}_0 .) It is true that if \mathbf{q} and \mathbf{p} were known analytically as functions of both θ and \mathbf{J}

(perhaps through perturbation theory or by solving the Hamilton-Jacobi equation analytically), then Eq. (26) could be used without much trouble. However, often one has less information than this, as was indicated in the introduction. In fact, it was the realization that Eqs. (7) and (26) were equivalent, and that Eq. (7) is more practical, that motivated us to write this paper. We turn now to a proof of this equivalence, which involves the topological properties of the group of symplectic matrices. In the process, we will also prove some other statements made above, such as that concerning the invariance of Eq. (7) under canonical transformations.

4. The Maslov Index and the Topology of the Symplectic Group

Equation (26) allows us to associate a Maslov index with any periodic symplectic matrix function, $S(\lambda)$, by setting $\mu = 2\pi n \det(A(\lambda) + iB(\lambda))$, whether or not $S(\lambda)$ is given by Eq. (13) or derived from an action orbit. This is definitely a useful generalization, as is shown by the applications below, and it causes us to shift our attention to the space of symplectic matrices, in which $S(\lambda)$ can be viewed geometrically as a closed curve. This space is the symplectic group manifold, which can be thought of as a surface imbedded in the space of all $2N \times 2N$ real matrices, i.e. the surface specified by the defining relation of the symplectic matrices, Eq. (14). This relation represents a set of constraints on the $4N^2$ numbers present in a $2N \times 2N$ matrix. In fact, since both sides of Eq. (14) are antisymmetric, there are $2N(2N - 1)/2$ independent constraints, which leave $N(2N + 1)$ independent components in a symplectic matrix. Thus, the symplectic group manifold can be thought of as an $N(2N + 1)$ -dimensional surface in $4N^2$ -dimensional matrix space.

The symplectic group manifold has a simple but nontrivial topological structure. This means that different closed curves in this space fall into different so-called homotopy classes, depending on whether they can be continuously deformed into one another. (Here and below we shall always mean "parameterized curve" when we say "curve." In the case we are mainly interested in, the parameterization is provided by the variable λ .) As was apparently first observed by Arnold,¹⁹ there is a close relationship between the topological properties of these curves in the symplectic group manifold (namely, the homotopy classes to which they belong), and

the associated Maslov indices. In this section we shall exploit such ideas to develop certain calculational tools, and to prove various facts. As we will show, there is definite computational power which comes from this topological point of view.

The topological methods we shall use properly belong to the subject of algebraic topology. An introduction to this has been given by Schulman,²⁰ and a more complete account may be found in Singer and Thorpe.²¹ It is not a particularly difficult subject, nor, as it turns out, do we place very heavy demands on it, since the topological structure of the symplectic group manifold is rather simple. As a result, a little geometrical intuition will suffice to follow all our arguments below, even with no particular background in this area of mathematics. The principal topological fact about the symplectic group manifold, from which follow most of the unproven statements we make below, is that this manifold is, topologically speaking, the Cartesian product of a simply connected space with a circle. It is the circle which provides all the nontrivial topological features of interest to us. This fact is proven in Appendix A of Ref. 15, by using various matrix manipulations. We will not repeat the proof here.

When thinking about the topological properties of the symplectic group manifold, it is a good idea to keep in mind an image of a certain three-dimensional object, consisting of the solid interior of an ordinary 2-torus, but not including the surface. Indeed, for $N = 1$, such an object is homeomorphic, i.e. topologically equivalent, to the symplectic group manifold, and even for larger N it provides an excellent intuitive guide. The (correct) idea conveyed by this picture is that the symplectic group manifold has a single "hole" in it, so that every closed curve is characterized by a winding number. A positive sense of traversal around the hole must be established by convention, but, once this is done, positive winding numbers can be distinguished from negative ones, since the curves are parameterized.

To be more precise about this, and to state the matter without reference to holes, we can say that every closed curve on the symplectic group manifold can be characterized by an integer, which we shall call the winding number, such that the following properties hold. First, two closed curves can be continuously deformed into one another, i.e. they belong to the same homotopy class, if and only if their winding

numbers are identical. Second, a curve which does not go anywhere, say, $S(\lambda) = S_0 = \text{const.}$ for all λ , has a winding number of 0. Third, if the parameterization of a curve is reversed, then the winding number changes sign. And fourth, if two curves which begin and end at the same point are concatenated, by going first around the first curve and then around the second, then the winding number of the compound curve is the sum of the two original winding numbers. (This concatenation process is the usual way of "multiplying" curves in homotopy theory.)

These facts are equivalent to saying that the fundamental group of the symplectic group manifold is \mathbf{Z}^1 , the set of the integers under addition. The fact that this group is Abelian simplifies certain things, and makes it easier to follow one's intuition. All the facts stated are in accordance with the intuitive image of the interior of the torus introduced above.

It is possible to establish a definite algorithm whereby the winding number of a periodic symplectic matrix $S(\lambda)$ can actually be computed. We shall denote this winding number by $\text{wn } S(\lambda)$, using the same notation "wn" for winding numbers in the symplectic group manifold as for periodic, nonzero closed curves of complex numbers in the complex plane. As was shown in Appendix A of Ref. 15, it turns out that one way to compute the winding number of a periodic symplectic matrix $S(\lambda)$ is to use the formula,

$$\text{wn } S(\lambda) = \text{wn } \det(A + iB). \quad (27)$$

In other words, the winding number in the complex plane which emerges from wave-packet evolution, when $S(\lambda)$ is given by Eq. (13), is the same as that in the symplectic group manifold. Therefore we can restate the relationship between the Maslov index and periodic symplectic matrices by writing

$$\mu = 2 \text{wn } S(\lambda). \quad (28)$$

This is the relationship which was recognized early by Arnold¹⁹ and other mathematicians. (Actually, Arnold worked with the manifold of Lagrangian planes, and not the symplectic group manifold. However, they are closely related.) Apparently,

however, they established this connection through WKB theory, or more precisely, Maslov's version of it,¹⁻⁴ and not through wave packets, as we have done here.

We will now use topological reasoning to prove several useful results. Let $S(t)$, $S_1(t)$ and $S_2(t)$ be any three periodic symplectic matrix functions, i.e. any three closed curves in the symplectic group manifold, and let S_0 be a constant symplectic matrix. Here we have set $t = \lambda/2\pi$; t is not time, but merely another parameter, designed to make the periods of our curves equal to unity instead of 2π , as is customary in homotopy theory. Then we have the following three relations, not all of which are independent:

$$\text{wn}(S_0 S(t)) = \text{wn}(S(t) S_0) = \text{wn}(S(t)); \quad (29)$$

$$\text{wn}(S(t)^{-1}) = -\text{wn}(S(t)); \quad (30)$$

$$\text{wn}(S_1(t) S_2(t)) = \text{wn}(S_1(t)) + \text{wn}(S_2(t)). \quad (31)$$

Note in particular that the left side of Eq. (31) is well defined, since the matrix product $S_1(t) S_2(t)$ is periodic with period unity if $S_1(t)$ and $S_2(t)$ individually are.

We prove Eq. (29) by continuously deforming the curve $S_0 S(t)$ or $S(t) S_0$ into $S(t)$. To do this, we call on the fact that the symplectic group manifold is connected (or more precisely, arc-wise connected), as the image of the interior of the torus would suggest, so that it is always possible to connect S_0 with the identity matrix I by means of some continuous curve of symplectic matrices. We denote this curve by $R(s)$, where s is a parameter ranging between 0 and 1, such that $R(0) = I$ and $R(1) = S_0$. Note that $R(s)$ is not a closed curve. Then for each value of s , the product $R(s) S(t)$ or $S(t) R(s)$ is a closed curve (in the variable t), which continuously deforms between $S(t)$ (for $s = 0$) and $S_0 S(t)$ or $S(t) S_0$ (for $s = 1$). Since the winding number cannot change under continuous deformations, Eq. (29) follows.

We prove Eq. (31) next. The idea is to continuously deform the closed curve $S_1(t) S_2(t)$ into the concatenation, or homotopic product, of $S_1(t)$ and $S_2(t)$. As noted above, and as is clear geometrically, winding numbers simply add under the homotopic product, so Eq. (31) will follow. However, the homotopic product is only defined if both curves have the same beginning and ending points, so we

must dispense with this issue first. We do so by setting $S_1'(t) = S_1(0)^{-1}S_1(t)$ and $S_2'(t) = S_2(t)S_2(0)^{-1}$, so that both $S_1'(t)$ and $S_2'(t)$ begin and end at the identity matrix. Then, by applying Eq. (29) to both sides of Eq. (31), we see that Eq. (31) will be true if and only if its primed equivalent is true. That is, we can, without loss of generality, assume that both $S_1(t)$ and $S_2(t)$ in Eq. (31) begin and end at the identity.

The homotopic product of $S_1(t)$ and $S_2(t)$ is a single curve $P(t)$ which crosses $S_1(t)$ on the first half of the domain of its independent variable, and $S_2(t)$ on the second half. In order to keep the period of $P(t)$ equal to unity, we set

$$P(t) = \begin{cases} S_1(2t), & 0 \leq t \leq \frac{1}{2}, \\ S_2(2t - 1), & \frac{1}{2} \leq t \leq 1. \end{cases} \quad (32)$$

To prove Eq. (31), we continuously deform the matrix product $S_1(t)S_2(t)$ into the homotopy product $P(t)$, by again invoking a deformation parameter s . We set

$$S(s, t) = \begin{cases} S_1(t(1+s)), & 0 \leq t \leq \frac{s}{1+s}, \\ S_1(t(1+s))S_2(t(1+s) - s), & \frac{s}{1+s} \leq t \leq \frac{1}{1+s}, \\ S_2(t(1+s) - s), & \frac{1}{1+s} \leq t \leq 1. \end{cases} \quad (33)$$

As s varies from 0 to 1, $S(s, t)$ represents a closed curve (in t) which continuously varies between $S_1(t)S_2(t)$ at $s = 0$ and $P(t)$ at $s = 1$. Therefore Eq. (31) is proven. This is quite a powerful result, that matrix products behave just like homotopic products, insofar as winding numbers are concerned.

Finally, Eq. (30) follows easily from Eq. (31), by setting $S_1(t) = S(t)$ and $S_2(t) = S(t)^{-1}$. On the left we get the winding number of the identity matrix, which is zero.

Equations (29-31) can be used to prove a large number of alternatives to Eq. (27) for computing the Maslov index. For example, by noting that the matrix J of Eq. (15) is symplectic and constant, we can identify it with S_0 in Eq. (29).

Then, decomposing $S(t)$ according to Eq. (16), we have

$$\begin{aligned} \text{wn det}(\mathbf{A} + i\mathbf{B}) &= \text{wn } \mathbf{S} = \text{wn } \mathbf{J}\mathbf{S} \\ &= \text{wn} \begin{pmatrix} \mathbf{C} & \mathbf{D} \\ -\mathbf{A} & -\mathbf{B} \end{pmatrix} = \text{wn det}(\mathbf{C} + i\mathbf{D}). \end{aligned} \quad (34)$$

Thus, $\mathbf{C} + i\mathbf{D}$ will work as well as $\mathbf{A} + i\mathbf{B}$ for computing the Maslov index. When this is used in Eq. (26), it shows that $q(\lambda)$ can be replaced by $p(\lambda)$, without changing the Maslov index. The same result could also have been obtained by studying wave packet evolution in momentum space.

As another example, Eq. (29) implies that $\mathbf{S}(t)$ and $-\mathbf{S}(t)$ have the same winding numbers, since $-\mathbf{I}$ is a constant symplectic matrix. When this is combined with the fact that $\tilde{\mathbf{S}} = -\mathbf{J}\mathbf{S}^{-1}\mathbf{J}$, as follows from Eq. (14), we see that $\tilde{\mathbf{S}}$ and \mathbf{S}^{-1} also have the same winding numbers (but opposite that of $\mathbf{S}(t)$ and $-\mathbf{S}(t)$). Thus, by Eq. (30), we have

$$\begin{aligned} -\text{wn } \mathbf{S} &= \text{wn } \mathbf{S}^{-1} = \text{wn } \tilde{\mathbf{S}} \\ &= \text{wn} \begin{pmatrix} \tilde{\mathbf{A}} & \tilde{\mathbf{C}} \\ \tilde{\mathbf{B}} & \tilde{\mathbf{D}} \end{pmatrix} = \text{wn det}(\tilde{\mathbf{A}} + i\tilde{\mathbf{C}}) = \text{wn det}(\tilde{\mathbf{B}} + i\tilde{\mathbf{D}}). \end{aligned} \quad (35)$$

However, the determinant does not change when we take the transpose, and a winding number in the complex plane changes sign when we take the complex conjugate. Therefore $\mathbf{A} - i\mathbf{C}$ and $\mathbf{B} - i\mathbf{D}$ will also work as well as $\mathbf{A} + i\mathbf{B}$ for computing Maslov indices. Altogether, we have shown that

$$\begin{aligned} \text{wn } \mathbf{S} &= \text{wn det}(\mathbf{A} + i\mathbf{B}) = \text{wn det}(\mathbf{C} + i\mathbf{D}) \\ &= \text{wn det}(\mathbf{A} - i\mathbf{C}) = \text{wn det}(\mathbf{B} - i\mathbf{D}), \end{aligned} \quad (36)$$

and many other equivalent formulas can be derived as well. The argument used in Sec. 3 to show that $\mathbf{A} + i\mathbf{B}$ can never be singular is easily extended to all these other matrices. In particular, this will show that the matrix \mathbf{M} of Eq. 5 is always nonsingular, as claimed.

Now let us go back to the periodic symplectic matrix $S(\lambda)$ given by Eq. (13), which occurs in wave packet evolution, where $q(\lambda)$ and $p(\lambda)$ represent orbits generated by one of the actions, say J_k . Furthermore, let us decompose this matrix according to Eq. (22). As noted previously, the middle matrix is just the identity, and the third one is constant. Therefore, by Eq. (29), we have

$$\text{wn} \left(\frac{\partial(q, p)}{\partial(q_0, p_0)} \right) = \text{wn} \left(\frac{\partial(q, p)}{\partial(\theta, J)} \right). \quad (37)$$

But, by combining this with Eqs. (26) and (36), we find

$$\mu_k = 2 \text{wn} \det \left(\frac{\partial q(\lambda)}{\partial q_0} + i \frac{\partial q(\lambda)}{\partial p_0} \right) = 2 \text{wn} \det \left(\frac{\partial q(\lambda)}{\partial \theta} - i \frac{\partial p(\lambda)}{\partial \theta} \right), \quad (38)$$

as well as many other formulas that are easy to write down. This establishes that the Maslov indices of Eqs. (7) and (26) are identical, as we have claimed.

Let us now consider what happens to Eq. (7) under a canonical transformation of the form $(q, p) \rightarrow (q', p')$. (We can evaluate Eq. (7) along some curve in phase space, such as the action orbit, Γ_k .) If we write μ and μ' for the two Maslov indices obtained from Eq. (7) by using the two sets of canonical variables indicated, then we can relate them by using the chain rule,

$$\frac{\partial(q', p')}{\partial(\theta, J)} = \frac{\partial(q', p')}{\partial(q, p)} \cdot \frac{\partial(q, p)}{\partial(\theta, J)}, \quad (39)$$

and by applying Eq. (31), to obtain

$$\mu' = \mu + 2 \text{wn} \left(\frac{\partial(q', p')}{\partial(q, p)} \right). \quad (40)$$

It makes sense to talk about the winding number in the final term on the right in this equation, since the symplectic matrix indicated is obtained by evaluating the Jacobian of the canonical transformation $(q, p) \rightarrow (q', p')$ along the given closed curve in phase space. As long as this transformation is smooth and well defined along this curve, then the Jacobian will also be well defined, and periodic.

The process of associating a periodic symplectic matrix with a closed curve in phase space, by evaluating the Jacobian of some canonical transformation along it,

is an interesting one, because it does not require that the curve in question lie on an invariant torus. Furthermore, if the curve in phase space is continuously deformed, then the corresponding winding number cannot change, so long as the Jacobian matrix remains continuous and well defined. In fact, if the phase space loop can be contracted to a point while these conditions are met, then the winding number must be zero. This will be the case for the second term on the right in Eq. (40), if the canonical transformation $(q, p) \rightarrow (q', p')$ is smooth and well defined on some simply connected region in phase space which includes the curve in question, as was mentioned in Sec. 2. In this case, we have $\mu = \mu'$, and Eq. (7) is indeed invariant under canonical transformations.

One may well wonder why the same contraction argument could not also be applied to the winding numbers of the first and third symplectic matrices shown in Eq. (39), which correspond to the Maslov indices μ' and μ . Apparently this argument would indicate that both μ and μ' should always vanish, and we know this is not true. The answer is that the canonical transformation (q, p) or $(q', p') \rightarrow (\theta, \mathbf{J})$ is not well defined on a simply connected region containing the action orbit Γ_k , because the angle θ_k is not defined when the action J_k vanishes. In other words, the action orbit Γ_k cannot be contracted to a point without pulling it through (or onto) a point where $J_k = 0$. On the other hand, as long as such singularities are avoided, the curve can be deformed without changing the Maslov indices.

Finally, let us return to the question of what to do if we wish to use an initial wave packet with different second moments of \hat{q} and \hat{p} than those afforded by the standard coherent state of Eq. (12). Heller¹⁴ has solved the problem of propagating a Gaussian wave packet in the quadratic approximation with any arbitrary Gaussian as initial conditions, and it turns out that the solution can still be represented in the form of Eq. (17), except that A, B, C, D are no longer the submatrices of the symplectic matrix S of Eq. (13). Instead, they are the submatrices of another symplectic matrix, $S' = SS_0$, where S_0 is a constant symplectic matrix which is related to the choice of initial state. The precise rules for determining S_0 are given in Sec. 8 of Ref. 15; we will not go into them here, except to note that the Maslov index of S' is the same as that of S , on account of Eq. (29). In other words, no matter what initial Gaussian state we choose, it is always the leading square root

factor which is responsible for the Maslov index, and this Maslov index is always the same.

5. Conclusions

In this paper we have given a fairly complete accounting of the Maslov index, as it occurs in wave packet evolution. Something we have not done is to relate the Maslov index we discuss here to the one which occurs in WKB theory. Since the Maslov index and the EBK rules can be derived entirely within wave packet theory, as indicated in Sec. 3, there seems to be no logical necessity of doing this. Furthermore, we wanted to avoid a lengthy excursion into the subject of caustic counting, which is not necessary in wave packet theory.

It would also be interesting to explore the meaning of the Maslov index for phase spaces which are not flat, such as the spherical phase space which occurs in rigid body motion. There seems to be some uncertainty for such systems as to when and how the Maslov index should be used. In general, it seems to us, the semiclassical mechanics of such systems is not well understood, and we hope to be able to shed some light on this subject in the future.

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