Quantum localization and the rate of exploration of phase space

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Nonstationary phase-space distributions $\rho(t)$ are shown to sweep out phase space at a rate \mathcal{R} which can be determined from the autocorrelation function, $P(t) = h^N \text{Tr}[\rho \rho(t)]$. It is demonstrated that, after the initial decay of $P(t)$, subsequent recurrences (increases) of $P(t)$ cause permanent slowdowns in the rate \mathcal{R} . Such slowdowns may cause localization of quantum eigenstates, whereas no such implications apply to the classical stationary distributions. The localization is discussed in terms of the fraction of the available phase space which the dynamics accesses, and the phase-space distribution of individual eigenfunctions.

I. INTRODUCTION

In this paper we focus on (1) the concept of the rate at which phase space is explored, given a nonstationary initial distribution, and (2) the importance of this rate to localization of the quantum dynamics and of the eigenstates, relative to distributions determined by prior constraints. This work began as a framework for understanding "scar" localization' of certain eigenstates of classically chaotic Hamiltonian systems. The scars are nonstatistical concentrations of probability around some periodic orbits with the shortest periods and smallest Lyapunov exponents. The scars have no analog in classical stationary distributions of chaotic systems.

The context of this paper has been expanded beyond the concept of periodic orbit scarring to encompass localization under much more general circumstances. Loosely speaking, localization happens whenever the rate of phase-space flow slows down below the maximum possible for a given initial distribution. Such slowdown occurs after recurrences; i.e., when the moving distribution comes back to partially overlap the initial distribution. In this more general context, we shall be able to shed some light on localization of driven rotor systems,² localization by cantori, 3 localization in the quasiperiodic regime, scattering resonance localization, and Anderson localization.

We usually discuss localization in its weak form, namely, a partial localization to certain subdomains. Weakly localized eigenfunctions have high density in a certain subdomain but are not exponentially damped outside of the subdomain. We shall nonetheless refer to this as "localization."

In many circumstances we are able to predict, from semiclassical arguments, when weak localization will occur. This was possible in the case of the periodic orbit scarring, for example. Strong localization of the Anderson type is more difficult to handle.

The concept of the rate of exploration of phase space, and the allied concepts of the number of phase-space cells accessed in the infinite time limit and the fraction $\mathcal F$ of available phase space explored, are useful alternatives to the usual participation ratio ideas familiar from localization theory. The latter focus on the "participation" of in-

dividual eigenstates in a set of localized states, whereas the former emphasizes the eigenstate content of particular localized states. The two points of view are intimately related but by no means identical.

The paper is organized as follows. In Sec. II some concepts and definitions necessary to discuss phase-space flow in classical and quantum mechanics are defined. The basic implications of our definition of the rate of exploration of phase space are presented in Sec. III. Section IV gives some examples of the rate of exploration of phase space; Sec. V discusses the amount of phase space which is eventually accessed, and reviews the related issues of available phase space in classical and quantum mechanics. Section VI discusses the implications of recurrences (and the associated rate reduction) for quantum localization.

II. DEFINITIONS

Consider a phase-space distribution ρ , with

$$
Tr(\rho) = \int \int \rho(\mathbf{p}, \mathbf{q}) d\mathbf{p} d\mathbf{q} = 1.
$$
 (1)

The density ρ has the dimensions of (action)^{$-N$} for N degrees of freedom. Therefore, $Tr(\rho^2)$ has the dimension of $(\arctan)^{-N}$, or in other words an inverse of a volume in phase space.

The density $\rho(\mathbf{p}, \mathbf{q})$ can be purely classical or a Wigner transform⁵ of a quantum wave function:

$$
\rho(\mathbf{p}, \mathbf{q}) = \left(\frac{1}{\pi \hbar}\right)^N \int_{-\infty}^{\infty} e^{2i\mathbf{p}\cdot\mathbf{s}/\hbar} \varphi^*(\mathbf{q} + \mathbf{s}) \varphi(\mathbf{q} - \mathbf{s}) d\mathbf{s} \tag{2a}
$$

More generally, ρ may arise from a quantum density ρ_{Ω} .

$$
\rho(\mathbf{p}, \mathbf{q}) = \left[\frac{1}{\pi \hbar}\right]^N \int_{-\infty}^{\infty} e^{2i\mathbf{p}\cdot\mathbf{s}/\hbar} \rho_Q(\mathbf{q}-\mathbf{s}, \mathbf{q}+\mathbf{s}) d\mathbf{s} . \tag{2b}
$$

We want to be able to define the volume ρ occupies in bhase space. This is conceptually simple if ρ is zero in some parts of phase space, and some fixed number elsewhere, such that the total probability is unity. In that

case $\rho = V^{-1}$ everywhere it does not vanish, so that $Tr(\rho) = 1$, and

$$
\int \int \rho^2 d\mathbf{p} d\mathbf{q} = \int \int_V V^{-2} d\mathbf{p} d\mathbf{q} = V^{-1}
$$
 (3)

or

$$
volume = \frac{1}{Tr(\rho^2)} \tag{4}
$$

For more general distributions which vary smoothly over phase space, Eq. (4) is still a reasonable definition for the phase-space volume (see Fig. 1).

As an example, if ρ arises from a pure state density as in Eq. (2a), then

$$
\int \int \rho^2(\mathbf{p}, \mathbf{q}) d\mathbf{p} d\mathbf{q} = h^{-N}, \qquad (5)
$$

and the volume occupied is one cell of volume h^{-N} , as it should be.

Suppose now that ρ is a nonstationary distribution $\rho(t)$, evolving under the influence of the Hamiltonian H. We ask: How rapidly does $\rho(t)$ sweep out new regions of phase space that it has not visited before? To answer this question, we need a measure of where $\rho(t)$ has visited. A natural choice is

$$
\rho^{av}(\mathbf{p}, \mathbf{q}, T) = \frac{1}{T} \int_0^T \rho(\mathbf{p}, \mathbf{q}, t) dt
$$
 (6)

This average density will obey

$$
h^N \text{Tr}[(\rho^{\text{av}})^2] \equiv \frac{1}{\mathcal{N}_T} \le 1 \tag{7}
$$

This defines \mathcal{N}_T , the number of phase-space cells accessed. The density $\rho^{av}(\mathbf{p}, \mathbf{q}, T)$ clearly is nonvanishing only where $\rho(\mathbf{p}, \mathbf{q}, t)$ has visited, but both distributions "feather out" rather than cut off abruptly in phase space. That is to say, there is no sharp distinction between a region that has been visited by $\rho(\mathbf{p}, \mathbf{q}, t)$ and one that has not, but the number of phase-space cells visited still has meaning. Figure ¹ helps to motivate this point.

Combining the equations above and using the fact that $Tr[\rho(t)\rho(t')] = Tr[\rho\rho(t'-t)]$ we have

FIG. 1. Three cases showing the distribution of phase-space probability and the resulting $\mathcal{N}_{\mathcal{T}}$. The first two cases are selfevident; the third shows how partial overpopulation or underpopulation of phase-space cells is treated by the measure, Eq. (8).

$$
\frac{1}{\mathcal{N}_T} = h^N \text{Tr}[(\rho^{\text{av}})^2] = \frac{2}{T} \int_0^T \left(1 - \frac{\tau}{T}\right) P(\tau) d\tau , \quad (8a)
$$

where the survival probability $P(\tau)$ is

$$
P(\tau) = h^N \text{Tr}[\rho \rho(\tau)] \tag{8b}
$$

Note that in the case that ρ corresponds to a pure quantum state density $|\varphi\rangle\langle\varphi|$, P is obtainable from the spectral distribution $S(E)$ of the state $|\varphi\rangle$, as follows:

$$
S(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{iEt/\hbar} \langle \varphi | \varphi(t) \rangle dt . \qquad (9a)
$$

By inverse Fourier transform,

$$
\langle \varphi | \varphi(t) \rangle = \int_{-\infty}^{\infty} e^{-iEt/\hbar} S(E) dE , \qquad (9b)
$$

and of course $P(t) = |\langle \varphi | \varphi(t) \rangle|^2$. For the case of a pure state density, $S(E)$ is often an experimentally obtainable spectrum. So the quantity $P(t)$, and via Eq. (8), \mathcal{N}_T , are often easily (if indirectly) measured.

The spectrum $S(E)$ fully resolved into δ -function peaks:

$$
S(E) = \sum_{n} p_n^{\varphi} \delta(E - E_n) , \qquad (10a)
$$

where

$$
p_n^{\varphi} = |\langle \varphi | E_n \rangle|^2. \tag{10b}
$$

The quantities p_n^{φ} for all *n* and fixed φ are the projections of the localized state $|\varphi\rangle$ onto the various eigenstates $|E_n\rangle$. The appropriate generalization of this to a quantum density matrix ρ_o is

$$
S(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{iEt/\hbar} \text{Tr}(e^{-iHt/\hbar} \rho_Q) dt \tag{11}
$$

[We have written Eq. (11) in the usual quantum formulation rather than the Wigner-Weyl phase-space formulation; the two are equivalent.] The same relation, Eq. (10a), holds for this case, with p_n^{φ} replaced by ρ_{nn} .

We shall need a smoothed version of $S(E)$, which is most easily generated by limiting the time integration:

$$
S_T(E) = \left(\frac{1}{2\pi\hbar}\right) \int_{-T}^{T} e^{iEt/\hbar} \operatorname{Tr}(e^{-iHt/\hbar}\rho) dt \qquad (12)
$$

for T chosen according to the degree of smoothing desired. This envelope $S_T(E)$ constrains $S(E)$ in the sense that a local smoothing of $S(E)$, with a function $\Omega_T(E - E')$, where

$$
\Omega_T(E - E') = \left[\frac{1}{2\pi\hbar}\right] \int_{-T}^T e^{-i(E - E')t/\hbar} dt
$$

$$
= \frac{\sin[(E - E')T/\hbar]}{\pi(E - E')} , \qquad (13)
$$

must give $S_T(E)$ as

$$
S_T(E) = \int_{-\infty}^{\infty} \Omega_T(E - E') S(E') dE'
$$

=
$$
\sum_n \Omega_T(E - E_n) p_n^{\varphi} .
$$
 (14)

The smoothed spectral distribution $S_T(E)$ is called the strength function, or simply the envelope, of $S(E)$.

III. THE RATE $\mathscr R$

A. Qualitative features

Typically, there are three regimes in the history of \mathcal{N}_T , for a bounded system with an initially localized density ρ . (1) The initial transient, including a rapid rise of $\mathcal{R} = d\mathcal{N}_T/dt$ followed possibly by some decline, leading $\mathcal{A} = a \mathcal{A} + r \mathcal{A}$ conomical possibily by some decline, reading
to (2) a plateau in \mathcal{R} , i.e., a linear increase in \mathcal{N}_T , the number of phase-space cells accessed. (3) Onset of the decline of the rate \mathcal{R} , which may occur in steps caused by recurrences in $P(t)$. The rate may temporarily become negative (see below), but it will approach zero and remain there asymptotically.

These three regimes are simple to understand if one imagines the nature of an initially localized distribution ρ and its subsequent classical dynamics (the quantal case will differ from the classical, especially in regime 3, but the distinct regimes will be present). In Fig. 2 we see two cases of initially localized distributions which start to explore phase space, thus $P(t)$ declines and \mathcal{N}_T increases. In case A the initial region is visited by part of the moving distribution in a decaying-periodic way, which is a common behavior. In case B the system revisits the initial region only after a long sojourn, and when it does start to arrive back it is quite disorganized, leading to the $P(T)$ shown.

The rate $\mathscr R$ is easily shown, by differentiation of Eq. (8a), to be

$$
\mathcal{R} = \frac{\frac{1}{2} \int_0^T \left[1 - \frac{2\tau}{T} \right] P(\tau) d\tau}{\left[\int_0^T \left[1 - \frac{\tau}{T} \right] P(\tau) d\tau \right]^2} . \tag{15}
$$

The rate $\mathscr R$ is not guaranteed to be strictly positive, for reasons which are apparent from Fig. 3. The "lapping" of the already-covered regions of phase space leads to an uneven distribution ρ^{av} , as seen in Fig. 3, which tem-

FIG. 2. Two typical scenarios for $P(t)$, $\mathcal{N}_{\mathcal{T}}$, and \mathcal{R} . Note $\mathcal{R} = \frac{1}{2\pi\hbar \int_{-\infty}^{\infty} [S_T(E)]^2 dE}$
that recurrences decrease \mathcal{R} and reduce \mathcal{N}_{∞} .

FIG. 3. Showing the case of a one-dimensional harmonic oscillator, and the way it explores phase space for the first period and somewhat beyond. Note the double coverage that occurs as $p(t)$ laps itself. This lapping, which is most severe in this periodic situation, causes an uneven phase-space distribution to temporarily develop. Successive lappings do the same, but the effect diminishes with time because an average overall time is taken.

porarily causes \mathcal{N}_T to diminish. This effect is most severe in the case shown, namely, a strictly periodic phase-space density.

From Eq. (15) it is seen that the steady-state rate (for large enough T and before any recurrences) approaches

$$
\mathscr{R} = \frac{1}{2 \int_0^T P(\tau) d\tau} = \frac{1}{\int_{-T}^T P(\tau) d\tau} \ . \tag{16}
$$

B. The rate $\mathcal R$ and the energy distribution of the density ρ

1. Quantum case

The faster the decay in $P(t)$, the faster the rate of exploration of phase space. It is intriguing that this rate is obtainable from the energy distribution, as we show next. Quantum mechanically, the energy dispersion of the nonstationary density ρ necessarily implies a decay of the autocorrelation function $P(t)$ which is related to the energy dispersion by the time-energy uncertainty principle. In this discussion we are necessarily restricted to pure state densities $\rho = |\varphi\rangle \langle \varphi |$.

The basic idea is to establish a link between $\int_{-\pi}^T P(t)dt$ and the envelope function $S_T(E)$, which carries the information about the energy distribution. The key ingredient is the equation

$$
\langle \varphi | \varphi(t) \rangle = \int_{-\infty}^{\infty} e^{-iE't/\hbar} S(E') dE'
$$

=
$$
\int_{-\infty}^{\infty} e^{-iE't/\hbar} S_T(E') dE', \qquad (17)
$$

provided $-T \le t \le T$. This follows directly from the definitions and the properties of Fourier transforms. From this and the equation

$$
\int_{-\infty}^{\infty} \Omega_T (E - E') \Omega_T (E' - E'') dE' = \Omega_T (E - E'')
$$
 (18)

follows

$$
\int_{-T}^{T} P(t)dt = 2\pi\hbar \int_{-\infty}^{\infty} [S_T(E)]^2 dE
$$
 (19)

and thus

$$
\mathcal{R} = \frac{1}{2\pi\hbar \int_{-\infty}^{\infty} \left[S_T(E) \right]^2 dE} \tag{20}
$$

The integral $\int_{-\infty}^{\infty} S_T(E)^2 dE$ is an interesting measure of the localization of $S_T(E)$. If $S_T(E)$ is confined to a single lump, say a Gaussian

$$
S_T(E) = [2\pi (\Delta E)^2]^{-1/2} \exp[-(E - E_0)^2 / 2(\Delta E)^2],
$$

then

$$
\int_{-\infty}^{\infty} [S_T(E)]^2 dE = \frac{1}{2\sqrt{\pi} \Delta E} \tag{21}
$$

2. Classical case

Classically, there is no basis for the time-energy connection, since for example a very dispersed phase-space density could have both large energy uncertainty and slow decay of $P(t)$. However, if we require that the classical density ρ comes from a quantum-mechanical pure state density, the restriction of $Tr(\rho^2) = h^{-N}$ is imposed. This places localization requirements on ρ . The time-energy correlation then makes sense classically too. Equation (20) is then valid for those times, which we call T^* , in the plateau (region 2), with $S_T(E)$ replaced by the classical phase-space trace $S_C(E) = Tr[\rho \delta(E - H)]$. As T increases, recurrences may happen, and these will destroy the near equality of $S_T(E)$ and $S_C(E)$. Further insight into the classical case is provided in the Appendix.

IV. SIMPLE EXAMPLES

A. Quantum tunneling resonance

In Fig. 4 an unbounded potential with a well, a barrier, and associated quasibound levels is shown. Suppose now that a wave packet is launched inside the well, as shown.

FIG. 4. One-dimensional potential with quasibound resonances. A wave packet launched inside the well, as shown at the top, will oscillate inside and, at the same time, leak out to the continuum by tunneling. The resulting $P(t)$ will have an exponential decay of the recurrences, as idealized in case A of Fig. 2. The wave functions at the energies of the resonance have enhanced probability inside the well, as shown. Off resonance, the opposite is true. One way to understand the reduction in $\mathscr R$ is shown at the bottom. Complete leakage out of the well occurs at long times, but the original smooth energy distribution $S_T^*(E)$ is now organized into narrow energy bands corresponding to the resonances; these travel along the x axis in elongated packets; they fail to explore the regions between the packets.

The resulting correlation function $P(t)$ will be of type A in Fig. 2, because the recurrences due to the return of the wave packet to its starting position are damped by the amplitude that tunnels through the barrier. This leads to an approximately exponential decay of the recurrences. The recurrences cause the rate \mathcal{R} to drop, but because of the exponential decay the rate does not asymptotically reach zero.

The asymptotic rate can be obtained from Eq. (16). Physically, the nonvanishing asymptotic rate corresponds to the continued exploration of phase space, as the distribution $\rho(x, p, t)$ moves along x, in narrow horizontal bands. These bands (Fig. 4, bottom) correspond to the resonance energies and their width in the momentum (vertical) direction corresponds to the width of the individual resonances.

We can model this behavior with the following form for $P(t)$:

$$
P(t) = \sum_{n=0}^{\infty} e^{-(\Delta E)^2 (t - n\tau_0)^2 / \hbar^2} e^{-\lambda t} . \tag{22}
$$

Then

$$
\int_0^T P(\tau)d\tau \simeq \frac{\sqrt{\pi\hbar}}{\Delta E} \left[\frac{\nu_0}{2\lambda}\right],
$$
\n(23)

where $v_0 = \tau_0^{-1}$. This gives

$$
\mathcal{R} = \frac{\Delta E}{\hbar \sqrt{\pi}} \left[\frac{\lambda}{v_0} \right].
$$
 (24)

We have assumed, in the approximate evaluation of the integral, that $\lambda \tau_0 \ll 1$ and $\Delta E / h \gg \lambda$. The rate \mathcal{R} is reduced by a factor of λ/ν_0 compared with Eqs. (20) and (21). This is λ/ν_0 times slower than what it would have been if the barrier did not exist. This factor is normally very small for a tunneling problem. Classically, the rate would have rapidly reached zero, because there would be no tunneling and the phase space inside the well would be quickly explored.

The exponentially decaying recurrences are a common behavior, corresponding to case A of Fig. 2. They appear again in the case of the unstable periodic orbit, discussed below. They lead to the conclusion that in certain regions some of the eigenfunctions are a factor of v_0/λ times larger than "expected," as explained in Sec. VI. Figure 5 shows $P(t)$ and the resulting envelopes $S_T^*(E)$, $S_T(E)$, and $S(E)$.

B. Many harmonic oscillators

Consider a set of nearly degenerate harmonic oscillators. We launch a wave packet with initial momentum zero, but stretch all the oscillators approximately equally. Because of the near-degeneracy of the oscillators, the wave packet nearly returns to its initial state after one period, and only slowly winds its way into new phase space thereafter, as the slightly different frequencies dephase. Again, we have a situation corresponding to case A of Fig. 3, namely, damped recurrences. [However, in contrast to the previous example, $P(t)$ does not decay per-

FIG. 5. The time development of $S_T(E)$ is for the idealized case of exponentially damped Gaussian recurrences is illustrated here. After the initial decay, but before the first recurrence, $S_T^*(E)$ is determined. Times T after the set of exponentially damped recurrences give $S_T(E)$. Future recurrences, not shown, eventually determine $S(E)$, the fully resolved spectrum.

manently, but increases again in regime 3.] Since the classical and quantum phase-space dynamics are identical for harmonic oscillators, i.e., $\rho^{\text{classical}}(t) = \rho^{\text{quantum}}(t)$ if $\rho^{\text{classical}}(0) = \rho^{\text{quantum}}(0)$, the diminution of $\mathscr R$ is a purely classical effect. For many sets of nearly degenerate frequencies and displacement of the oscillators, the decay in the recurrences will be nearly exponential, and Eq. (24) pertains again. Regime 3 is delayed in coming for a nearly degenerate set of frequencies, so the system explores phase space for a long time but at a reduced rate \mathcal{R} . For a more random set of frequencies, \mathcal{R} tends to be much higher, but regime 3 sets in much sooner. A harmonic system or indeed any separable system accesses only a small fraction of the total phase space available, where the available phase space is defined by a superposition of microcanonical densities with the superposition being weighted by the energy density of ρ .

C. Unstable periodic orbit

Systems of two or more degrees of freedom have periodic orbits which may be stable or unstable. If the dynamics is chaotic, all the periodic orbits are unstable. Isolated unstable orbits may also exist in integrable systems.

Suppose we select an initially localized phase-space density ρ , centered on the vicinity of a portion of such a periodic orbit. The time-evolved density $\rho(t)$ will return to this vicinity after the orbital period has elapsed, but $p(t)$ will have spread along the unstable manifolds and contracted along the stable ones. The result is a series of recurrences in $Tr[\rho \rho(t)]$ at multiples of the period of the orbit, which again damp out. The short-time dynamics (a few periods) of such an initial phase-space density is the same classically or quantum mechanically, for sufficiently small \hbar . Therefore both classical and quantum systems slow down their rate of exploration of phase space due to the periodic orbit recurrences. The recurrences can be shown to be exponentially damped.¹ Apparently, the unstable periodic orbit causes a reduction of the rate by λ/ν_0 , for nonstationary states launched on the orbit, where λ is the stability parameter and v_0 is the frequency of the orbit. Such unstable periodic orbits are the source of scar localization in classically chaotic systems. '

D. Phase-space bottlenecks, cantori

Suppose we divide phase space into two regions, A and B. We launch a localized state in A. Suppose too that, classically, slow diffusion into region B occurs. A prime example of this behavior is a cantorus,³ a kind of remnant torus which divides A from B and which leaks slowly. Classically, the diffusion can be slow enough that recurrences of $Tr[\rho \rho(t)]$ while $\rho(t)$ is still confined to region A will drastically slow down the exploration of phase space. Region A is fully explored on a time scale short compared to the diffusion. This happens in classical and quantum mechanics, but the consequences on the quantum system are a permanent localization, as explained in Sec. VI.

V. THE LONG-TIME LIMIT

A. The number of phase-space cells explored as $T \rightarrow \infty$

Equation (8) gives the number of phase-space cells which are eventually accessed as

$$
\frac{1}{\mathcal{N}_{\infty}} = h^{N} \text{Tr}[(\rho^{\text{av}})^{2}]
$$
\n
$$
= \lim_{T \to \infty} \left[\frac{2}{T} \int_{0}^{T} \left[1 - \frac{\tau}{T} \right] P(\tau) d\tau \right]
$$
\n
$$
= \lim_{T \to \infty} \left[\frac{1}{T} \int_{0}^{T} P(\tau) d\tau \right].
$$
\n(25)

Equation (25) is true both classically and quantum mechanically. In the quantum case, for a nondegenerate spectrum (the degenerate case is slightly more complicated) we can write explicitly, in the case that the initial density ρ arose from a localized pure quantum state $|\varphi\rangle$ as $\rho = |\varphi\rangle \langle \varphi|,$ ^{6,7}

$$
P(\varphi \mid \varphi) \equiv \frac{1}{\mathcal{N}_{\infty}}
$$

= $\sum (\mathbf{p}_n^{\varphi})^2$, (26a)

where

$$
p_n^{\varphi} = |\langle \varphi | E_n \rangle|^2. \tag{26b}
$$

The quantities p_n^{φ} are the spectral intensities which are the coefficients of the delta functions in $S(E)$ [see Eq. (9)].

Equation (26a) is related to the participation ratio familiar in solid state contexts.⁴ The participation ratio requires the p_n^{φ} for a set of localized $|\varphi\rangle$ and fixed eigenstate $|E_n\rangle$; here we need p_n^{φ} for fixed $|\varphi\rangle$ and all $|E_n\rangle$. The two are obviously related in the qualitative information they contain about the degree of localization.

B. Digression into quantum ergodicity

In order to discuss the concept of localization, we need to define what we mean by complete delocalization. That is, if we are going to accuse a particular eigenstate or a given time evolution of being localized, we have to have a reference system firmly in mind. This cannot be a uniform distribution in phase space, for that would violate things we supposedly know about $\rho^{av}(\infty)$. For example, we might know the value of

$$
\langle E \rangle = \text{Tr}[\rho(0)H] = \text{Tr}(\rho^{\text{av}}H) , \qquad (27)
$$

at $t = 0$, before any dynamics of $\rho(t)$ is known.

We are now entering somewhat subtle territory in the study of ergodicity in quantum mechanics, $6 - 10$ involving the concept of the known prior constraints on the dynamics, against which the eventual phase-space flow is judged. These constraints include $\langle E \rangle$ for instance, and they certainly affect the question at hand, namely: How many phase-space cells could the system have accessed, given only what we knew about it at first (the prior constraints)?

The issue of prior constraints is just as crucial in classical dynamics. Classical Hamiltonian systems are always trivially ergodic in the sense that phase space is uniformly covered on *some* manifold (e.g., the energy shell, or an N torus). Indeed, as Lichtenberg and Lieberman put it, "In a sense, ergodicity is universal, and the central question is to define the subspace over which it exists."¹¹ We may call the system nonergodic with respect to some smaller set of constraints or constants of the motion. The concepts of localization or nonergodicity arise when the dynamics accesses a region or manifold of lower dimensionality than the prior constraints imposed. A classical system is ergodic or not depending on our choice of the prior constraints.

An example is a system free to rotate. If total energy is the only prior constraint, then all such systems will be localized. Only when the additional prior knowledge of the conservation of angular momentum is added is it possible for the system to be called ergodic. We say, in effect, that we already know about certain localizations and we then incorporate them; the interesting questions then become: Is there any localization beyond what we knew about to begin with?

The concept of ergodicity in quantum mechanics must be expected to have the same characteristics: We must specify what the known constraints or constants of the motion are before we can speak of ergodicity or the available phase-space manifold. Only those parts of phase space satisfying the constraints are available.

It would seem natural to introduce the constraints,

$$
\mu_0 = \operatorname{Tr}[\rho(0)] ,
$$

\n
$$
\mu_1 = \operatorname{Tr}[\rho(0)H] ,
$$

\n
$$
\mu_2 = \operatorname{Tr}[\rho(0)H^2] ,
$$

\n
$$
\vdots
$$

\n(28)

But each new constraint further restricts the available phase space until, when all the moments are known, there can be no "surprises"; what is available is just what is in fact accessed. The system, with enough prior constraints known, becomes trivially ergodic, just as in classical mechanics. It is interesting to see how this happens in more detail.

Taylor expansion of the propagator $\exp(-iHt/\hbar)$ shows that powers of H contain dynamical information. Each higher power of H in effect introduces more knowledge about the dynamics. We expand the propagator and evaluate $\langle \varphi | \varphi(t) \rangle$ in terms of the moments:

$$
\langle \varphi | \varphi(t) \rangle = \langle \varphi | (1 - iHt/\hbar - H^2t^2/2\hbar^2 + \cdots) | \varphi \rangle
$$

= $\mu_0 - i\mu_1 t/\hbar - \mu_2 t^2/2\hbar^2 + \cdots$ (29a)

More generally, for a density ρ ,

$$
\mathbf{Tr}(e^{-iHt/\hbar}\rho) = \mu_0 - i\mu_1 t/\hbar - \mu_2 t^2/2\hbar^2 + \cdots \qquad (29b)
$$

The quantity $Tr[\exp(-iHt/\hbar)\rho]$ is somewhat unusual. It plays the role of $\langle \varphi | \varphi(t) \rangle$ in the case that a mixedstate density matrix applies. [See Eq. (9b).]

Given enough moments, it is possible to completely determine the p_n^{φ} . Indeed, the Lanczos algorithm¹² specifically generates the spectrum $S(E)$ from the moments μ_n .

The concept of localization, then, is void without specifying the frame of reference, i.e., the constraints that the dynamics voluntarily obeys and which we have incorporated as given. These we call the "prior" constraints.

In a given physical situation there is a natural set of prior constraints, to match one's state of presumed ignorance about the dynamics. There are also other ways to summarize these constraints than to list the moments one by one. One idea is to employ the *envelope*, $S_T(E)$, or strength function, of the spectral distribution $S(E)$ [see Eqs. (12)–(14)]. We may obtain $S_T(E)$ by direct Fourier transform of $Tr[\exp(-iHt/\hbar)\rho]$ truncated at time T. Alternately, we may use a finite number of moments in the Lanczos method to obtain the spectral density $S_M(E)$, where M is the number of moments taken. For short times, this is very similar to the direct Fourier transform, but we shall use $S_T(E)$. This envelope is very precisely defined in the typical case that $Tr[\exp(-iHt/\hbar)\rho]$ decays nearly to zero and stays there for some time. The envelope which corresponds to knowing a few moments or the very short-time dynamics is given by the Fourier transform

$$
S_T^*(E) = \left(\frac{1}{2\pi\hbar}\right) \int_{-T^*}^{T^*} e^{iEt/\hbar} \text{Tr}(e^{-iHt/\hbar} \rho) dt \tag{30}
$$

for T^* chosen in the region following the initial decay but preceding any recurrences (i.e., in region 2). The star signifies this special choice. This envelope $S_T^*(E)$ constrains $S(E)$ in the sense that a local smoothing of $S(E)$ yields $S_T^*(E)$, as in Eq. (14).

C. The number of available phase-space cells

The task of finding the number of available phase-space cells is now reduced to minimizing $\sum_n (p_n^{\varphi})^2$ subject to the envelope constraint. The envelope can be considered to give a local constraint, namely, that the sum of the p_x^{φ} in a given small-energy region around E give a result proportional to $S_T^*(E)$. To minimize the sum locally around E is to assign similar intensities to all the p_n^{φ} , with the

only variations being smooth ones imposed by the requirements of $S_T^*(E)$. A trivial example serves to illustrate. Suppose there are N p_n^{ϕ} and we assume the envelope S^* is rectangular with height ΔE^{-1} and width ΔE . Then if all $p_n^{\varphi} = 1/N$, it follows that $P(\varphi | \varphi) = \sum_n (p_n^{\varphi})^2 = 1/N$ is a minimum. Any fluctuations in the p_n^{φ} cause the sum to increase. The worst case is when all the p_n^{φ} vanish, except one, which must then be 1. The sum then is 1. Note that one, which must then be 1. The sum then is 1. Note that
in this case, $\mathcal{N}_{\infty} = 1$, whereas $\mathcal{N}_{\infty} = N$ in the case where all the p_n^{φ} shared the strength S^* equally.

When we make the p_n^{φ} as smooth as possible subject to the envelope, and account for the local density of states, we find that the set of constraint-obeying p_n^{φ} which minimize the sum are⁷

$$
p_n^{\varphi*} = \frac{S_T^*(E_n)}{D_T^*(E_n)} , \qquad (31)
$$

where $D_T^*(E_n)$ is the density of states

$$
D_T^*(E_n) = \sum_n \Omega_T^*(E_n - E_{n'})
$$
\n(32)

and the asterisk signifies the special p_n^{φ} which maximize \mathcal{N}^* , i.e.,

$$
\frac{1}{\mathcal{N}^*} = \sum_n (p_n^{\varphi*})^2 = P^*(\varphi \mid \varphi)
$$

$$
\simeq \int \frac{[S_T^*(E)]^2}{D_T^*(E)} dE . \tag{33}
$$

In classical mechanics, a very similar form applies: $⁷$ </sup>

$$
\frac{1}{\mathcal{N}^*} = P^*(\varphi | \varphi)
$$

=
$$
\int \frac{[S_C(E)]^2}{D_C(E)} dE,
$$
 (34)

where $S_C(E) = Tr[\rho \delta(E - H)]$ and $D_C(E) = Tr[\delta(E - H)].$

The set of $p_n^{\varphi*}$ are smoothly varying from one *n* to the next. In fact, we must expect some fluctuations, because the $p_n^{\varphi*}$ represent the square of a matrix element

$$
\int \varphi^*(\mathbf{x}) \Psi_n(\mathbf{x}) d\mathbf{x} , \qquad (35)
$$

where $\Psi_n(x)$ are the eigenstates. In the case of a spatially Gaussian random eigenfunction $\Psi_n(x)$, the matrix element would also be Gaussian random,¹³ accounting for the secular variation due to the envelope. Once this is done, one obtains a χ^2 distribution for the matrix elements squared, p_n^{φ} , just as in the statistical theory of nuclear reactions. '

The set of p_n^{φ} which (1) obey the envelope constraints, and (2) maximize $\mathcal N$ subject to the imposition of χ^2 fluctuations is called the quantum ergodic set, $p_n^{\varphi,QE}$. Stechel has provided a rigorous theory of quantum ergodicity based on the p_n^{φ} , ¹⁰ and has shown that

$$
\mathcal{N}^{QE} = \frac{\mathcal{N}^*}{3} \tag{36}
$$

That is, the χ^2 fluctuations in the p_n^{φ} cause $\frac{2}{3}$ of the phase space to become unavailable. This may be viewed as a consequence of the nodal structure of the eigenfunctions,

which causes a locally fluctuating phase-space distribution, rather than an absolutely smooth one, even for the most ergodiclike eigenstates. The fluctuations cause $Tr(\rho^2)$ to be larger, and therefore $\mathcal N$ to be smaller.

However, instead of discussing a pure quantum state φ , we may coarse grain over several nearby φ 's, leading to a mixed-state density matrix ρ which smooths out the local fluctuations but which is still confined to a small region in phase space. For such coarse-grained initial densities, the full \mathcal{N}^* is attainable. Kay⁸ has given a related theory of coarse-grained quantum ergodicity.

D. The break time

Classical mechanics allows an infinite amount of time for the questions surrounding the ergodicity of the flow to be answered. The rate $\mathcal R$ can become very slow, due to recurrences, and yet the phase space eventually may be completely explored. An excellent example of this is temporary confinement inside a cantorus, mentioned in Sec. IV D.

Bounded quantum-mechanical systems are a different matter. They have a discrete spectrum, and a finite spacing between the levels. Very roughly speaking, no new regions of phase space can be visited after a break time $\mathcal{T}_B = hD(E)$, where $D(E)$ is the density of states. There are many qualitative arguments leading to this conclusion. For example, consider two different states $|\varphi_a\rangle$ and φ_b , or to simplify the notation, |a) and |b). We suppose these states are in very different regions of phase space, but share similar envelopes, i.e., $S_T^{a*}(E) \simeq S_T^{b*}(E)$. The similar envelopes assure us that flow from region a to region b is permitted by the constraints. The question before us is: Can $\rho^{a}(t)$ stay away from ρ^{b} for times longer than \mathcal{T}_B , but visit there later? The measure of the visitation is of course $Tr[\rho^{a}(t)\rho^{b}]$. The asymptotic flow from a to b is $P(a | b)$, where

$$
P(a \mid b) = \lim_{T \to \infty} \left[\frac{1}{T} \int_0^T \text{Tr}[\rho^a(t)\rho^b] dt \right]
$$

$$
= \sum_n (p_n^a p_n^b) . \tag{37}
$$

In the case of a pure state, we have

$$
\operatorname{Tr}[\rho^{a}(t)\rho^{b}]=\left|\sum_{n}a_{n}b_{n}e^{-iE_{n}t/\hbar}\right|^{2},\qquad(38)
$$

where $a_n = \langle a | E_n \rangle$, etc. Equation (37) shows that for $P(a \mid b)$ to differ substantially from zero, both p_n^a and p_n^b must be nonvanishing for some set of n 's. In fact, the more terms in the sum in Eq. (38) that contribute (because both a_n and b_n are substantial for the same n), the longer the possible delay in $Tr[\rho^{a}(t)\rho^{b}]$ rising above zero. But this delay cannot go past the break time: Up until \mathcal{T}_B , the phase factors $exp(-iE_n t/\hbar)$ for adjacent *n* maintain phase coherence; but after that time they essentially become random phase factors, since their arguments become large multiples of π . Moreover, these factors vary with time, while they remain random. There is no way continuously many random superpositions of the $a_n b_n$ can all

vanish; i.e., there must be a visitation of ρ^b by $\rho^a(t)$ near or before \mathcal{T}_R .

The break time is evidently an approximate concept. Clusters of levels with a spacing much smaller than the average may exist, and it will take much longer than the break time to dephase these levels and explore the last corners of phase space. In the case of a classical Hamiltonian which is chaotic, it is becoming well established that energy-level spacings for high enough energy or small enough \hbar obey the Wigner surmise spacing distribution, $14,15$ which abhors small spacings (manifested by a linear level repulsion at small spacing). Thus the concept of a break time actually becomes better established for a classically chaotic system.

In an unbound system such as the quantum resonance considered above, there is no break time because the density of states is infinite. Nonetheless, recurrences slow down the rate \mathcal{R} , and so the amount of phase space explored per unit time is affected. Whether this is a pure quantum effect simply depends on whether the recurrences are quantum effects. In the case of Anderson localization, $\mathscr R$ evidently reaches zero, even though there is a continuum of 1evels present.

VI. QUANTUM LOCALIZATION

A. Localization in the first guise: The fraction $\mathcal F$

The fraction $\mathcal F$ of available phase space which is actually accessed by the dynamics in the long-time limit is simpIy defined as

$$
\mathcal{F} = \frac{\mathcal{N}_{\infty}}{\mathcal{N}^*} \tag{39}
$$

Corresponding to the prior constraint envelope $S_T^*(E)$ there is a rate \mathcal{R}^* , which is the rate in the region T^* after the first decay and before the first recurrence of $Tr[\rho \rho(t)].$ This is the maximum rate for the density ρ ; it can only decrease due to recurrences. It is simple to demonstrate that phase space must be explored at the maximum possible rate \mathscr{R}^* for the density ρ (i.e., the initial rate before any recurrences) up until \mathcal{T}_B , or else $\mathcal F$ cannot approach unity: From Eq. (33) we have

$$
\mathscr{N}^* \simeq \frac{1}{\int \frac{[S_I^*(E)]^2}{D_I^*(E)}} dE
$$

$$
\simeq \frac{D^*}{\int [S_I^*(E)]^2 dE}, \qquad (40)
$$

where D^* is the average density of states. Multiplying the numerator and denominator by Planck's constant gives, from Eq. (20) and $\mathcal{F}_B = hD^*$,

$$
\mathscr{N}^* = \mathscr{R}^* \mathscr{T}_B \tag{41}
$$

This simple relation, derived with the assumption that the density of states can be treated as a constant over the energy interval ΔE , is a consistency check on the meaning of the three quantities involved. It confirms that if the rate

 $\mathscr R$ should fall below $\mathscr R^*$, then $\mathscr N_{\infty} < \mathscr N^*$. Put another way, recurrences must be put off until close to the break time or the phase space will be incompletely explored. This is consistent with the notion that recurrences cause a decrease in \mathcal{R} , together with the concept of a finite time allowed to explore phase space.

The reader will be convinced, with a little thought, that the recurrences are indeed put off until roughly \mathcal{T}_B in the ideal case that the p_n^{φ} are smoothly distributed under the envelope $S^*(E)$, as in Eq. (31). Fluctuations will cause earlier recurrences, but in the case of χ^2 random fluctuations, these are not drastically earlier and cause only a $\frac{2}{3}$ reduction in the phase space accessed. This is a negligible amount on two counts: First, coarse graining will remove the effect; second, the \mathcal{F} 's expected from quasiperiodic motion in a many-degree-of-freedom system can be orders of magnitude smaller than 1. This results from the vast majority of the p_n^{φ} being exponentially close to zero.

Recurrences and the p_n^a . The envelope $S_T(E)$ for T after the initial decay of $Tr[\exp(-iHt/\hbar)\rho]$ but before any recurrences, i.e., $S_T^*(E)$, is some smooth shape which defines the envelope constraint (the prior constraint) we have been discussing. It maintains its original shape, independent of T, as long as $Tr[\exp(-iHt/\hbar)\rho] \approx 0$. As soon as a recurrence happens, $S_T(E)$ begins to develop additional structure. (See Fig. 5.) The new structure represents new constraints on the p_n^d , but these are not the agreed-upon prior constraints. Since the p_n^{φ} are forced to live under the new roof, so to speak, of the now more highly structured $S_T(E)$, they are forced to fluctuate relative to the $p_n^{\varphi,QE}$. The new fluctuations will increase $P(\varphi | \varphi)$ and therefore decrease \mathcal{N}_{∞} and \mathcal{F} , the fraction of phase space explored.

We can calculate the amount of localization, as measured by its effect on $\mathcal F$, that a given recurrence *imposes* on the dynamics, as

$$
\frac{1}{\mathcal{N}^{\dagger}} \simeq \int \frac{[S_T^{\dagger}(E)]^2}{D_T^{\dagger}(E)} dE
$$
\n(42)

[compare Eq. (33)]. $S_T^{\dagger}(E)$ is the envelope imposed on the system after some recurrences have taken place. The $\mathcal F$ is reduced at least as low as $\mathcal N^*/\mathcal N^*$. For example, the common case of the exponentially damped recurrences gives

$$
\mathcal{N}^{\dagger} = \frac{\lambda}{v_0} \mathcal{N}^* < \mathcal{N}^* \tag{43}
$$

Also, the rate \mathcal{R}^{\dagger} after the series of recurrences damps out and before any other recurrences take place is $\mathscr{R}^{\dagger} = (\lambda/\nu_0)\mathscr{R}^*$, as already noted in connection with Eq. (24).

The crux of the matter is that a short-time recurrence (before \mathcal{T}_B) imposes an $S_T^{\dagger}(E)$ with more structure than $S_T^*(E)$; this in turn means that the "best" the dynamics can do thereafter is to sample $\mathcal{N}^{\dagger} < \mathcal{N}^*$ phase-space cells. Of course, it may sample much less than this, if further recurrences happen before \mathcal{T}_B , but it can sample no more than this. This permanent effect on the quantum phasespace exploration due to a temporary phenomenon has no parallel in classical mechanics.

We are often able to make rigorous statements about the short-time dynamics, via semiclassical means, for example. This means we can predict weak localization of the quantum dynamics and even of the eigenfunctions (see below) from short-time approximations. This was the strategy for the proof that some eigenfunctions suffer partial localization around certain periodic orbits in classically chaotic systems (so-called scar localization).

B. Localization in the second guise: The eigenfunctions

I. Qualitative statements

Starting with a pure state $|\varphi\rangle$, we can project eigenfunctions of the Hamiltonian H out of the dynamics of $|\varphi(t)\rangle$ as

$$
|E_n\rangle = \eta_n \int_{-\infty}^{\infty} e^{iE_n t/\hbar} |\varphi(t)\rangle dt , \qquad (44)
$$

where η_n is a normalization constant, and E_n is the eigenvalue for $|E_n\rangle$. Now, for those η_n which are not too large, i.e., for the $|E_n\rangle$ which have the largest components in $|\varphi\rangle$, the phase-space distribution of $|E_n\rangle$ (that is, its Wigner transform) can be large only where $\rho^{\varphi}(t)$ traveled. If $\rho^{\varphi}(t)$ visited only part of the available phase space, then $|E_n\rangle$ can have significant probability only there.

2. Dynamics of $\rho(t)$ and local of $|E_n\rangle$

We can make these arguments quantitative. From Eq. (37), it is obvious that

$$
p_n^{\beta} p_n^{\varphi} \le P(\beta \mid \varphi) \tag{45}
$$

where $|\beta\rangle$ is an arbitrary state. Here, we suppose $P(\beta | \varphi)$ is small, and we use Eq. (45) to check if $|E_n\rangle$ has a significant component in $|\beta\rangle$:

$$
|\langle E_n | \beta \rangle|^2 \le \frac{P(\beta | \varphi)}{p_n^{\varphi}}.
$$
 (46)

This important equation says that if $|\varphi(t)\rangle$ does not access $|\beta\rangle$ very much in the course of time, and also $|\varphi\rangle$ has a large component in $|E_n\rangle$ (p_n^{φ}), then $|E_n\rangle$ cannot be found to have a large component in β . Equation (46) quantifies the localization of the eigenfunctions which re sults if $|\varphi(t)\rangle$ fails to explore $|\beta\rangle$ within the break time \mathcal{T}_B .

3. Localization of certain $| E_n \rangle$ to $p^{\varphi}(0)$ [and $p^{\varphi}(t)$]

The necessary result of failure to explore one part of available phase space is a heavier concentration elsewhere. This is true of the dynamics of $\rho(t)$ and of the eigenfunctions E_n). The p_n^{φ} are a direct measure of the overlap between an eigenstate $|E_n\rangle$ and a test state $|\varphi\rangle$. We have seen that recurrences cause oscillations in $S_T^{\dagger}(E)$. The p_n^{φ} residing under a "mountain" in S_T^{\dagger} must be larger, on the average, than those p_n^{φ} in the valleys. More important is the fact that this overlap is also higher than the expected overlap based on S_T^* , which is indicated by the smooth low-resolution envelope shown in grey in Fig. 5. The ratio $S_T^{\dagger}(E)/S_T^*(E)$ gives the average local deviation of the probabilities p_n^{φ} from the expectations of the prior distribution. The presence of certain p_n^{φ} which are larger than they ought to be, given only the prior constraint $S_T^*(E)$, means certain $|E_n\rangle$ are partially localized to the region of $|\varphi\rangle$. The degree of localization is at least $S_T^{\dagger}(E)/S_T^*(E)$; this ratio can only increase if we remain in the mountain regions of the developing $S_T^{\dagger}(E)$. Concomitantly, there are states which stay out of the region occupied by $\langle \varphi \rangle$. It is certainly worth noting that since

$$
|\langle \varphi(0) | E_n \rangle| = |\langle \varphi(t) | E_n \rangle| , \qquad (47)
$$

the localization of certain $| E_n \rangle$ to (or away from) $| \varphi \rangle$ applies also to $| \varphi(t) \rangle$ for any t.

C. Examples of the localization

1. Scattering resonance

A viable analog to $\mathcal F$ in the case of an unbound potential is the ratio of the asymptotic rate \mathcal{R}^{\dagger} to the initial constraint rate \mathcal{R}^* , i.e., $\mathcal{F} = \mathcal{R}^{\dagger}/\mathcal{R}^*$. This ratio is just $\mathcal{F} = \lambda / v_1$ in the example of the barrier tunneling of Sec. IV A.

Contact may be made with a more traditional view of resonance localization in scattering theory by asking how large the wave function is inside the well, as a function of the scattering energy. We adopt the usual scattering normalization $\langle E | E' \rangle = \delta(E - E')$. A calculation yields the continuum wave function normalization factor as $\eta_E^{-1} = h\sqrt{S(E)}$:

$$
\eta_E^{-2}\delta(E-E') = \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' e^{i(Et-E't')/\hbar} \langle \varphi(t') | \varphi(t) \rangle
$$

\n
$$
= \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' e^{iE(t-t')/\hbar} e^{i(E-E't')/\hbar} \langle \varphi(0) | \varphi(t-t') \rangle
$$

\n
$$
= 2\pi \hbar \delta(E-E') \int_{-\infty}^{\infty} e^{iE u/\hbar} \langle \varphi(0) | \varphi(t-t') \rangle du = (2\pi \hbar)^2 \delta(E-E') S(E) .
$$
\n(48)

We obtain then

$$
|\langle \varphi | E \rangle|^2 = S(E) . \tag{49}
$$

[Note that $S(E)$ is a continuous function of E.] Thus, on the resonance energies, there is an enhancement

 $S(E)/S_T^*(E)$ of the overlap with a test state $|\varphi\rangle$. This is not a fluke, but representative of the enlargement of the local norm of the resonant wave function inside the potential well. For example, Eq. (47) applies, and for the first period of the motion of the wave packet $|\varphi(t)\rangle$ covers the whole relevant phase space inside the well, in the one di-

mensional case and in the limit $v_0 \gg \lambda$.

In the important case of the exponentially decaying recurrences, we get

$$
\frac{S(E)}{S_T^*(E)} = \frac{\lambda}{\tau_0} \sum_{m = -\infty}^{\infty} \frac{\exp\left[\frac{-4\pi^2 m^2 \hbar^2}{2\tau_0^2 (\Delta E)^2} + \frac{(E - E_0)^2}{2(\Delta E)^2}\right]}{\frac{\lambda^2}{4} + \left[\frac{(E - E_0)}{\hbar} - \frac{2\pi m}{\tau_0}\right]^2}.
$$
\n(50)

[This equation should not be taken too literally in the wings, i.e., large $|E - E_0|$, since the assumption of strict exponential decay is not good near $t\simeq 0$. The damage this does is in the wings of $S(E)$.] The ratio $S(E)/S_T^*(E)$ maximizes at the peaks in $S(E)$ with the value

$$
\frac{S(E)}{S_T^*(E)} = 4\frac{\nu_0}{\lambda} \tag{51}
$$

This enhancement is relative to that standard established by the prior constraints, which are contained in $S_T^*(E)$, consisting of a single smooth lump. The prior constraint envelope did not "know" about the resonances; information about them only appeared after $T \simeq \tau_0 > T^*$.

2. The average overlap with a test state

Suppose we average this ratio $S(E)/S_T^*(E)$ over an energy interval comparable or greater in extent than the energy spacing of the resonances, $h\nu_0$. We recall that if $\Omega_T(E - E')$ is used to perform the average, then $S(E)$ becomes $S_T^*(E)$, and thus the average enhancement becomes nearly one. This is a universal phenomenon: If we take an energy interval $\Delta E^* \simeq T^* / h$, the *average* projection of all the eigenstates in the interval onto a localized test state $|\varphi\rangle$ having the envelope $S_T^*(E)$ is $p_n^{\varphi,QE}$. Put more loosely, the average of consecutive eigenstates over an interval ΔE around energy E becomes more and more like a microcanonical distribution smeared over ΔE around E. This is true independent of the nature of the dynamics.

3. Quasiperiodic motion and 1ocalization to invariant tori

If the dynamics is classically quasiperiodic, there is a quantifiable tendency for the eigenfunctions to localize on the invariant tori, which are the classical stationary distributions.¹⁶ This localization will be reflected in the early and drastic reduction in $\mathcal R$ due to recurrences. As in the harmonic-oscillator case, which is an example of the quasiperiodic motion we are discussing, the localization in this case is the same classically and quantum mechanically.

There is a caveat: Quantum tunneling can occur, leading to a leakage in phase space which is not permitted classically. Such tunneling corresponds to exponentially small splittings in the energies of pairs or clusters of levels. As $h\rightarrow 0$, the classical and quantal $\mathscr R$ will track each other for times which increase exponentially as $exp(const \times \hbar^{-1})$, which is much longer than \mathcal{F}_B . Recall that such tunneling is in violation of the notion that the dynamics is all over by \mathcal{T}_B .

The possibility of tunneling reminds us that there is no rule which says that the classical exploration of phase space is more (or less) extensive than the quantum mechanical. Recurrences together with the break time effect can, and often do, make the quantum motion more localized than the classical. Tunneling has the opposite effect.

Comparisons of classical versus quantum wave-packet dynamics, using the Wigner phase-space picture, have been the subject of several studies.¹⁶

4. Anderson localization

As mentioned above, we can often make quantitative statements about weak localization of the long-time dynamics or of the eigenfunctions from short-time information about the dynamics. Whether an eigenstate is strongly localized (e.g., confined to a region, via exponential damping of the eigenstate outside the region, even though no known constraints binding it there exist) is really an infinite-time question and therefore much harder to approach.

As an illustration, consider a random potential in two dimensions with a wave packet launched somewhere on the potential. If the wave packet simply leaves and never returns, the eigenstates must be extended. However, the random features of the potential will cause amplitude to be reflected back, resulting in recurrences with the initial state, and causing a reduction in \mathcal{R} . The reflections off the potential features and thus the reduction of the rate may be entirely quantum mechanical; an analogous swarm of classical trajectories need not show the recurrences. In this sort of system it will be fairly easy to confirm weak localization. But the issue of whether the recurrences completely shut down $\mathcal R$ to zero seems to be as subtle in the present formulation as it is in the traditional ones.

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APPENDIX: CLASSICAL TIME-ENERGY UNCERTAINTY CORRELATIONS

Here we consider the time-energy relation for classical phase-space distributions which could have arisen as Wigner transforms of pure quantum states.

We estimate $P(t) = Tr[\rho \rho(t)]$ by approximation of the short-time dynamics of $\rho(t)$. The short-time dynamics of $\rho(\mathbf{p}, \mathbf{q}, t)$ is simply

$$
\rho(\mathbf{p}, \mathbf{q}, t) = \rho(\mathbf{p} + \nabla_{\mathbf{q}} H t \mathbf{q} - \nabla_{\mathbf{p}} H t), \qquad (A1)
$$

through order t . If we assume that the distribution is localized enough to get out of its own way, so to speak, in a short time, then we may write

$$
\int_0^T P(\tau)d\tau = \int_0^T \text{Tr}[\rho \rho(\tau)]d\tau
$$

= $\int_{-\infty}^{\infty} d\mathbf{p} \int_{-\infty}^{\infty} d\mathbf{q} \int_0^T d\tau \rho(\mathbf{p}, \mathbf{q}) \rho(\mathbf{p} + \nabla_{\mathbf{q}} H \tau, \mathbf{q} - \nabla_{\mathbf{p}} H \tau)$
= $\int_{-\infty}^{\infty} d\mathbf{s} \int_{-\infty}^{\infty} du \int_0^T d\tau \rho(\mathbf{s}, u) \rho(\mathbf{s}, u - |\nabla H| \tau)$ (A2)

Defining
$$
\rho(s) = \int \rho(s, u) du
$$
, we have, for *T* large enough, $\lim_{\Delta t \to 0} \sup \sup_{\rho(s) = \Delta t} \rho(s) = \int_0^T P(\tau) d\tau = \frac{h}{2} \int_{-\infty}^{\infty} d\mathbf{s} \frac{\rho^2(s)}{|\nabla H(s)|} \approx \frac{h}{2} \frac{\int_{-\infty}^{\infty} \rho^2(s) ds}{|\nabla H|}, \qquad \int_{-\infty}^{\infty} \rho^2(s) ds$ \n(A3)

where the approximation is valid for distributions well enough localized in phase space. From Eqs. (Al) and (A3) we have

$$
\mathscr{R} = \frac{|\nabla H|}{h \int_{-\infty}^{\infty} \rho^{2}(\mathbf{s}) d\mathbf{s}} \tag{A4}
$$

The integral $\int_{-\infty}^{\infty} \rho^2(s) ds$ is an interesting measure of the localization of $\rho(\tilde{s})$ along s. If $\rho(s)$ is confined to a single

ump, say a Gaussian (specializing to one degree of free-
dom) $\rho(s) = (1/2\pi\sigma^2)^{1/2} \exp(-s^2/2\sigma^2)$, then

$$
\int_{-\infty}^{\infty} \rho^2(s)ds = \frac{1}{2\sqrt{\pi}\sigma} \quad .
$$
 (A5)

(A3) With $\Delta E = |\nabla H| \sigma = (\partial H / \partial s) \delta s$, we have

$$
\mathcal{R} = \frac{1}{\sqrt{\pi}\hbar} \Delta E \tag{A6}
$$

where $\Delta E = (\partial H/\partial s)\sigma = (\partial H/\partial s)$. The rate then goes as ΔE for a single lump distribution for $\rho(s)$. However, if $\rho(s)$ is distributed over several different regions, then the rate $\mathscr R$ is not directly related to the usual measure of the energy uncertainty.

- E. J. Heller, Phys. Rev. Lett. 53, 1515 (1984); E. J. Heller, in Proceedings of the Cuernauaca Conference on Quantum Chaos, edited by T. Seligman and G. Casati (Springer-Verlag, New York, in press).
- 2G. Casati, B. V. Chirikov, F. M. Izraelev, and Joseph Ford, Stochastic Behavior in Classical and Quantum Hamiltonian Systems, Vol. 93 of Lecture Notes in Physics, edited by G. Casati and J. Ford (Springer-Verlag, New York, 1979); G. Casati, and I. Guaneri, Commun. Math. Phys. 80, ¹ (1984).
- ³R. S. MacKay, J. D. Meiss, and I. C. Percival, Physica D 13, 55 (1984); M. J. Davis, J. Chem. Phys. 83, 1016 (1985); M. J. Davis and S. K. Gray, ibid. 5389 (1986); R. C. Brown and R. Wyatt (unpublished); W. A. Lin and L. E. Reichl, Physica D 17, 165 (1985).
- 4P. W. Anderson, Phys. Rev. 103, 1492 (1958); D. J. Thouless, Phys. Rep. 13C, 95 (1974); S. Fishman, D. R. Grempel, and R. E. Prange, Phys. Rev. Lett. 49, 509 (1982).
- 5J. E. Moyal, Proc. Cambridge Philos. Soc. 45, 99 (1949).
- ⁶K. S. J. Nordholm and Stuart A. Rice, J. Chem. Phys. 61, 2031 (1974); 61, 768 (1974).
- 7E. J. Heller, J. Chem. Phys. 72, 1337 (1980); E. J. Heller and

M. J. Davis, ibid. 86, 2118 (1982); E. B. Stechel and E. J. Heller, Annu. Rev. Phys. Chem. 35, 563 (1984).

- 8K. G. Kay, J. Chem. Phys. 79, 3026 (1983).
- ⁹E. Thiele and J. P. Stone, J. Chem. Phys. 80, 5187 (1984).
- ⁰E. B. Stechel, J. Chem. Phys. 82, 364 (1985).
- ¹¹A. J. Lichtenberg and M. A. Lieberman, Regular and Stochastic Motion (Springer-Verlag, New York, 1983).
- ¹²C. Lanczos, J. Res. Natl. Bur. Stand. **45**, 255 (1950); A. Nauts and R. E. Wyatt, Phys. Rev. A 30, 872 (1984).
- ¹³M. V. Berry, Chaotic Behavior of Deterministic Systems (Les Houches Summer School Lectures, 1981) (North-Holland, Amsterdam, 1983), p. 171.
- ⁴T. A. Brody, J. Flores, J. B. French, P. A. Mello, A. Pandey, and S. S. M. Wong, Rev. Mod. Phys. 53, 385 {1981).
- ¹⁵E. P. Wigner, Ann. Math. 53, 36 (1951); 62, 548 (1955); 65, 203 (1957); 67, 325 (1958).
- 16M. J. Davis and E. J. Heller, J. Chem. Phys. 73, 4720 (1980); J. S. Hutchinson and R. E. Wyatt, Phys. Rev. A 23, 1567 (1981); N. Moiseyev and A. Peres, J. Chem. Phys. 79, 5945 (1983); J. Brickmann, P. Gofmann, and P. C. Schmidt, Int. J. Quantum Chem. 28, 109 (1985}.