Regular and chaotic propagators in quantum theory

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Quantum-mechanical propagators of regular and chaotic systems are qualitatively different. The rms time average of a chaotic propagator is uniformly spread over the entire Hilbert space, while that of a regular propagator is large in some domains and small in others. Moreover, the instantaneous (complex) value of the propagator appears to follow a regular pattern for regular systems and is "random" for chaotic systems.

Classical Hamiltonian systems have two types of qualitatively different orbits.[1,2] Those of integrable systems are multiply periodic in time and are constrained to lie on n-dimensional tori in the $2n$-dimensional phase space. They are called "regular." On the other hand, the orbits of a nonintegrable system explore part or all of the energy surface, which is $(2n-1)$-dimensional. They are called "chaotic" because any small deviation from the initial data grows exponentially. Even when the initial data are perfectly known, the motion is unpredictable for long times, if we use a *finite* computer.[3] Intermediate cases also exist. In particular, there are systems having mostly regular orbits in some regions of their phase space, and mostly chaotic orbits in other regions.[4–6]

These properties are reflected in various ways in the quantum analogs of these Hamiltonian systems. If we use a "reasonable" basis in Hilbert space (i.e., a basis consisting of eigenfunctions of reasonable operators[7,8] such as position, momentum, angular momentum, etc.), then the eigenfunctions of a regular Hamiltonian are "localized." Most of their components (in the above basis) are vanishingly small. Only a small minority of the components are large. This is related to the existence of selection rules. On the other hand, the eigenfunctions of a chaotic Hamiltonian have many small "random" components. The corresponding Wigner functions[9] occupy the entire available phase space, with an amplitude roughly proportional to the microcanonical probability density at the corresponding energy. These properties, first conjectured by Percival,[10] are now firmly established by a large body of theoretical arguments[11–16] and numerical simulations.[17–21]

In this paper, we show that there are, not unexpectedly, significant morphological differences in the propagators (Green's functions) of regular versus chaotic systems. The propagator $G_{mn}(t)$ is defined (in any arbitrary basis) by

$$G_{mn}(t)=\sum_E u_{Em}u_{En}^{*}e^{-iEt/\hbar} . \tag{1}$$

In Eq. (1) the sum is taken over all the energy levels of the Hamiltonian (its spectrum is assumed discrete, for simplicity) and the u_{Em} are the corresponding normalized eigenfunctions:

$$\sum_m H_{km}u_{Em}=Eu_{Ek} . \tag{2}$$

The name "propagator" is due to the fact that an arbitrary initial state vector $\psi_m(0)=\sum_E c_E u_{Em}$ evolves into

$$\psi_m(t)=\sum_E c_E u_{Em}e^{-iEt/\hbar} \tag{3}$$

$$=\sum_n G_{mn}(t)\psi_n(0) . \tag{4}$$

In particular, we have the combination law

$$\sum_n G_{mn}(t')G_{ns}(t'')=G_{ms}(t'+t'') . \tag{5}$$

Notice that

$$G_{nn}(t)=(v_n,e^{-iHt/\hbar}v_n) \tag{6}$$

is equal to the "survival" amplitude, after a time t, of a state initially equal to the basis vector v_n.

The difference between regular and chaotic propagators arises from the fact that in the regular case the unitary matrix u_{Em} is sparse (most elements are very close to zero, only a few are large) while in the chaotic case it is pseudorandom.[22] (It is not truly random, of course, because of the orthonormality constraints.) By virtue of Eq. (1), the same properties are likely to hold for $G_{mn}(t)$, as soon as t is large enough so that the initial constraint $G_{mn}(0)=\delta_{mn}$ is washed away by the dephasing of the various components.

This is best seen if we consider the time average of $|G_{mn}|^2$, which we shall denote by angular brackets. Assuming for simplicity that the energy levels are not degenerate, we have

$$\langle |G_{mn}|^2\rangle=\sum_E |u_{Em}|^2|u_{En}|^2 . \tag{7}$$

This expression was first obtained by Nordholm and Rice[17] who called it P_{mn}. Its properties were further discussed by Heller[14] who denoted it as $P(m\,|\,n)$. Notice that

$$\sum_m \langle |G_{mn}|^2\rangle=1 . \tag{8}$$

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Thus, if many $|u_{Em}|$ have roughly the same order of magnitude (in a chaotic system) so do the $\langle |G_{mn}|^2 \rangle$ and their value is roughly the inverse of the number of energy levels involved. On the other hand, if the system is regular and therefore subject to selection rules, $|u_{Em}|^2$ and $|u_{En}|^2$ will rarely both be large for the same E, therefore most $\langle |G_{mn}|^2 \rangle$ will be very small. A few of them must of course be large, because of (8).

Here, it should be pointed out that even in the chaotic case, the $|u_{Em}|^2$ may be pseudorandom only for a limited range of values of E (roughly, within a standard deviation from the expectation value of E). This point was discussed in great detail by Heller[14] who introduced the notion of "spectral envelope." However, in the example given below, the chaotic state which we consider has a spectral envelope which is nearly flat over the entire energy spectrum, so that this question does not come up.

To illustrate these properties, we used the coupled-rotators model, with Hamiltonian[6,21]

$$H = L_z + M_z + L_x M_x \ . \tag{9}$$

Here, **L** and **M** are two independent angular momenta. The constants of motion of this system are H, L^2, and M^2. For some values of these constants, the *classical* system with Hamiltonian (9) is regular, for other values it is chaotic.[6] These properties are reflected in the quantum-mechanical spectrum[23,24] and matrix elements.[21]

For given values of $L^2 = \hbar^2 l(l+1)$ and $M^2 = \hbar^2 m(m+1)$, the Hamiltonian (9) is a finite matrix of order $(2l+1)(2m+1)$. It is convenient to use a basis $|j,k\rangle$ labeled by $j=(L_z+M_z)/\hbar$ and $k=(L_z-M_z)/\hbar$. If $l=m$, the Hilbert space splits into four disjoint subspaces, with j even or odd, and with states even or odd with respect to $k \to -k$. The Hamiltonian (9) has no matrix elements connecting these subspaces. In the following numerical example, the discussion will be restricted to the even-even subspace.

As in previous work,[21,23,24] we took $l=m=20$ and $\hbar = 0.170\,782\,5$. (This corresponds to $L=M=3.5$.)

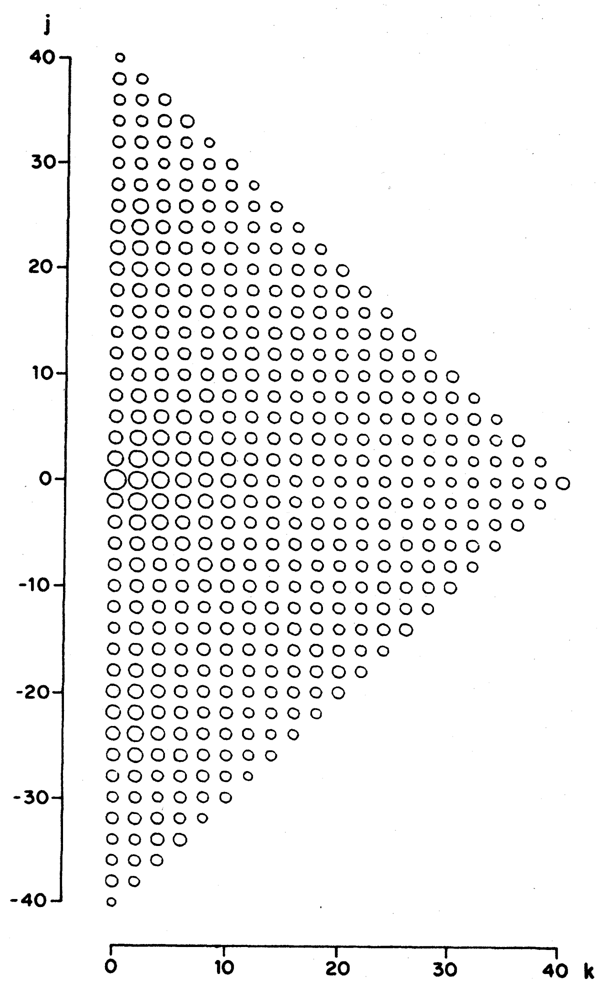

FIG. 1. Time average of the propagator from a chaotic state. The initial state is $|c\rangle = |0,0\rangle$. The area of each circle is proportional to $\langle |G_{mc}|^2 \rangle$.

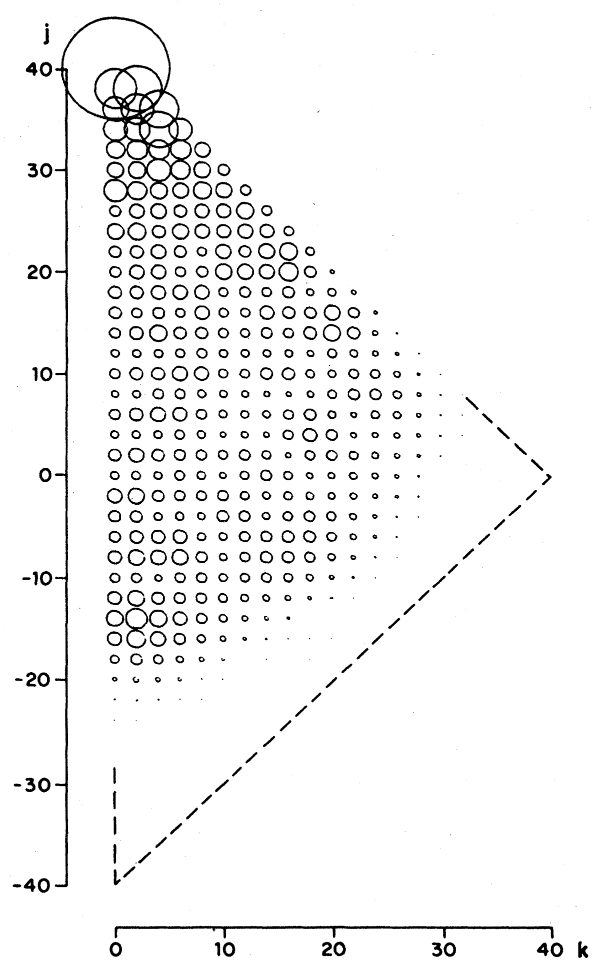

FIG. 2. Time average of the propagator from a regular state. The initial state is $|r\rangle = |40,0\rangle$. The area of each circle is proportional to $\langle |G_{mr}|^2 \rangle$, with the same scale as in Fig. 1.

Under these conditions, it was found[25] that some basis vectors, for example $|0,0\rangle$, have chaotic dynamics, namely, $e^{-iHt/\hbar}|0,0\rangle$ is very sensitive to a small perturbation of H. Other basis vectors, such as $|40,0\rangle$, which are mostly localized in the regular part of the classical phase space, have an evolution $e^{-iHt/\hbar}|40,0\rangle$ which is much less sensitive to small perturbations of the Hamiltonian.[25] In the present paper we shall compare the propagators $G_{mc}(t)$ and $G_{mr}(t)$, where $|c\rangle=|0,0\rangle$ and $|r\rangle=|40,0\rangle$ are the two basis vectors mentioned above, and $|m\rangle=|j,k\rangle$ runs over the entire Hilbert space (that is, its even-even subspace, having dimension $21^2=441$). From this point, m represents the *pair* of indices j and k.

First consider the time averages $\langle |G_{mc}|^2\rangle$ and $\langle |G_{mr}|^2\rangle$. They are shown in Figs. 1 and 2, respectively. As expected, the chaotic propagator is, on the average, nearly uniformly spread over the entire Hilbert space. This property is analogous to classical ergodicity. On the other hand, the propagator from a regular state is localized in a subset of states. It almost does not reach other parts of the Hilbert space.

Additional insight is obtained by comparing $G_{mc}(t)$ and $G_{mr}(t)$ themselves, rather than their time averages. Figure 3 shows the absolute values of the survival amplitudes $G_{cc}(t)$ and $G_{rr}(t)$. At first sight, it is surprising that the two curves are so different, since they refer to two states of the *same* system, i.e., to the *same frequency spectrum.* However, there are important differences in the way this spectrum is populated: Most components u_{Er} (i.e., $|r\rangle=|40,0\rangle$ and all values of E) are very small. The few large ones, shown in Table I, have nearly equidistant values of E (they are all within 0.2% of $E=6.794+0.213n$, with $n=0,\pm1$).[15] As a consequence, the motion is approximately quasiperiodic, as expected from the correspondence principle.[23,26] On the other hand, all the components u_{Ec} (for $|c\rangle=|0,0\rangle$) are small and their energy differences do not lead to any quasiperiodicity.

TABLE I. The most populated energy levels of the initial states.

$\|40,0\rangle$		$\|0,0\rangle$	
E	$\|u_{Er}\|^2$	E	$\|u_{Ec}\|^2$
6.801 926	0.381 937 6	±1.074 954	0.023 537 8
6.994 843	0.153 378 1	±11.056 02	0.017 808 1
7.019 689	0.114 185 5	±11.575 16	0.014 828 6
6.581 356	0.078 724 7	±2.298 508	0.013 251 7
6.791 842	0.060 114 6	0	0.012 087 5

We now turn to compare the time dependence of $G_{mc}(t)$ and $G_{mr}(t)$. Figure 4 shows $G_{mr}(t)$ for $t=31.326$ (this value of t was chosen because it corresponds to a minimum of $|G_{rr}|$). Regular patterns are easily seen: The amplitude and phase of G_{mr} vary smoothly with the Hilbert space index m (i.e., with j and k).

On the other hand, Fig. 5 shows $G_{mc}(t)$ for $t=3.045$, corresponding to a minimum of G_{cc}. The result looks

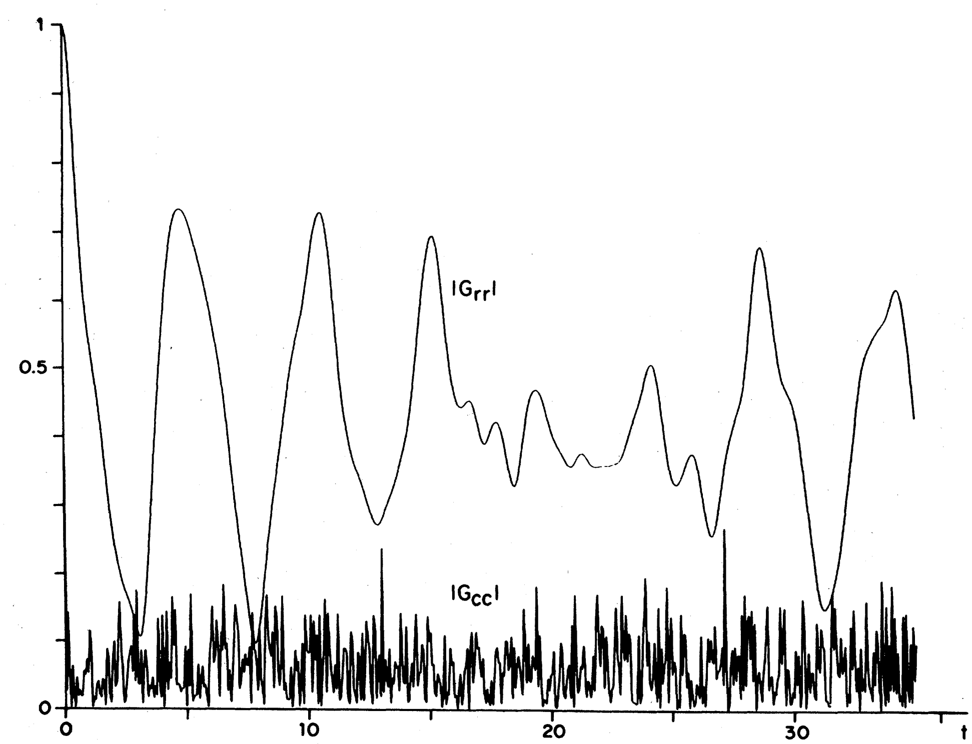

FIG. 3. The survival amplitudes $|G_{rr}(t)|$ and $|G_{cc}(t)|$. (The figure shows only the absolute values.)

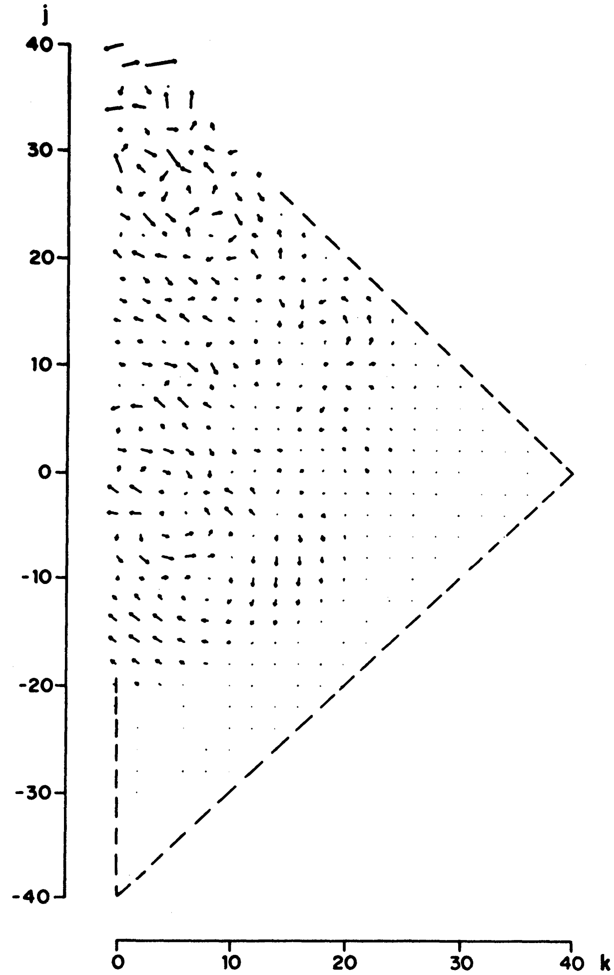

FIG. 4. The regular propagator $G_{mr}(t)$ for $t=31.326$. (Each arrow represents a complex number, as is usual.)

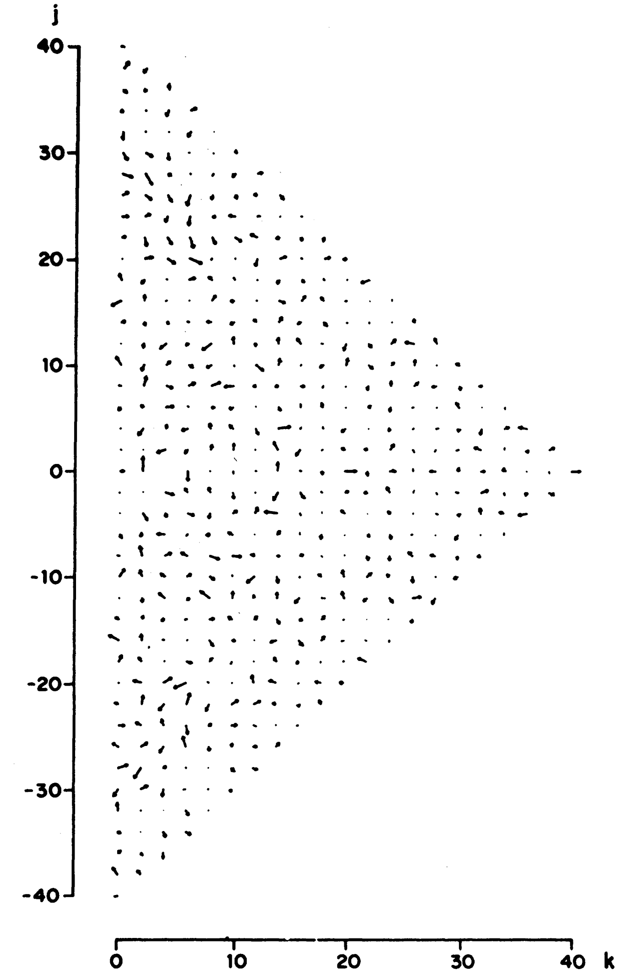

FIG. 5. The chaotic propagator $G_{mc}(t)$. Except for the symmetry discussed in Eq. (10), no regularity is apparent.

completely random. The only apparent regularity is a reflection symmetry

$$G_{-jk,c}=(-1)^{(j+k)/2}G^{*}_{jk,c} , \tag{10}$$

which is due to the fact that the spectrum of the Hamiltonian (9) consists of pairs of opposite eigenvalues (E and $-E$). This can be seen by considering a unitary transformation of H generated by a combined rotation of 180° around the L_x axis and the M_y axis[6] ($L_y\to -L_y$, $L_z\to -L_z$, $M_x\to -M_x$, and $M_z\to -M_z$). This rotation makes $H\to -H$ so that the spectrum must be symmetric with respect to $E=0$. As the initial state $|c\rangle=|0,0\rangle$ is invariant under the above combined rotation, it follows from time-reversal symmetry that $G_{-jk,c}$ must be proportional to $G^{*}_{jk,c}$. The proportionality constant $(-1)^{(j+k)/2}$ cannot be derived from symmetry arguments alone, since it depends on an arbitrary choice of phases.

Finally, let us consider the fluctuations of $|G_{mn}(t)|^2$ around its time average $\langle |G_{mn}|^2\rangle$, which is given by Eq. (7). Their rms average F is given by

$$\begin{aligned} F^2 &= \langle (|G_{mn}|^2 - \langle |G_{mn}|^2\rangle)^2\rangle \\ &= \langle |G_{mn}|^4\rangle - \langle |G_{mn}|^2\rangle^2 . \end{aligned} \tag{11}$$

The first term in the right-hand side (rhs) contains expressions such as $\exp[i(E_1-E_2+E_3-E_4)t/\hbar]$. If there are no "accidental" degeneracies of energy-level differences, these expressions have a nonvanishing time average only if $E_1=E_2$ and $E_3=E_4$, or $E_1=E_4$ and $E_2=E_3$. Collecting all the nonvanishing terms, we obtain

$$(F_{\rm nd})^2=\left[\sum_E |u_{Em}|^2|u_{En}|^2\right]^2=\langle |G_{mn}|^2\rangle^2 , \tag{12}$$

where the label "nd" means "no degeneracy." In other words, the first term in the rhs of (11) is equal to twice the second term. We thus get the remarkable result that, if there is no degeneracy in the energy-level differences, the rms fluctuation of $|G_{mn}(t)|^2$ is equal to the time average $\langle |G_{mn}|^2\rangle$.

If, however, some energy differences are equal, there will be additional terms for which $E_1-E_2+E_3-E_4=0$. In that case, the fluctuations will be *larger*. For example, in the double-rotator model, we may have $E_1+E_3=E_2+E_4=0$. It follows that

$$F^2=(F_{\rm nd})^2+\left|\sum_E u_{Em}u^*_{En}u_{-Em}u^*_{-En}\right|^2 . \quad (13)$$

Here, again, there is an essential difference between regular and chaotic states. If $|n\rangle$ is a regular state, so that most u_{En} are small (and very few are large) it is very unlikely to find any E for which both u_{En} and u_{-En} are large. Therefore the second term in the rhs of (13) is vanishingly small. On the other hand, if $|n\rangle$ is a chaotic state, all the u_{En} are more or less of the same order of magnitude, and the second term in the rhs of (13) may be comparable to the first one (it cannot exceed it, however, because of Schwarz's inequality). Numerical tests indeed confirm these qualitative predictions.

Although we tested these properties only for a particular model, they are likely to hold in general in the statistical mechanics of systems having discrete symmetries. For example, the reader is referred to a recent work of Davis and Heller[27] who investigated the dynamics of Gaussian wave packets and made a detailed comparison with the classical results. These authors denote $|G_{mn}(t)|^2$ as $P_{mn}(t)$.

In summary, we have found the following qualitative difference between regular and chaotic propagators, $G_{mr}(t)$ and $G_{mc}(t)$, respectively. The time average $\langle |G_{mc}|^2\rangle$ is spread nearly uniformly over the entire Hilbert space, while $\langle |G_{mr}|^2\rangle$ is restricted to some parts of that space. This is quite analogous to the situation in classical physics: Chaotic orbits explore the entire accessible phase space, while regular ones are constrained to Kolmogorov-Arnol'd-Moser tori.[1,2] Moreover, at any given instant, the amplitude and phase of $G_{mr}(t)$ depend rather smoothly on the Hilbert space index m—provided, of course, that the latter is a smooth function of the corresponding classical variables. (In our example, we took m as the pair jk, where j and k have elementary classical analogs.) On the other hand, $G_{mc}(t)$ does not show any simple dependence on m, other than the one required by symmetries of the Hamiltonian.

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[1] J. Ford, in *Fundamental Problems in Statistical Mechanics,* edited by E. G. D. Cohen (North-Holland, Amsterdam, 1975), Vol. III, pp. 215—255.

[2] M. V. Berry, in *Topics in Nonlinear Dynamics (La Jolla Institute),* Proceedings of the Workshop on Topics in Nonlinear Dynamics, edited by S. Jorna (AIP, New York, 1978), pp. 16—120.

[3] J. Ford, Phys. Today **36**, (4), 40 (1983).

[4] M. Hénon and C. Heiles, Astron. J. **69**, 73 (1964).

[5] R. A. Pullen and A. R. Edmonds, J. Phys. A **14**, L477 (1981).

[6] M. Feingold and A. Peres, Physica (Utrecht) D **9**, 433 (1983).

[7] L. G. Yaffe, Rev. Mod. Phys. **54**, 407 (1982).

[8] K. G. Kay, J. Chem. Phys. **79**, 3026 (1983).

[9] E. P. Wigner, Phys. Rev. **40**, 749 (1932).

[10] I. C. Percival, J. Phys. B **6**, L229 (1973).

[11] M. V. Berry, J. Phys. A **10**, 2083 (1977).

[12] M. V. Berry, Philos. Trans. R. Soc. London, Ser. A **287**, 237 (1977).

[13] A. Voros, in *Stochastic Behavior in Classical and Quantum Hamiltonian Systems,* edited by G. Casati and J. Ford (Springer, Berlin, 1979), pp. 326—333.

[14] E. J. Heller, J. Chem. Phys. **72**, 1337 (1980).

[15] M. V. Berry, J. H. Hannay, and A. M. Ozorio de Almeida, Physica (Utrecht) D **8**, 229 (1983).

[16] P. Pechukas, Phys. Rev. Lett. **51**, 943 (1983).

[17] K. S. J. Nordholm and S. A. Rice, J. Chem. Phys. **61**, 213, (1974); **61**, 768 (1974).

[18] D. W. Noid, M. L. Koszykowski, and R. A. Marcus, J. Chem. Phys. **71**, 2864 (1979).

[19] D. W. Noid, M. L. Koszykowski, M. Tabor, and R. A. Marcus, J. Chem. Phys. **72**, 6169 (1980).

[20] M. J. Davis, E. B. Stechel, and E. J. Heller, Chem. Phys. Lett. **76**, 21 (1980).

[21] M. Feingold, N. Moiseyev, and A. Peres, Phys. Rev. A **30**, 509 (1984).

[22] A. Peres, Phys. Rev. A **30**, 504 (1984).

[23] A. Peres, in *Chaotic Behavior in Quantum Systems,* edited by G. Casati (Plenum, New York, 1985).

[24] A. Peres, Phys. Rev. Lett. **53**, 1711 (1984).

[25] A. Peres, Phys. Rev. A **30**, 1610 (1984).

[26] N. Moiseyev and A. Peres, J. Chem. Phys. **79**, 5945 (1983).

[27] M. J. Davis and E. J. Heller, J. Chem. Phys. **80**, 5036 (1984).