Signatures of chaos in the modulus and phase of time-dependent wave functions

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For a classically chaotic two-dimensional bound system, based on the assumption that an initially-well-localized, semiclassical wave packet can be represented by a superposition of a large number of random plane waves at fixed times, we show that the modulus and phase of the wave function are independent random functions having a Rayleigh and a uniform one-point spatial distribution function, respectively. These predictions are confirmed through our numerical wave-packet study for one-quarter of the Sinai billiard. Streamline vortices can form around wave-function nodes, a fact first discovered by Dirac in 1931. For a classically chaotic billiard, the random plane-wave superposition approximation predicts that both the number of nodal points and the maximum number of vortices in a wave packet with initial wave number k is N, where N refers to the Nth eigenstate with wave number k_N which is closest to k.

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Much effort (see [1] for a review and references) has been devoted to the understanding of the quantum manifestation of classical chaos in two-dimensional (2D) bound systems in recent years. The main approach of such an endeavor, commonly referred to as quantum chaos or quantum chaology [2], has been statistical in nature. The results of various studies suggest that the statistical properties of energy eigenvalues, and both stationary and time-dependent wave functions of classically chaotic systems, exhibit generic behavior. For eigenvalues [1–3], the spectral statistics are well described by random-matrix theory. For spatially irregular wave functions, semiclassical energy eigenfunctions [4,5] and initially-well-localized, semiclassical wave packets [6,7] are quite accurately represented by a superposition of a large number of plane waves of equal wave-vector magnitude but random directions and phases. The random plane-wave superposition approximation (PWSA) was originally conjectured by Berry and co-workers [5,8] to be valid for semiclassical (high-lying) stationary states of classically chaotic systems with and without time-reversal symmetry. Recently, its validity has also been studied for nonchaotic, pseudointegrable billiards [7,9]. O'Connor, Gehlen, and Heller [10] found, numerically, that a superposition of a large number of random cosine waves exhibits a network of ridge structures in configuration space, instead of a speckle pattern as previously believed. These ridge structures have recently [11] been observed experimentally in water surface waves in a stadium-shaped ripple tank.

For time-dependent wave functions $\psi(\mathbf{r})$ (the time dependence in ψ is omitted because only spatial properties of the wave functions at *fixed times* are considered here, as we did in [6,7]), we have recently shown that the PWSA leads to the result that the real and imaginary parts [6,7]

$$\chi(\mathbf{r})=\mathrm{Re}\psi(\mathbf{r}) \quad \text{and} \quad \eta(\mathbf{r})=\mathrm{Im}\psi(\mathbf{r}) \tag{1}$$

are independent Gaussian random functions (processes) in position. The 2×2 pair-correlation-function (PCF) matrix has zero off-diagonal elements (cross PCF's) and identical diagonal elements (auto PCF's), which are expressed in terms of a Bessel function. To verify these predictions, spatial statistical properties (one- and two-point distribution functions and PCF's) of $\chi(\mathbf{r})$ and $\eta(\mathbf{r})$ were studied numerically for the chaotic $S4$ billiard (one-quarter of the Sinai billiard) [6,7] and a scattering version thereof [6]. Good agreement between the PWSA predictions and numerical results was obtained for initially-well-localized, semiclassical wave packets at times much longer than the classical time of flight, as determined by the initial mean speed of the wave packet, between the walls of the billiards. Berry and Robnik [5] have also suggested, on the basis of the PWSA, that the real and imaginary parts of the high-lying *stationary* states of a classically chaotic system without time-reversal symmetry are independent Gaussian random functions of position, and used it to predict the number of singularities (they occur at the joint zeros of the real and imaginary parts; in two dimensions, the zeros are points) in the eigenfunction's phase. For the Africa billiard [5], the predicted numbers agreed reasonably well with numerical results.

Dirac [12], and later Hirschfelder, Goebel, and Bruch [13], showed that quantum-mechanical streamlines (they follow the direction of the flux density $\mathbf{J}=\mathrm{Re}[-i\phi^*\nabla\phi]$) can form vortices around nodes of the wave function $\phi(\mathbf{r})$. For a given spatial dimensionality, a vortex can only occur if the node has the proper topology: in two dimensions, the node must be a point [13,14]. However, the existence of a node of the correct topology does not guarantee the existence of a vortex around it [13]. Furthermore, the vortex is quantized in the sense that the line integral of the "velocity" $\mathbf{v}=\mathbf{J}/\phi^*\phi$ along any closed path that encloses, but does not cross, the same node is given by [13,14]

$$m\oint \mathbf{v}\cdot d\mathbf{r}=n\hbar, \quad n=\pm1,\pm2,\ldots,$$

where m is the mass and $\hbar$ is Planck's constant. Vortices have been observed in various quantum time-independent and time-dependent scattering studies [14], including a previous (unpublished) wave-packet vortex study for the $S4$ billiard by us.

The aim of this paper is twofold. To date, we [6,7] have only treated the real and imaginary parts of the time-dependent wave function $\psi(\mathbf{r})$ at fixed times. Our main aim is to study the modulus and phase of $\psi(\mathbf{r})$ (also at fixed times); in particular, their individual one-point spatial distribution functions (DF) and their joint spatial distribution function(JDF) are derived on the basis of the PWSA and numerically verified for the $S4$ billiard. Second, we will show that the result of Berry and Robnik [5] for stationary states, with a slight reinterpretation, is also valid for wave packets, i.e., that the PWSA can also predict the number of nodal points in a billiard wave packet, and thus the maximum number of vortices the wave packet can have.

According to the PWSA [5,6,7], $\chi(\mathbf{r})$ and $\eta(\mathbf{r})$ are both Gaussian random functions, which means [15,16] that their individual n-point distribution functions are multivariate Gaussian functions. In particular, their individual DF's are predicted to be Gaussian functions with zero means and the same variance σ^2 [5–7]

$$P(f)=(2\pi\sigma^2)^{-1/2}\exp(-f^2/2\sigma^2)\ , \tag{2}$$

where f is either χ or η. For a billiard with total area S, the variance σ^2 is equal to $1/2S$ [5–7]. Moreover, χ and η are not only uncorrelated, but also independent [5–7]. Under these circumstances, it is possible to derive the DF's of the modulus

$$\rho=(\chi^2+\eta^2)^{1/2} \tag{3}$$

and phase

$$\theta=\tan^{-1}(\eta/\chi) \tag{4}$$

of the complex-valued wave function ψ. Since χ and η are independent and since we know their individual DF's [Eq. (2)], it is easy to show, using the transformation-of-variable technique [16], that the modulus ρ has a Rayleigh DF [17]

$$P(\rho)=\begin{cases}\sigma^{-2}\rho\exp(-\rho^2/2\sigma^2) & \text{for } \rho\geq 0\\ 0 \ \text{ elsewhere}\ ,\end{cases} \tag{5}$$

and the phase θ (radians) has a uniform DF

$$P(\theta)=\begin{cases}1/2\pi & \text{for } 0\leq\theta\leq 2\pi\\ 0 \ \text{ elsewhere}\ .\end{cases} \tag{6}$$

Furthermore, it can be shown [16] that ρ and θ are also independent, i.e., their JDF is given by

$$P(\rho,\theta)=P(\rho)P(\theta)\ . \tag{7}$$

To test predictions (5), (6), and (7), an initially-well-localized (in position and momentum), semiclassical ($k_{x,y}^{-1} \ll \alpha \ll \sqrt{S}$) 2D Gaussian wave packet

$$\psi(x,y)=(2\pi\alpha^2)^{-1/2}\exp(-[(x-x_0)^2+(y-y_0)^2]/4\alpha^2)$$
$$\times\exp(ik_x x+ik_y y) \tag{8}$$

was propagated numerically using a conditionally stable, explicit finite-difference scheme for the chaotic $S4$ billiard and, for comparison, the integrable square billiard. Details of the propagation scheme can be found in [6]. For our calculations, the initial wave-packet parameters $x_0=y_0=0.025$, $k_x=1500$, $k_y=2500$, and variance $\alpha^2=6.25\times 10^{-6}$ were chosen. The spatial grid size and time step used in the propagation scheme were 2.5×10^{-4} and 1.0×10^{-8}, respectively. Also, $\hbar=m(\text{mass})=1$. For the $S4$ billiard, a circle of radius 0.05 centered in a square of side length 0.1 was chosen. For the square billiard, a side-length of 0.05 was used. All physical quantities with dimensions are in arbitrary units. Previously [7], using the same initial wave-packet and propagation parameter values, we found that the spatial statistical properties of the real and imaginary parts of the wave function for the

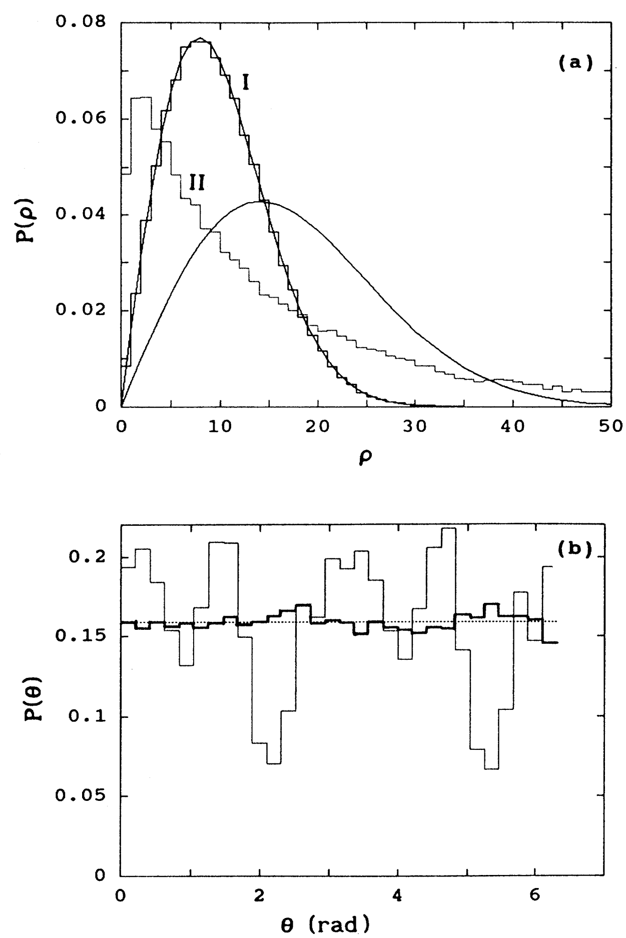

FIG. 1. One-point distribution functions of (a) modulus $P(\rho)$ and (b) phase $P(\theta)$ for the $S4$ billiard and the square billiard. In (a), histograms I and II are the numerical $P(\rho)$ for the $S4$ billiard and the square billiard, respectively. The smooth curves are the PWSA predictions for $P(\rho)$: the narrower curve is Eq. (5) plotted using the area of the $S4$ billiard; the wider curve is Eq. (5) plotted using the area of the square billiard. Shown in (b) are the numerical $P(\theta)$ for the $S4$ billiard (bold histogram) and square billiard (thin histogram). The horizontal dashed line is $1/2\pi$ [Eq. (6)] predicted by the PWSA.

$S4$ billiard agree well with the PWSA predictions after an initial "relaxation" period, whereas the corresponding properties for the square billiard do not.

Numerical results for the DF's $P(\rho)$ and $P(\theta)$ are shown in Figs. 1(a) and 1(b), respectively. For the $S4$ billiard, the agreement between the numerical DF's and their corresponding predictions (5) and (6) is good. In contrast, the DF's $P(\rho)$ and $P(\theta)$ for the square billiard deviate considerably from Eqs. (5) and (6), respectively, and they are nongeneric, depending on time. For the $S4$ billiard, the numerical JDF $P(\rho,\theta)$ (a cross section for a particular range of phase is shown in Fig. 2) is well fitted by Eq. (7), but the JDF for the square billiard is not.

Based on these results, we conclude that the modulus and phase (at fixed times) of an initially-well-localized, semiclassical wave packet of a classically chaotic system are independent random functions (variables), having a Rayleigh and uniform distribution function, respectively. Our analysis in this paper should also be equally valid for semiclassical eigenstates of classically chaotic systems that do not have time-reversal symmetry, e.g., the Africa billiard [5], since their real and imaginary parts should [5] also be independent Gaussian random functions, with DF's given by Eq. (2). Conversely, the result of Berry and Robnik [5] with regard to the number of nodal points in a semiclassical eigenstate of the Africa billiard should also be valid for an initially-well-localized, semiclassical wave packet [see Eq. (8)]. In [5] the number of nodal points in the Nth eigenstate ($N \rightarrow \infty$, i.e., semiclassical), with energy $E_N = \hbar^2 k_N^2/2m$, was predicted to be

$$Sk_N^2/4\pi \simeq N \;, \tag{9}$$

where S is the area of the billiard. The right-hand side of Eq. (9) was obtained [5] by noting that the left-hand side is the leading term in the expression for the average part of the spectral staircase function for a billiard.

For initially-well-localized, semiclassical wave packets in a billiard B, the derivation in [5] that led to the left-hand side of (9) also applies, and thus the number of nodal points is

$$Sk^2/4\pi \;, \tag{10}$$

where $k=(k_x^2+k_y^2)^{1/2}$ is the wave-packet initial wave number. If we replace k in (10) by k_N, the wave number of the Nth eigenstate of the billiard B that is closest to k, then the same argument [5] that led to the right-hand side of (9) also applies, and thus the number of nodal points (10) is approximately N.

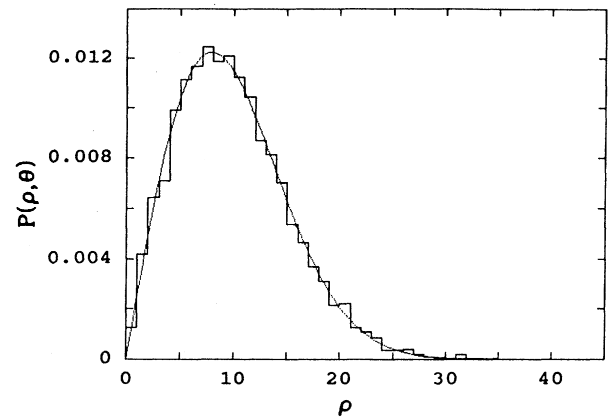

FIG. 2. Cross section of the numerical (histogram) joint distribution function $P(\rho,\theta)$ as a function of ρ for $\theta\in[2.94,3.15]$ and the corresponding prediction (smooth curve) of the PWSA [Eq. (7)] for the $S4$ billiard.

In two dimensions, streamline vortices can only occur around nodal points, but the existence of a nodal point is not a sufficient condition for the formation of a vortex [13]. Thus, for a chaotic billiard, the maximum number of vortices in a wave packet (or a stationary state without time-reversal symmetry) is evidently given by the right-hand side of (9), which is the number of nodal points predicted by the PWSA. Apart from the question of how many vortices can occur, another interesting question is: What is the distribution of vortex size? Also, what are the role of vortices in scattering systems [18], which exhibit chaos classically? It has been speculated [14] that the vortices play an important role in the dynamics of molecular collisions. These and other problems concerning vortices remained to be studied, and we hope to report our findings in the future.

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[18] See, for example, the review by U. Smilansky, in *Chaos and Quantum Physics,* edited by M. Giannoni, A. Voros, and J. Zinn-Justin (North-Holland, Amsterdam, 1990).