Title

On the Micromechanisms of Fatigue-Crack Propagation in Aluminum-Lithium Alloys: Sheet vs. Vlate Material

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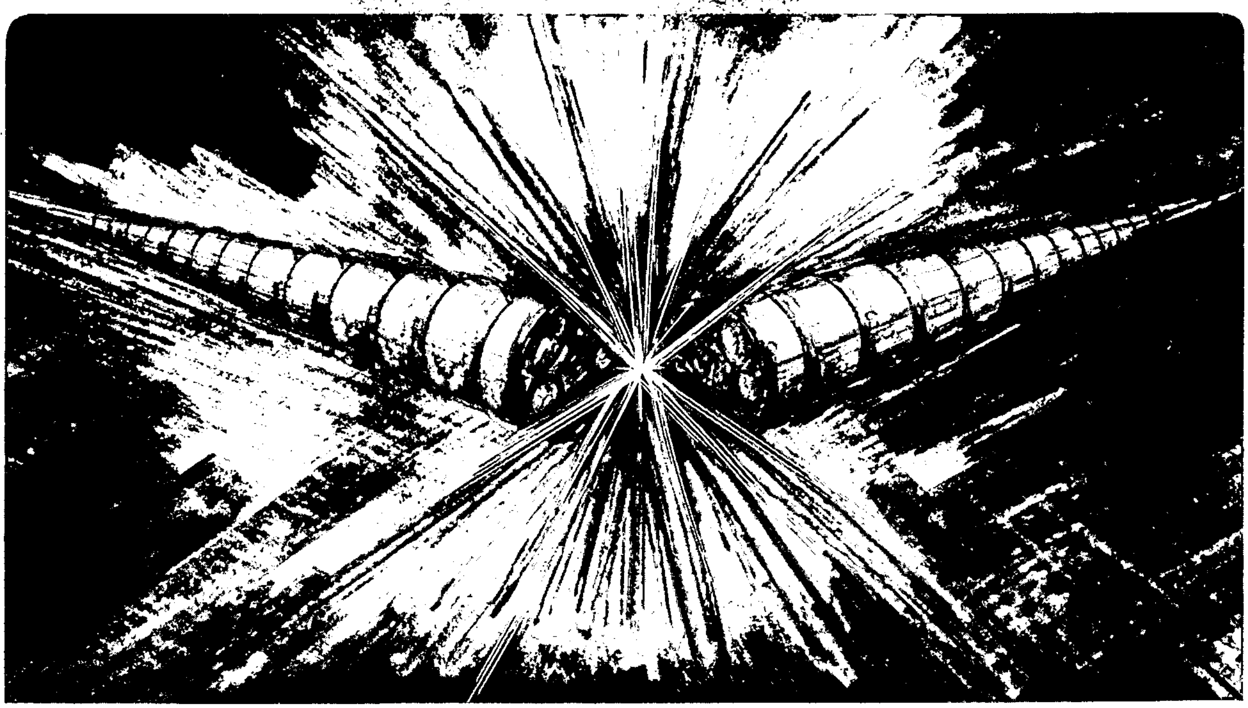

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Abstract

Traditional WKB theory yields wavefunctions which have divergences and are not invariant under any reasonable class of transformations. This letter presents alternative WKB wavefunctions which have no divergences and are symplectic invariants.

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WKB theory is an eminently practical theory, finding wide application in all branches of physical science. Its uses are by no means limited to the Schrödinger equation, but rather encompass all types of linear wave equations, including integral equations. Nevertheless, WKB theory has a number of shortcomings, both practical and theoretical.

From a practical point of view, WKB theory suffers from a lack of a uniform approximation for the wave function, due to divergences at caustics. The methods developed to handle this problem are either nonuniform, or specific to special configurations of turning points, or special to one dimension. Furthermore, these methods are generally awkward and esthetically unappealing. An exception to this is the set of methods developed by Heller,[1] about which I will say more.

From a theoretical point of view, it is notable that many features of traditional WKB theory are not invariant under any reasonable class of transformations in the phase space of ray trajectories. For example, the usual WKB approximation does not commute with the Fourier transform: the locations of turning points and the structure of Stokes' lines are not the same in momentum space as in configuration space. Ideally, one would like to have a WKB theory whose results are independent of the phase space coordinates in which the calculations are carried out. Such goals motivated an early paper by Einstein[2] on quantum mechanics, but have been absent from most work on WKB theory.

In this letter I shall present a formula for a normal mode of a self-adjoint wave equation (in quantum mechanics, an energy eigenfunction) which is a symplectic invariant. The precise meaning of this term will be given later. In addition to being a symplectic invariant, the result is a uniform approximation to the exact wave function, i.e. it has no infinities at caustics. For simplicity, the result is presented in the context of a one-dimensional system; similar techniques can be applied to integrable systems in several dimensions, and, with some modifications, to nonintegrable systems.

There are several avenues to this result, each more or less abstract. For the sake of clarity, the following approach is fairly concrete, being based on a picture developed by Maslov[3] and Percival.[4] We consider a one-dimensional wave equation, separable in time, which abstractly has the form $L\psi = 0$ for some linear operator L. Corresponding to L is a function $D(q,p,\omega)$ on a classical phase space, parameterized by the frequency ω, which serves as the Hamiltonian for the ray trajectories. As discussed by McDonald,[5] there are persuasive reasons for taking D to be the Weyl symbol of the operator L; by this definition, D is a symplectic invariant. In quantum mechanical applications, $D(q,p,\omega) = H(q,p) - E$, where H is the classical Hamiltonian and $E = \hbar\omega$; in other applications, D is a local dispersion relation. Here we identify p and k, and q and x, and we set $\hbar = 1$. The ray trajectories in phase space generated by D are assumed to be closed curves for some range of ω; thus, the system is bounded. Corresponding to this family of closed curves are the action–angle variables (I,θ).

We fix attention on one of these curves Γ, given by $I(q,p) = I_0 = \text{const.}$, a portion of which is shown in Fig. 1. In standard WKB theory, a WKB wavelet is associated with each branch of the projection of this curve onto the q-axis. The degree to which this wavelet represents the true wavefunction depends on the quantity $(\partial p/\partial q)_I$; the approximation is best when this quantity is zero, and becomes progressively worse as this quantity becomes large. It breaks down completely at the caustics, where $(\partial p/\partial q)_I$ is infinite.

A common strategy[4] for dealing with caustics is to switch to momentum space as one approaches a caustic, since this replaces $(\partial p/\partial q)_I$ by $(\partial q/\partial p)_I$ as the criterion of the goodness of the approximation; the latter is small when the former is large. Continuity of the WKB wavelet on Γ is guaranteed by using the Fourier transform on some overlap region, evaluated by stationary phase; the result is a phase shift which accumulates as one moves around Γ, giving finally the Maslov index as a part of the quantization condition.

We propose here to use not just the position and momentum representations, but rather a large number of intermediates, one for each of a number of small segments on Γ, with each representation chosen to be optimal on its particular segment. We divide the curve Γ into N small segments, (say) evenly spaced in the angle variable θ, with $\Delta\theta = 2\pi/N$. The beginning of the n-th segment is marked by the point $\varsigma = (\xi, \eta)$ in Fig. 1. We associate with each segment two canonical coordinate systems, $z_n = (q_n, p_n)$ and $Z_n = (Q_n, P_n)$. The system $z_n = (q_n, p_n)$ is related to $z = (q, p)$ by a simple translation in phase space, namely $z_n = z - \varsigma$. The system $Z_n = (Q_n, P_n)$ is in turn related to $z_n = (q_n, p_n)$ by a fixed symplectic matrix R, according to $z_n = RZ_n$. For R we write

$$R = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{1}$$

where we take $a = \partial q/\partial\theta$, $b = \partial q/\partial I$, $c = \partial p/\partial\theta$, $d = \partial p/\partial I$, all evaluated at (ξ, η).

The effect of these conventions is to make Γ appear in the (Q_n, P_n) coordinates as a curve passing through the origin, tangent to the Q_n-axis. Furthermore, the coordinates (Q_n, P_n) produce locally a copy of the (θ, I) coordinate mesh, although (Q_n, P_n) form straight lines everywhere, and (θ, I) gradually curve as one moves away from (ξ, η). Thus, the range in Q_n is $0 \le Q_n \le \Delta\theta$. To lowest order in $\Delta\theta$, the Hamilton-Jacobi equation is trivial to solve in the

(Q_n, P_n) coordinates; the action is $S_n(Q_n, I) = \alpha_n + (I - I_0)Q_n$, where α_n is a constant to be determined, and the local WKB wavelet is simply

$$\phi_n(Q_n) = e^{i\alpha_n}, \tag{2}$$

where we have set $I = I_0$.

This wavelet from the n-th segment is transformed from the Q_n representation successively to the q_n-representation and finally to the q-representation. The first step involves a unitary transformation corresponding to the symplectic matrix R, which will be denoted by $M(R)$. This unitary transformation is a member of the metaplectic group, which has been invesitgated by Bargmann[6] and others. There are two such unitary transformations $M(R)$ for a given symplectic matrix R, differing by a sign, and my notation $M(R)$ will denote one of these, suitably chosen. For a specific R, it does not matter which is chosen. But when R varies continuously through the space of symplectic matrices, as does R in Eq. (1) as we move around the curve Γ, then it is necessary to choose the sign for each R so that $M(R)$ also forms a continuous family. The matrix elements of $M(R)$ in the q-basis are given by

$$\langle q|M(R)|q'\rangle = \frac{\pm 1}{\sqrt{2\pi i b}} \exp\left[\frac{i}{2b}\left(aq'^2 - 2q'q + dq^2\right)\right], \tag{3}$$

when $b \neq 0$. When $b \to 0$, the matrix element of $M(R)$ becomes singular, in the manner of a δ-function, but $M(R)$ itself is continuous and well behaved.

Transforming from the q_n-basis to the q-basis involves another unitary transformation $T(\varsigma)$, which corresponds to the displacement ς in phase space. This is a member of the Heisenberg-Weyl group of operators, and is given explicitly by $T(\varsigma) = \exp[i(\eta\hat{q} - \xi\hat{p})]$, where $\hat{q}, \hat{p}$ are operators. Combining these transformations, we have

$$\langle q|WKB,n\rangle = \Delta\theta e^{i\alpha_n}\langle q|T(\varsigma)M(R)|0\rangle, \tag{4}$$

where the left side denotes the n-th WKB wavelet in the q-basis. When we combine this with a similar expression for the $(n+1)$-st segment and demand continuity, just as Percival has done for four segments, we find $\Delta\alpha = \alpha_{n+1} - \alpha_n = \frac{1}{2}(p\Delta q - q\Delta p)$. We also demand continuity between segment 0 and segment $N-1$, when we have gone completely around Γ. This reproduces the EBK quantization condition, which requires that the action I_0 on Γ satisfy $I_0 = n + \frac{1}{2}$.

Finally, we add up the contributions from all the segments and take the limit $N \to \infty$, and we obtain the total q-space wave function

$$\psi(q) = c\int_0^{2\pi} d\theta\, e^{i\alpha}\langle q|T(\varsigma)M(R)|0\rangle, \tag{5}$$

where c is a normalization constant, and where ς and R are functions of θ, being evaluated along the curve Γ. The phase $\alpha = \alpha(\theta)$ is given by

$$\alpha(\theta) = \frac{1}{2}\int_0^{\theta} d\theta\left(p\frac{dq}{d\theta} - q\frac{dp}{d\theta}\right). \tag{6}$$

I shall now explain the term "symplectic invariant." A given linear, inhomogeneous canonical transformation on the classical phase space corresponds to a definite displacement ς_0 in phase space and a definite symplectic matrix R_0. These in turn can be placed into correspondence with a unitary transformation composed of $T(\varsigma_0)$ and $M(R_0)$, acting on wave functions. A formula will be called a symplectic invariant if transforming the wave functions by the unitary operator has the same effect as transforming the classical coordinates by the given linear canonical transformation. By this definition, Eq. (5) is a symplectic invariant. For example, if $\varsigma = \varsigma(\theta)$ and $R = R(\theta)$ in Eq. (5) are referred to the coordinates (q', p'), with $q' = p$, $p' = -q$, then the wave function which emerges is the Fourier transform of the one given, i.e. the answer emerges in the momentum representation.

Explicitly evaluating the operators in Eq. (5), we find

$$\psi(q) = c \int_0^{2\pi} d\theta \, \frac{e^{i(\alpha + \eta q - \xi\eta/2)}}{\sqrt{2\pi i \left(\frac{\partial q}{\partial I}\right)_\theta}} \exp\left[\frac{i}{2}\left(\frac{\partial p}{\partial q}\right)_\theta (q - \xi)^2\right], \tag{7}$$

in which form the symplectic invariance is less apparent. Again, α, ξ and η are functions of θ as we move around Γ, as are the partial derivatives shown.

An apparent drawback to this result is the singularity of the integrand as $\partial q/\partial I \to 0$. But there is an avenue around this difficulty, which uses the coherent state basis,[7] and which always yields nonsingular integrands. I will report on this in more detail in the future; for now I merely note that the results are closely related to the techniques developed by Heller.[1]

Equations (5) and (7) can also be understood in terms of a propagator formalism. Effectively, we have replaced the exact propagator by an approximation which is composed of Heisenberg and metaplectic operators, referred to a certain classical trajectory. Similar approximations have been used in classical mechanics.[8] The details of this connection will be given in the future.

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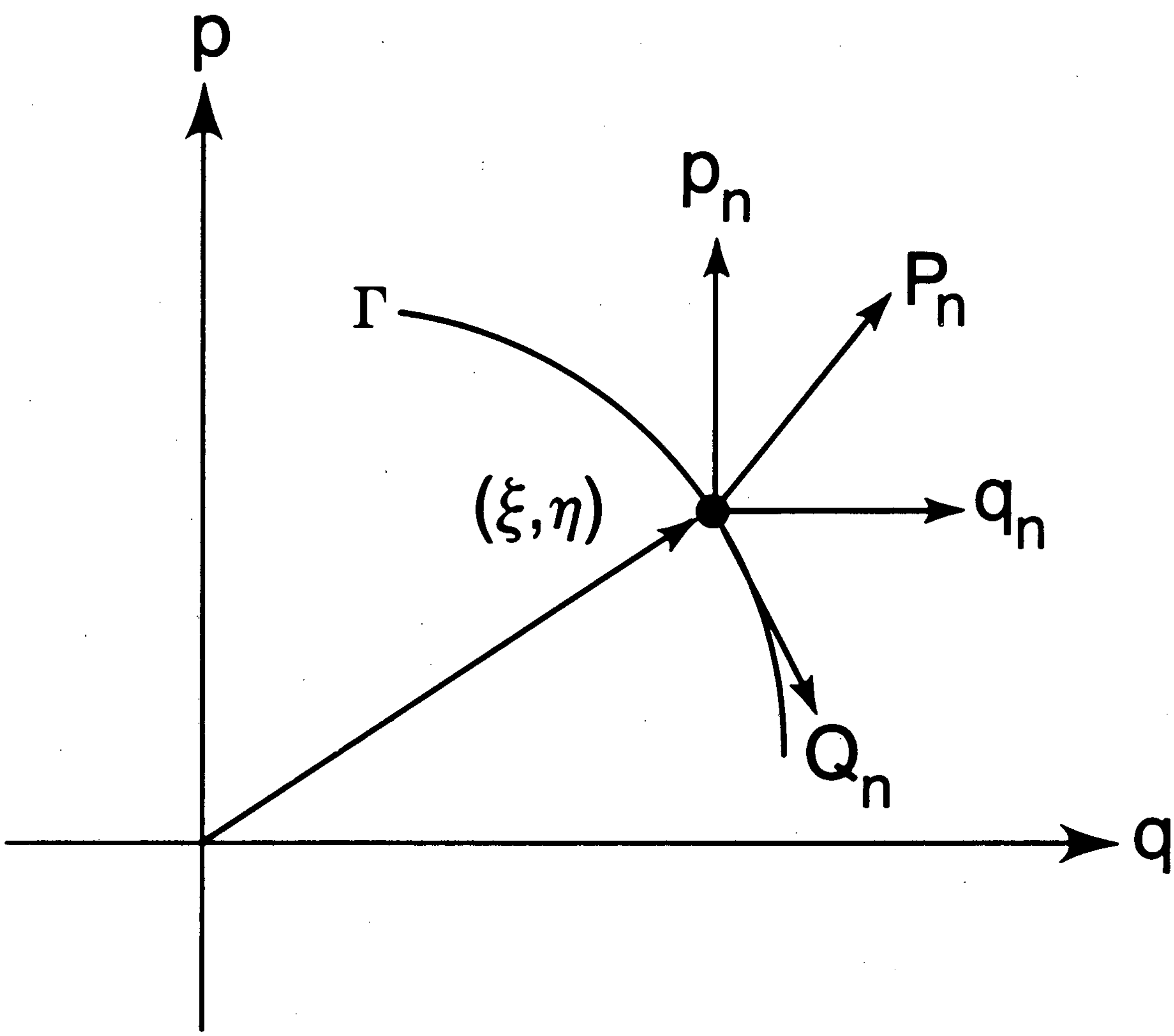
Figure Captions.

Fig. 1. Coordinate systems in phase space.



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