Band Husimi distributions and the classical-quantum correspondence on the torus

Itzhack Dana
Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel

Yaakov Rutman and Mario Feingold
Department of Physics, Ben-Gurion University, Beer-Sheva 84105, Israel

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Band Husimi distributions (BHDs) are introduced in the quantum-chaos problem on a toral phase space. In the framework of this phase space, a quantum state must satisfy Bloch boundary conditions (BCs) on a torus and the spectrum consists of a finite number of levels for given BCs. As the BCs are varied, a level broadens into a band. The BHD for a band is defined as the uniform average of the Husimi distributions for all the eigenstates in the band. The generalized BHD for a set of adjacent bands is the average of the BHDs associated with these bands. BHDs are shown to be closer, in several aspects, to classical distributions than Husimi distributions for individual eigenstates. The generalized BHD for two adjacent bands is shown to be approximately conserved in the passage through a degeneracy between the bands as a nonintegrability parameter is varied. Finally, it is shown how generalized BHDs can be defined so as to achieve physical continuity under small variations of the scaled Planck constant. A generalization of the topological (Chern-index) characterization of the classical-quantum correspondence is then obtained. [S1063-651X(98)03011-6]

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I. INTRODUCTION

The main objective of ''quantum chaos'' is to understand the correspondence between classically nonintegrable systems and their quantum counterparts in the semiclassical limit [1]. During the past two decades, significant progress has been made in the study of this correspondence with the discovery of phenomena such as dynamical localization [1–3], ''scarring'' of eigenstates by unstable periodic orbits [1,4–6], and statistical properties of the eigenspectrum [1,7]. However, the relation between classical phase-space structures and corresponding quantum-dynamical entities is still far from being completely understood.

In this paper we introduce quantum-mechanical distributions that, in the semiclassical limit, are expected to approach in a natural way classical distributions on both regular and chaotic phase-space structures. This will be done in the framework of a toral phase space, where, as shown in a recent series of works [8–10], some interesting insights in the quantum-chaos problem can be achieved. Quantum dynamics can be reduced to a torus if two conditions are satisfied (see Sec. II for more details). First, the classical map for the system is strictly periodic in all the phase-space coordinates. The simplest nonintegrable system possessing this property is the ''kicked-Harper'' (KH) model [8–15] with the Hamiltonian

$$H = A\cos(v) + A\cos(u)\sum_{s=-\infty}^{\infty}\delta(t/\tau - s), \qquad (1)$$

where u and v are dimensionless conjugate phase-space variables (with the Poisson bracket $\{u,v\}=1/I$, I being some classical action), A is the amplitude, and τ is the time period. The system (1) is exactly related [14] to the problem of periodically kicked charges in a uniform magnetic field under resonance conditions [16]. In the limit $\tau \to 0$, Eq. (1) reduces to the integrable Harper Hamiltonian $H_0 = A\cos(u) + A\cos(v)$. The transition from integrable to chaotic phase-space structure, as the dimensionless classical parameter $\gamma = A\tau/2\pi I$ is increased from 0, is shown in Fig. 1. The second condition for quantum dynamics on a torus is that a scaled $\hbar$, denoted here by ρ ($[\hat{u},\hat{v}] = 2\pi i\rho = i\hbar/I$), assumes rational values $\rho = q/p$ (q and p are coprime integers). The admissible quantum states are then those that satisfy Bloch quasiperiodic boundary conditions (BCs) on the torus; see Sec. II. The energy or quasienergy spectrum consists of precisely p levels and, as the BCs are varied, each of these levels spans a band.

The advantage of this framework is that it allows for a characterization of the classical-quantum correspondence by means of integer topological invariants, the Chern indices [8–10], associated with the p bands. The Chern index σ for a band is analogous to the quantum Hall conductance carried by a magnetic band in a perfect crystal [17–24] and is a measure of the sensitivity of the eigenstates in the band to variations in the BCs [8–10,25]. For $q=1$, the toral phase space coincides with the basic unit cell of periodicity of the system. In this case, where the classical-quantum correspondence can be established in the simplest and most natural way, σ can assume, in principle, all values. Several arguments [8,9,25], supported by numerical evidence, then indicate that if the Husimi distribution of an eigenstate is localized, in a semiclassical regime ($\rho \ll 1$), on classical regular orbits (e.g., Kol'mogorov-Arnol'd-Moser tori or periodic orbits) the corresponding band has $\sigma = 0$. On the other hand, eigenstates whose Husimi distribution is spread over the classical chaotic region should correspond to bands with $\sigma \neq 0$. The transition from a nearly integrable regime [e.g., Fig. 1(a)], where almost all $\sigma = 0$, to a fully chaotic regime [e.g., Fig. 1(d)], where almost all $\sigma \neq 0$, as a nonintegrability parameter is varied, takes place via degeneracies between ad-

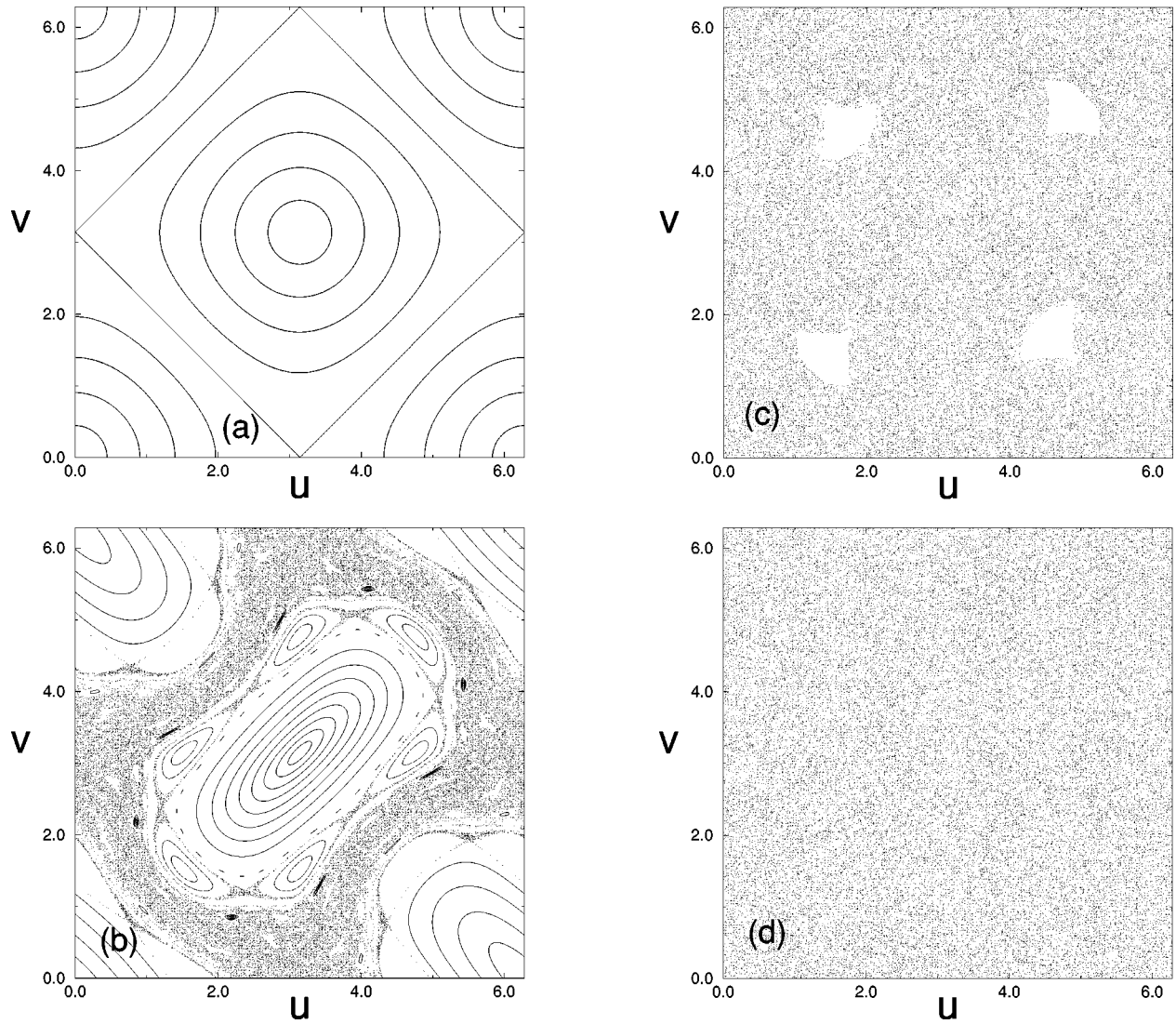

FIG. 1. Classical Poincaré maps of typical orbits of the kicked-Harper (KH) model (1) for different values of the nonintegrability parameter $\gamma = A\tau/2\pi I$: (a) $\gamma = 0.001$ (nearly integrable regime), (b) $\gamma = 0.26$ (mixed regime) (notice, for future reference, the island chains of periods 6 and 8 surrounding the central elliptic point), (c) $\gamma = 0.56$ (the chaotic region occupies a large fraction of the phase space), and (d) $\gamma = 0.95$ (strongly chaotic regime).

jacent bands. In the passage through a degeneracy between bands b and b', the Chern indices σ_b and $\sigma_{b'}$ change, respectively, by $\pm\Delta\sigma$, where, generically [19,26], $|\Delta\sigma| = 1$. A ''diffusion'' of Chern indices [27] occurs then in the transition above.

Despite this characterization of the classical-quantum correspondence for small ρ, the eigenstates may not be considered close to classical phase-space structures, strictly speaking, for any ρ. This is because of the following reasons. (a) While the BCs satisfied by a quantum state have a well-defined physical meaning (see Sec. III), they are of a purely quantum nature. In particular, the strong dependence of the eigenstates on the BCs for $\sigma \neq 0$ and, in several cases (see Sec. III), also for $\sigma = 0$, has no classical counterpart. (b) The Husimi distribution of an eigenstate always assumes p zeros in the torus; see Sec. II. Because of this fact, an eigenstate cannot tend, in the semiclassical limit, to the microcanonical uniform distribution on the chaotic region [8,28]. (c) In the general case of $q \neq 1$, the exact eigenstates may be viewed as arising from quantum tunneling between degenerate classical orbits located in q adjacent unit cells [9–11]. As a consequence, σ is always nonvanishing [10] and the topological characterization of the classical-quantum correspondence cannot be extended straightforwardly to this general case.

We show in this paper that a natural way to overcome these difficulties is simply to average uniformly the Husimi distributions of the eigenstates in a band over all the BCs. In what follows we refer to the result of this averaging as the *band Husimi distribution* (BHD). The BHDs turn out to be closer, in several aspects, to classical distributions than Husimi distributions for individual eigenstates. It is well known [5,6] that smoothing a probability distribution over a range ΔE of energy levels has the effect of washing out purely quantum structures such as scars. As ΔE is increased, this effect increases and the smoothed probability distribution (e.g., the spectral Wigner function in Ref. [6]) becomes closer to a classical distribution. In our case the smoothing is done not over a range of *discrete* energy levels but over the *continuous* range of one band, corresponding essentially to a *single* level in the framework of a toral phase space. This is

thus the *minimal* smoothing in this framework and it is performed just for the sake of eliminating the purely quantum effects of individual BCs. The BHD may be viewed as the representative Husimi distribution for a level in the torus. In several important cases, we shall find it necessary to generalize the concept of BHD by considering the average of BHDs associated with a set of adjacent bands.

This paper is organized as follows. In Sec. II we summarize the relevant known facts about quantum dynamics on a torus [8–10]. In Sec. III the concept of BHD for a single band is introduced. In Sec. IV the concepts of generalized band (set of adjacent bands) and the associated BHD are introduced and studied. In Sec. V the generalized BHD for two adjacent bands near a degeneracy of these bands is studied. In Sec. VI we show how to define generalized BHDs for $q\neq 1$ in order to achieve physical continuity under small variations in ρ. In this way, the topological characterization of the classical-quantum correspondence is extended to the general case of $q\neq 1$. Conclusions are presented in Sec. VII.

II. QUANTUM DYNAMICS ON A TORUS

We provide here some relevant background on quantum dynamics on the torus [8–10] using, for later convenience, the notation of Ref. [10], where a general formulation of the problem was presented. Consider a classical area-preserving map strictly periodic in the phase space (u,v) with a $2\pi\times 2\pi$ unit cell, which is the basic torus T^2. The one-step quantum evolution operator corresponding to the classical map is $\hat{U}(\hat{u},\hat{v})$, where $[\hat{u},\hat{v}]=2\pi i\rho$. If ρ is a rational number, $\rho=q/p$ (q and p are coprime integers), there exists a pair of ''smallest'' commuting phase-space translations

$$\hat{D}_1=e^{i\hat{u}/\rho},\quad \hat{D}_2=e^{ip\hat{v}}. \tag{2}$$

Because of $[\hat{u},\hat{v}]=2\pi i\rho$, $\hat{D}_1$ ($\hat{D}_2$) is a translation by 2π ($2\pi q$) in the v (u) direction. Since $\hat{U}(\hat{u},\hat{v})$ is periodic in both $\hat{u}$ and $\hat{v}$ with period 2π, it commutes with $\hat{D}_1$ and $\hat{D}_2$. There exist therefore simultaneous eigenstates Ψ of $\hat{U}$, $\hat{D}_1$, and $\hat{D}_2$:

$$\hat{U}|\Psi_{b,\mathbf{w}}\rangle=e^{-i\omega_b(\mathbf{w})}|\Psi_{b,\mathbf{w}}\rangle,$$

$$\hat{D}_1|\Psi_{b,\mathbf{w}}\rangle=e^{iw_1/\rho}|\Psi_{b,\mathbf{w}}\rangle,\quad \hat{D}_2|\Psi_{b,\mathbf{w}}\rangle=e^{ipw_2}|\Psi_{b,\mathbf{w}}\rangle, \tag{3}$$

where b is a ''band'' index (see below), $\omega_b(\mathbf{w})$ is the quasienergy, and $\mathbf{w}=(w_1,w_2)$ is a Bloch wave vector varying in the ''Brillouin zone'' (BZ) $0\leqslant w_1<2\pi\rho$, $0\leqslant w_2<2\pi/p$, a torus to be denoted T_{BZ} in what follows. Now, for each given value of $\mathbf{w}$, Eqs. (3) can be interpreted as quasiperiodic BCs satisfied by the eigenstates $|\Psi_{b,\mathbf{w}}\rangle$ in the ''quantum'' toral phase space T_Q^2: $0\leqslant u<2\pi q$, $0\leqslant v<2\pi$. It can be shown [10] that for each $\mathbf{w}$ the quasienergy spectrum consists precisely of p levels $\omega_b(\mathbf{w})$, $b=1,\ldots,p$. As the BCs are varied (by varying $\mathbf{w}$ in the BZ), each level broadens into a ''band.''

In the absence of band degeneracies [$\omega_b(\mathbf{w})\neq\omega_{b'}(\mathbf{w})$ for all $\mathbf{w}$ and $b'\neq b$], $|\Psi_{b,\mathbf{w}}\rangle$ must be periodic in the BZ up to a constant phase factor depending, in general, on $\mathbf{w}$. The phase of $|\Psi_{b,\mathbf{w}}\rangle$ may be chosen so that $|\Psi_{b,\mathbf{w}}\rangle$ will be exactly periodic in one direction, say w_1, but then it will be periodic in w_2 only up to a phase factor that, in its simplest form, has a phase that is linear in w_1 [10]:

$$|\Psi_{b,w_1+2\pi\rho,w_2}\rangle=|\Psi_{b,\mathbf{w}}\rangle, \tag{4}$$

$$|\Psi_{b,w_1,w_2+2\pi/p}\rangle=\exp(i\sigma_b w_1/\rho)|\Psi_{b,\mathbf{w}}\rangle. \tag{5}$$

Here the constant σ_b must be an integer in order for Eq. (5) to be consistent with Eq. (4). It is easy to see from Eqs. (4) and (5) that $2\pi\sigma_b$ is the total phase change of $|\Psi_{b,\mathbf{w}}\rangle$ when going around the BZ boundary counterclockwise. This phase change is independent of phase transformations of $|\Psi_{b,\mathbf{w}}\rangle$. In fact, the integer σ_b is a topological number, the *Chern index*, which can be expressed in a form manifestly invariant under phase transformations [see Ref. [8] and expression (28) below].

The general form of $|\Psi_{b,\mathbf{w}}\rangle$ in the v representation is [10]

$$\Psi_{b,\mathbf{w}}(v)=\langle v|\Psi_{b,\mathbf{w}}\rangle=\sum_{m=0}^{p-1}\phi_b(m;\mathbf{w})\psi_{w_1+2\pi m\rho,w_2}(v), \tag{6}$$

where $\phi_b(m;\mathbf{w})$ are expansion coefficients and $\psi_{\mathbf{w}}(v)$ are kq functions [29],

$$\psi_{\mathbf{w}}(v)=\sum_{l=-\infty}^{\infty}\exp(ilw_1/q)\,\delta(v-w_2+2\pi l/p). \tag{7}$$

Without the label b, Eq. (6) is the most general expression of a quantum state in the v representation for given BCs (i.e., given $\mathbf{w}$). A completely analogous expression is obtained in the conjugate (u) representation by Fourier transforming Eq. (6). These expressions imply, essentially, a discretization of the toral phase space T_Q^2 into p^2 points, $u_{m_1}=w_1+2\pi m_1\rho$, $v_{m_2}=w_2+2\pi m_2/p$, $m_1,m_2=0,\ldots,p-1$, with $\phi(m_1;\mathbf{w})$ being the probability amplitude for u to assume the value u_{m_1}. The corresponding amplitude for $v=v_{m_2}$ is the discrete Fourier transform of $\phi(m_1;\mathbf{w})$. This discretization was studied by Hannay and Berry [30] in the special case of $q=1$ ($T_Q^2=T^2$) and $\mathbf{w}=\mathbf{0}$ (strict periodicity). They used the p amplitudes $\phi(m;\mathbf{w}=\mathbf{0})$ to investigate the evolution of a quantum state in the cat maps.

A most useful representation of $|\Psi_{b,\mathbf{w}}\rangle$ is the coherent-state representation $\Psi_{b,\mathbf{w}}(\mathbf{R})=\langle\mathbf{R}|\Psi_{b,\mathbf{w}}\rangle$, where $\mathbf{R}\equiv(u,v)$ and $|\mathbf{R}_0\rangle$ is a coherent state,

$$\langle v|\mathbf{R}_0\rangle=\left(\frac{\alpha^2}{2\pi^2\rho}\right)^{1/4}\exp\left[-\frac{\alpha^2(v-v_0)^2}{4\pi\rho}-\frac{iu_0}{2\pi\rho}(v-v_0/2)\right]. \tag{8}$$

Here α is the ''squeezing parameter,'' related to the parameters of the harmonic oscillator for which the quantum evolution of the state (8) is nondispersive. An equivalent expression for a coherent state depends on u_0 and v_0 only through the complex number $z_0=u_0/\alpha-i\alpha v_0$ (see, e.g., Refs. [28,31]), giving an analytic representation $\Psi_{b,\mathbf{w}}(z)$. For future convenience, however, we shall use the representation $\Psi_{b,\mathbf{w}}(\mathbf{R})$, choosing, as in Ref. [28], the symmetric value $\alpha=1$.

Important properties of $\Psi_{b,\mathbf{w}}(\mathbf{R})$ concern its zeros, in both the $\mathbf{R}$ and $\mathbf{w}$ variables. At fixed $\mathbf{w}$, $\Psi_{b,\mathbf{w}}(\mathbf{R})$ always assumes exactly p zeros $\mathbf{R}=\mathbf{R}_{0,j}(\mathbf{w})$ $(j=1,\ldots,p)$ in T_Q^2 (counting possible but nongeneric zero multiplicities). This property was proved in Ref. [28] for $q=1$ and $\alpha=1$, but it can be easily generalized to all q and α, using Eq. (6), together with Eqs. (7) and (8). It is also well known [28] that the p zeros $\mathbf{R}_{0,j}(\mathbf{w})$, like the p amplitudes $\phi_b(m;\mathbf{w})$ in Eq. (6), completely determine the wave function $\Psi_{b,\mathbf{w}}(\mathbf{R})$. At fixed $\mathbf{R}$, the number $N_0(\mathbf{R})$ of zeros $\mathbf{w}=\mathbf{w}_0(\mathbf{R})$ of $\Psi_{b,\mathbf{w}}(\mathbf{R})$ in the BZ is not smaller than $|\sigma_b|$ [32]. These properties imply that the p zeros $\mathbf{R}_{0,j}(\mathbf{w})$ must wind around T_Q^2 at least $|\sigma_b|$ times when $\mathbf{w}$ is varied in the BZ. Thus, if for some $\mathbf{R}=\mathbf{R}'$, $\Psi_{b,\mathbf{w}}(\mathbf{R}')$ does not vanish in the BZ, $\sigma_b=0$. We shall refer to the union of all $\mathbf{R}'$ as the *localization domain* of $\Psi_{b,\mathbf{w}}(\mathbf{R})$, for reasons that will become clear in the following paragraph. As $\mathbf{w}$ is varied over the entire BZ, the p zeros $\mathbf{R}_{0,j}(\mathbf{w})$ never enter this domain (see also Ref. [25]).

In a nearly integrable situation [e.g., very small A in the KH model (1)] and in a semiclassical regime ($\rho\ll 1$), most eigenstates $\Psi_{b,\mathbf{w}}(\mathbf{R})$ will be localized on regular classical orbits and the corresponding bands are usually very narrow (almost independent of $\mathbf{w}$). A good approximation to the Husimi probability distribution $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$ in its localization region is given by [8,34]

$$|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2 \approx \frac{\mathcal{N}}{V(\mathbf{R})}\exp\left\{-\frac{1}{2\pi\rho}\left[\frac{\overline{H}_0(\mathbf{R})-E_b}{V(\mathbf{R})}\right]^2\right\}, \quad (9)$$

where $\overline{H}_0(\mathbf{R})$ is the energy function for an effective integrable Hamiltonian H_0 in this nearly integrable situation, E_b is an energy eigenvalue of H_0 approximating the very narrow band $[E_b\approx\omega_b(\mathbf{w})\hbar/\tau]$, $V(\mathbf{R})$ is the phase-space velocity for H_0, and $\mathcal{N}$ is a normalization constant. The relation (9) manifestly shows that the eigenstates are quite insensitive to variations in $\mathbf{w}$ in the region of phase space where they are localized. In particular, the p zeros $\mathbf{R}_{0,j}(\mathbf{w})$ should never enter this region, thus implying a finite localization domain (as defined above). We therefore expect that eigenstates that are localized on regular classical orbits for $\rho\ll 1$ should belong to bands with $\sigma_b=0$ (see also Sec. III).

It is important to remark here that the value $\sigma_b=0$ may occur only for $q=1$ since σ_b has to satisfy the Diophantine equation $p\sigma_b+q\mu_b=1$, where μ_b is a second integer [10,20]. For $q\neq 1$, the exact eigenstates are quite ''nonclassical'' since they may be viewed as arising from quantum tunneling between q degenerate classical orbits located in the q adjacent unit cells defining T_Q^2 [9–11]. Thus, even in a completely integrable situation, the p zeros $\mathbf{R}_{0,j}(\mathbf{w})$ always cover the torus T_Q^2 when $\mathbf{w}$ varies in the BZ [9].

In a strongly chaotic situation, where a typical orbit fills the entire phase space T^2, the p zeros $\mathbf{R}_{0,j}(\mathbf{w})$ for $q=1$ are expected to be distributed almost uniformly in $T_Q^2=T^2$ [28] and to explore the entire T^2 as $\mathbf{w}$ is varied in the BZ [8]. Almost all the bands should therefore be characterized by nonvanishing σ_b. The transition from a nearly integrable situation (almost all $\sigma_b=0$) to a strongly chaotic one (almost all $\sigma_b\neq 0$), as a nonintegrability parameter is varied, takes place via successive degeneracies between adjacent bands [8,9] (see also the Introduction).

III. BAND HUSIMI DISTRIBUTIONS

We start this section by considering in more detail the nature of the BCs (3) using the KH system (1) as a model. The nearly integrable regime for this system corresponds to very small values of the classical parameter $\gamma=A\tau/2\pi I$ [see Fig. 1(a)]. In this regime, the system is well described by the Harper Hamiltonian $H_0=A\cos(u)+A\cos(v)$. For $\rho=1/p$, p odd, the energy spectrum of H_0 consists of p bands $E_b(\mathbf{w})$, $b=1,\ldots,p$, in order of increasing energy. Only the central band $[b=(p+1)/2]$ has a nonvanishing Chern index $\sigma_b=1$ [17]. In the semiclassical regime $p\gg 1$, the eigenstates of this band are concentrated on the separatrix orbit [see Fig. 1(a)], which is not contractible to a point. On the other hand, the eigenstates of the other bands, which have vanishing Chern indices, are concentrated on orbits that are contractible to a point.

This state of matters persists also for γ not very small, when the separatrix orbit breaks into a stochastic layer, and island chains emerge from the H_0 contractible orbits. For example, for $\rho=1/11$, the Chern indices σ_b appear to be the same as in the Harper case in the entire interval $\gamma\leqslant 0.26$ [9,35]. Namely, only the central quasienergy band features a nonvanishing Chern index $\sigma_b=1$. We have studied numerically the sensitivity of the eigenstates to variations in the BCs (i.e., variations in $\mathbf{w}$) for several values of γ in the interval above. We find that eigenstates in $\sigma_b=0$ bands sufficiently ''far'' from the central band (i.e., b close to 1 or 11) are indeed almost insensitive to variations in $\mathbf{w}$ (large localization domain). This is not the case, however, for bands sufficiently close to the central band. While the Chern index for these bands vanishes, the sensitivity of the eigenstates to variations in $\mathbf{w}$ is quite strong (very small or empty localization domain), almost as strong as that of eigenstates in the central band. This is clearly illustrated in Figs. 2 and 3. In general, we expect strong sensitivity to variations in $\mathbf{w}$ in $\sigma_b=0$ bands that are sufficiently close to $\sigma_b\neq 0$ bands.

This sensitivity has no classical analog since $\mathbf{w}$ is a purely quantum characterization of the eigenstates, which are concentrated on different regions of T_Q^2 for different values of $\mathbf{w}$. In fact, by comparing Eqs. (3) with the definitions (2) of the operators $\hat{D}_1$ and $\hat{D}_2$, we see immediately that $\mathbf{w}$ is just a *quasicoordinate* of $\mathbf{R}=(u,v)$:

$$w_1 \Leftrightarrow \rho\left(\frac{u}{\rho} \bmod 2\pi\right), \quad w_2 \Leftrightarrow \frac{1}{p}(pv \bmod 2\pi).$$

To understand this better, consider, for given $\mathbf{w}=\mathbf{w}'$, the ''displaced'' quantum state

$$\hat{D}(z_0)|\Psi_{b,\mathbf{w}'}\rangle = \exp(z_0\hat{a}^\dagger - z_0^*\hat{a})|\Psi_{b,\mathbf{w}'}\rangle, \quad (10)$$

where $z_0=u_0+iv_0$ and $\hat{a}=(\hat{u}+i\hat{v})/4\pi\rho$ is the annihilation operator. It is easy to verify, using the well-known commutation relation for the phase-space translations $\hat{D}(z_0)$ [36], that the state (10) satisfies the BCs (3) with the displaced value of $\mathbf{w}=\mathbf{w}'+\mathbf{R}_0$ $[\mathbf{R}_0=(u_0,v_0)]$. On the other hand, using the expression (8) (for $\alpha=1$), we find that the coherent-state representation of the state (10) is given by

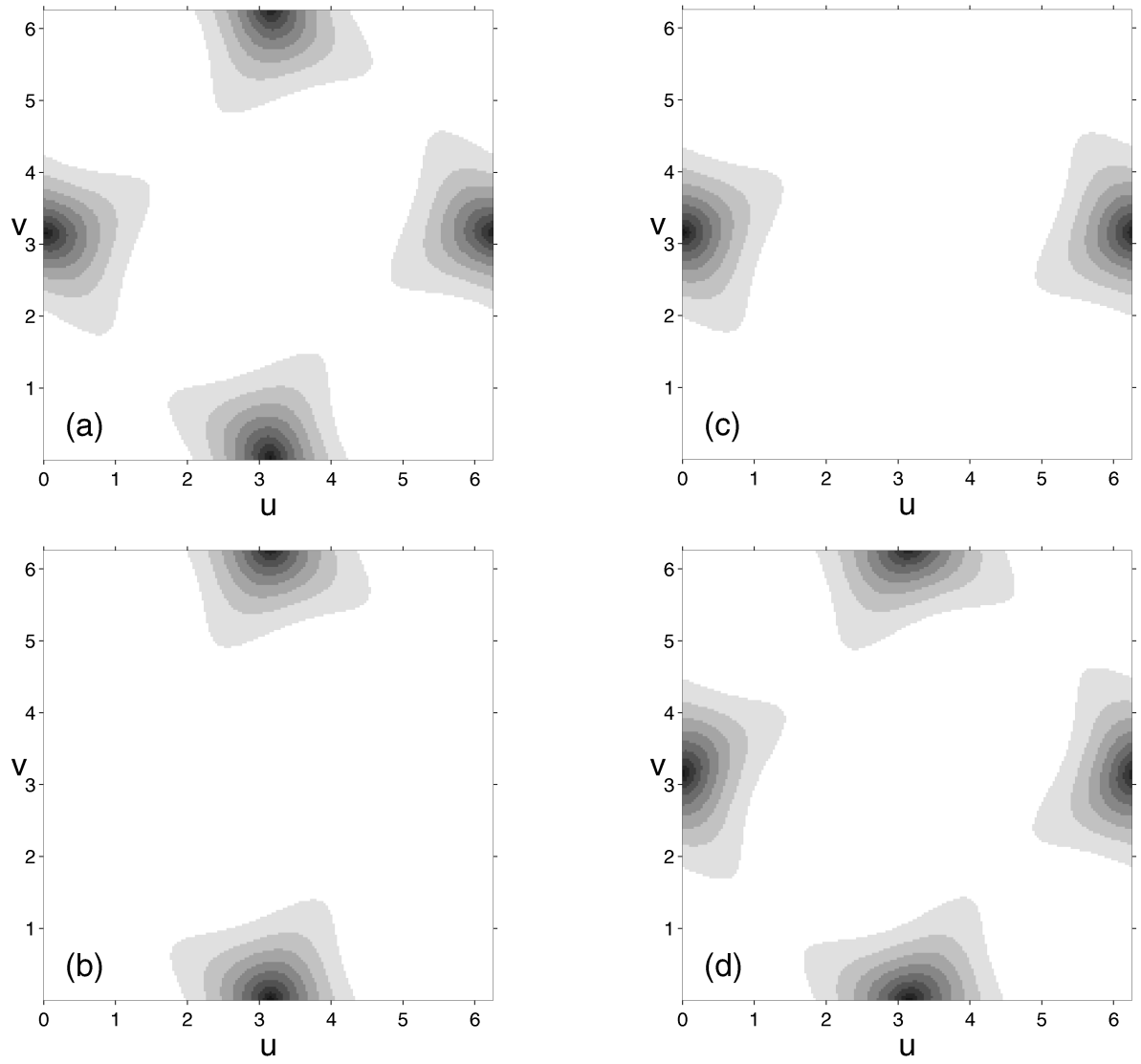

FIG. 2. Density plots of Husimi distributions $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$ for the KH model with parameters $\gamma=0.26$ [compare with Fig. 1(b)] and $\rho=1/11$. The central band $b=6$ (with Chern index $\sigma_6=1$) is considered for different values of $\mathbf{w}$ in the BZ: (a) $\mathbf{w}=(0,0)$, (b) $\mathbf{w}=(\pi/11,0)$, (c) $\mathbf{w}=(0,\pi/11)$, and (d) $\mathbf{w}=(\pi/11,\pi/11)$. In these plots, as well as in Figs. 3–5, we use a power-law density scale (with power $\approx 1/3$) and ten gray tones, with darker tones corresponding to higher values of the distribution. In cases (b) and (c), $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$ is concentrated on one of the two hyperbolic fixed points, while in cases (a) and (d) it is concentrated on both points.

$$\langle \mathbf{R}|\hat{D}(z_0)|\Psi_{b,\mathbf{w}'}\rangle = \exp[i(uv_0-u_0v)/4\pi\rho]\Psi_{b,\mathbf{w}'}(\mathbf{R}-\mathbf{R}_0). \tag{11}$$

Thus the shifted function $\Psi_{b,\mathbf{w}'}(\mathbf{R}-\mathbf{R}_0)$ is, up to a phase factor, the coherent-state representation of a quantum state characterized by the displaced value of $\mathbf{w}=\mathbf{w}'+\mathbf{R}_0$. This is a vivid illustration of the notion of ''quasicoordinate of $\mathbf{R}$'' for $\mathbf{w}$.

From Eq. (11) one may get the impression that there is always strong sensitivity to variations in the BCs. However, since $\hat{D}(z_0)$ does not commute, for general z_0, with the evolution operator $\hat{U}$, the displaced state (10) will not be, in general, an eigenstate. Still, one has the expansion

$$\langle \mathbf{R}|\hat{D}(z_0)|\Psi_{b,\mathbf{w}'}\rangle = \sum_{b'=1}^{p} c_{b,b'}(\mathbf{R}_0,\mathbf{w})\Psi_{b',\mathbf{w}}(\mathbf{R}),$$

where the coefficients $c_{b,b'}(\mathbf{R}_0,\mathbf{w})=\langle \Psi_{b',\mathbf{w}}|\hat{D}(z_0)|\Psi_{b,\mathbf{w}'}\rangle$. Assume, for example, that $\Psi_{b,\mathbf{w}}(\mathbf{R})$ is almost insensitive to variations in $\mathbf{w}$ (large localization domain). Then, from Eq. (11) and $\mathbf{w}=\mathbf{w}'+\mathbf{R}_0$ it follows that the coefficient $c_{b,b}(\mathbf{R}_0,\mathbf{w})$ should be relatively small for almost all $\mathbf{w}$ if R_0 is larger than the typical width of the localization domain. If, on the other hand, $\Psi_{b,\mathbf{w}}(\mathbf{R})$ is highly sensitive to variations in $\mathbf{w}$, the coefficients $c_{b,b'}(\mathbf{R}_0,\mathbf{w})$, for $b'\approx b$, may be relatively large for ''many'' pairs $(\mathbf{R}_0,\mathbf{w})\neq\mathbf{0}$. For example, in the cases shown in Figs. 2 and 3, these pairs include $[\mathbf{R}_0=(\pi,\pi),\mathbf{w}=(0,\pi/11)]$ [i.e., $\mathbf{w}'=(\pi/11,0)$; compare Fig. 2(b) with Fig. 2(c) and Fig. 3(b) with Fig. 3(c)] and $[\mathbf{R}_0=(\pi,\pi),\mathbf{w}=(\pi/11,\pi/11)]$ [i.e., $\mathbf{w}'=(0,0)$; compare Fig. 2(a) with Fig. 2(d)].

Because of the purely quantum nature of $\mathbf{w}$ and the BCs, it is natural to perform a uniform average over $\mathbf{w}$ in the Brillouin zone in order to obtain ''more classical'' quantities. In this paper we shall consider the average of the Husimi

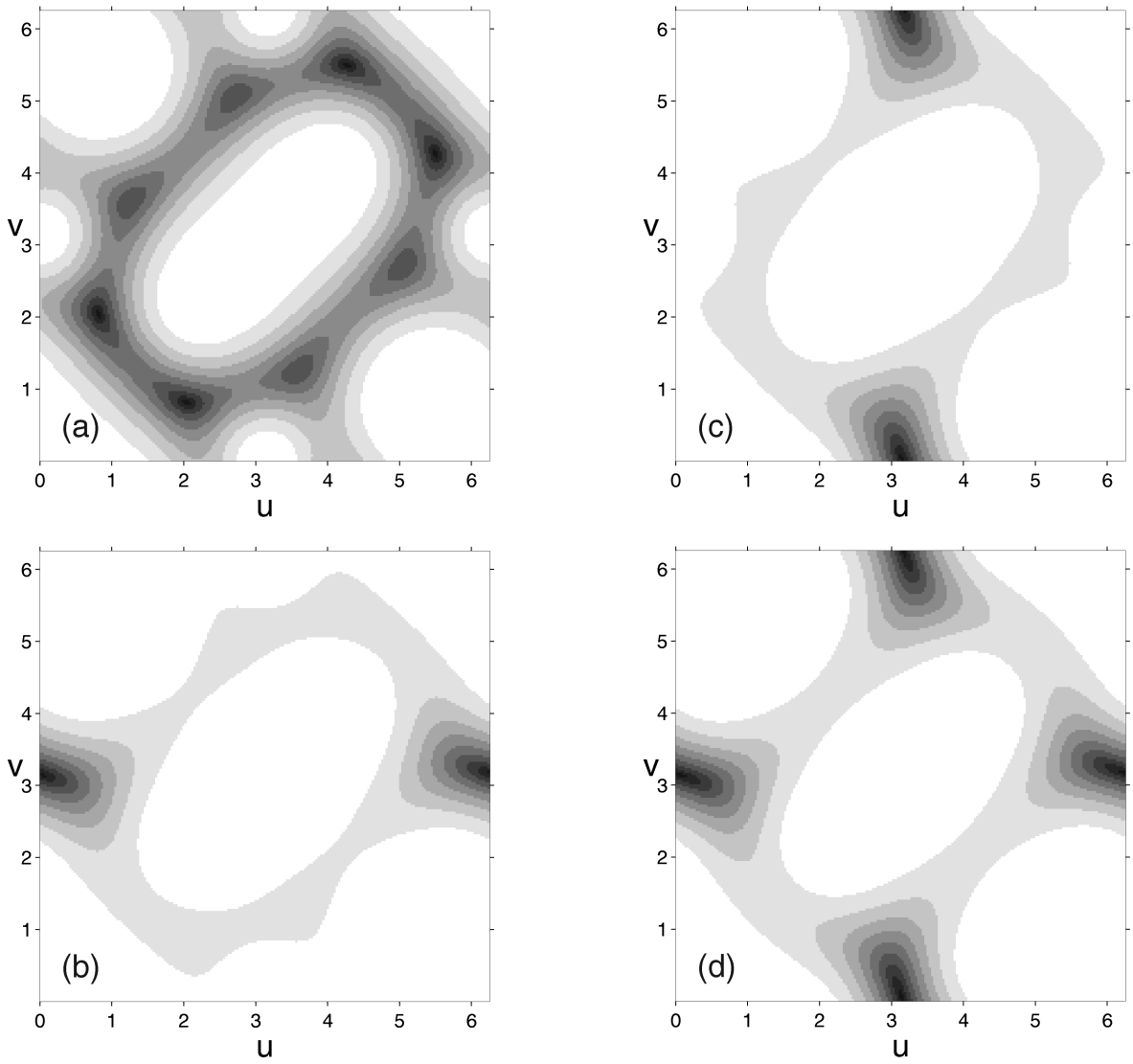

FIG. 3. Similar to Fig. 2, but for band $b=5$ with Chern index $\sigma_5=0$. Despite the fact that $\sigma_5=0$, we observe strong sensitivity to variations in $\mathbf{w}$, as in the case of Fig. 2. In (a) $[\mathbf{w}=(0,0)]\,|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$ is concentrated on the island chain of period 8 [see Fig. 1(b)]. Notice that the localization regions in the case of plots (b) and (c) are reversed relative to the corresponding plots in Fig. 2. (d), on the other hand, is qualitatively similar to Fig. 2(d).

probability distribution $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$, giving the *band Husimi distribution* (BHD) for band b:

$$P_b(\mathbf{R})=\frac{1}{|T_{\mathrm{BZ}}|}\int_{T_{\mathrm{BZ}}} d\mathbf{w}|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2, \tag{12}$$

where $|T_{\mathrm{BZ}}|=4\pi^2q/p^2$ is the area of the Brillouin zone. The BHD (12) corresponds to the *minimal* smoothing of a probability distribution in the framework of a toral phase space, namely, the smoothing over the continuous range of a single band. We now show that this smoothing is sufficient to make the BHD more classical than an individual Husimi distribution $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$ in several aspects. First, we notice from Eqs. (3) that $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$ is periodic only with unit cell T_Q^2, i.e., the quantum phase space, which differs from the classical one T^2 whenever $q\neq 1$. Now, using the relation [10]

$$\hat{D}(-2\pi s)|\Psi_{b,\mathbf{w}}\rangle=\exp(isw_2/\rho)|\Psi_{b,w_1-2\pi s,w_2}\rangle$$

(s integer) as well as Eq. (11) in Eq. (12), we easily find that

$$P_b(\mathbf{R})=\frac{1}{q}\sum_{s=0}^{q-1} P_b^{(q)}(u+2\pi s,v), \tag{13}$$

where $P_b^{(q)}(\mathbf{R})$ is defined as in Eq. (12), but the integral is performed over $1/q$ of the BZ, i.e., $0\leqslant w_1,w_2<2\pi/p$, and $|T_{\mathrm{BZ}}|$ is replaced by $|T_{\mathrm{BZ}}|/q$. It is then clear from Eq. (13) that $P_b(\mathbf{R})$, unlike $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$, is periodic with unit cell T^2 for *general* q. This allows one to impose on $P_b(\mathbf{R})$ the normalization condition

$$\int_{T^2} d\mathbf{R}\,P_b(\mathbf{R})=1. \tag{14}$$

This makes $P_b(\mathbf{R})$ analogous to a classical probability distribution on the classical phase space T^2.

Second, $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$ always assumes p zeros $\mathbf{R}_{0,j}(\mathbf{w})$ ($j=1,\ldots,p$) in T_Q^2 (see Sec. II). These zeros give $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$

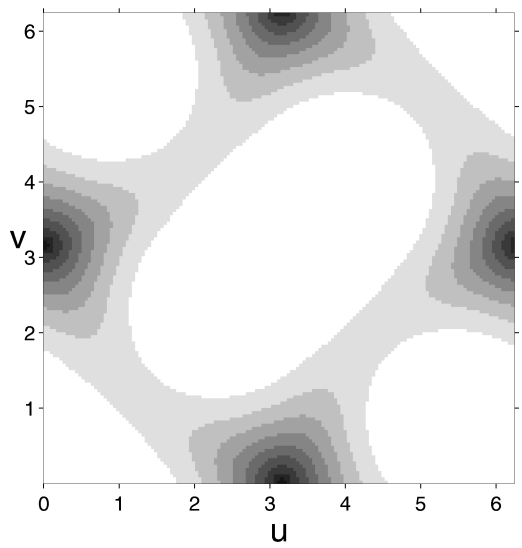

FIG. 4. Band Husimi distribution (BHD) for the case considered in Fig. 2 ($b=6$). The BHD was calculated by averaging $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$ over 20×20 values of $\mathbf{w}$, uniformly distributed in the BZ. This BHD, with a localization region similar to that of Figs. 2(a) and 2(d), is close to a classical probability distribution for the stochastic layer in Fig. 1(b) (see the text).

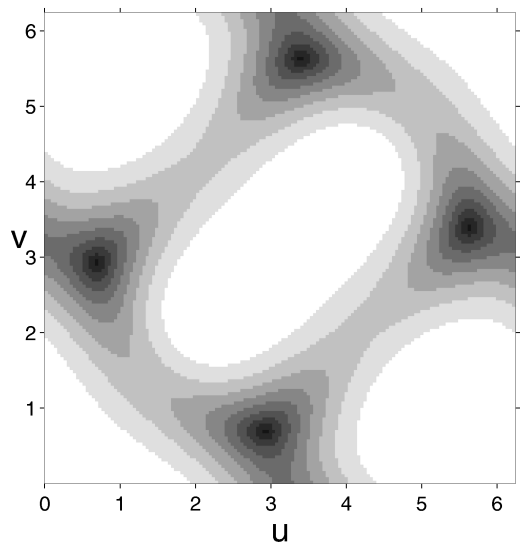

FIG. 5. Similar to Fig. 4, but for the case considered in Fig. 3 ($b=5$). The BHD appears to be concentrated on four of the six islands of an island chain of period 6, surrounding the main island chain of this period in Fig. 1(b). The localization region for this BHD is representative for band $b=5$ but is qualitatively different from that of $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$ for all the special values of $\mathbf{w}$ considered in Fig. 3.

a rather ''nonclassical'' appearance, for example, they do not allow $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$ to approach, in the semiclassical limit, the microcanonical uniform distribution in the chaotic region (strong-chaos regime) [8,28]. On the other hand, the BHD *never vanishes* in the phase space [$P_b(\mathbf{R})>0$ for all $\mathbf{R}$ in T^2], simply because the p zeros $\mathbf{R}_{0,j}(\mathbf{w})$ ($j=1,\ldots,p$) generally vary with $\mathbf{w}$ and, by definition [see Eq. (12)], a BHD involves an integration over all $\mathbf{w}$. It is therefore possible for a BHD to resemble a classical probability distribution. For example, in Fig. 4 we show the BHD for the case considered in Fig. 2 ($b=6$). The relatively high probability density near the hyperbolic points $\mathbf{R}=(\pi,0),(0,\pi)$ can be easily understood from classical considerations. The band $b=6$ corresponds to a ''broken'' separatrix orbit (that is, a homoclinic orbit in the chaotic layer) and the phase-space velocity on this orbit vanishes as one approaches the hyperbolic points. Accordingly, the approximate formula (9) suggests that the BHD should assume relatively high values near these points. Figure 5 shows that the localization region of the BHD for band $b=5$ is completely different from that of individual Husimi distributions (see Fig. 3). Although this band has $\sigma_b=0$, it exhibits strong sensitivity to variations of the BCs. The representative or dominant localization region for such a band can be found only by inspecting its BHD. In the strongly chaotic regime ($\gamma\gg 1$) and in the semiclassical limit, the BHDs are expected to approach the microcanonical uniform distribution.

Finally, consider the special but important case of bands with $\sigma_b=0$, which is possible only for $q=1$ (see Sec. II). Here an eigenstate $\Psi_{b,\mathbf{w}}(\mathbf{R})$ can always be written as a symmetry-adapted sum [20,22]

$$\Psi_{b,\mathbf{w}}(\mathbf{R})=\sum_{l_1,l_2=-\infty}^{\infty}\exp[-ip(l_1w_1+l_2w_2)]\langle\mathbf{R}|\hat{D}_1^{l_1}\hat{D}_2^{l_2}|\varphi_b\rangle, \tag{15}$$

where $\hat{D}_1$ and $\hat{D}_2$ are the basic phase-space translations (2) and $|\varphi_b\rangle$ is some square-integrable state, which is analogous to a Wannier function [20,22,24]. Inserting Eq. (15) into Eq. (12), we easily obtain the exact expression

$$P_b(\mathbf{R})=\sum_{l_1,l_2=-\infty}^{\infty}|\langle u+2\pi l_1,v+2\pi l_2|\varphi_b\rangle|^2. \tag{16}$$

While the Wannier function $\langle\mathbf{R}|\varphi_b\rangle$ is not invariant under gauge transformations in which the eigenstates are multiplied by phase factors $\exp[i\theta(\mathbf{w})]$ [24], the BHD (16) is gauge invariant. In a nearly integrable situation and in a semiclassical regime, $|\langle\mathbf{R}|\varphi_b\rangle|^2$ may be identified with the ''quasimode'' of Ref. [37], which is well localized on a classical regular orbit and, in the limit $\rho\to 0$, tends pointwise to zero outside this orbit. Similarly, the BHD (16) tends pointwise to zero outside the periodic repetition of the orbit on all unit cells (l_1,l_2). It is therefore a periodic version of the quasimode, appropriate for a toral phase space. A good approximation to the BHD should be given by the right-hand side of Eq. (9), which, like Eq. (16), is essentially independent of $\mathbf{w}$ and is periodic with unit cell T^2. The difference $Z_{b,\mathbf{w}}(\mathbf{R})\equiv|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2-P_b(\mathbf{R})$ is the sum of the overlaps of the quasimode $\langle u+2\pi l_1,v+2\pi l_2|\varphi_b\rangle$ [in unit cell (l_1,l_2)] with a quasimode in a different unit cell. The function $Z_{b,\mathbf{w}}(\mathbf{R})$ is thus of a purely quantum nature and it is entirely responsible to the p zeros of $\Psi_{b,\mathbf{w}}(\mathbf{R})$ and to the sensitivity of $\Psi_{b,\mathbf{w}}(\mathbf{R})$ to variations of $\mathbf{w}$ for $\mathbf{R}$ outside the localization domain. This clarifies the classical nature of the BHD in this case.

IV. GENERALIZED BANDS AND BHDs

In several important situations, some of which will be considered in the following sections, it is necessary to gen-

eralize the concept of BHD by smoothing over more than a single band, namely, over a set of N adjacent bands $b=b_1,\ldots,b_N$. This gives the *generalized* BHD

$$P_{b_1-b_N}(\mathbf{R})=\frac{1}{N}\sum_{b=b_1}^{b_N}P_b(\mathbf{R}). \tag{17}$$

The additional smoothing over bands should give a more classical BHD, as when smoothing over many levels in a bounded quantum system [6]. The ''maximal'' smoothing is, of course, that over all the p bands. From the completeness of the eigenstates (6), together with the normalization condition (14), we find in this case that

$$\frac{1}{p}\sum_{b=1}^{p}P_b(\mathbf{R})=\frac{1}{|T^2|},$$

where $|T^2|=4\pi^2$ is the area of the classical torus. Thus, as one could expect, the generalized BHD in this case is just the uniform distribution over phase space.

The set of N adjacent bands can be considered as a single entity, a *generalized band* (GB). One may perform arbitrary linear combinations of GB eigenstates at fixed $\mathbf{w}$ to obtain general states satisfying given BCs (3) on the torus. While these states are generally not eigenstates of the evolution operator, they are ''almost stationary'' provided the energy or quasienergy width of the GB is sufficiently small [10]. The set of all these states, for all $\mathbf{w}$, is the space of the GB. A natural starting basis for this space is, of course, the set of N eigenstates $\Psi_{b,\mathbf{w}}(\mathbf{R})$, $b=b_1,\ldots,b_N$, at each fixed value of $\mathbf{w}$. An arbitrary basis will then be given by

$$\overline{\Psi}_{n,\mathbf{w}}(\mathbf{R})=\sum_{b=b_1}^{b_N}B_b^{(n)}(\mathbf{w})\Psi_{b,\mathbf{w}}(\mathbf{R}), \tag{18}$$

$n=1,\ldots,N$. To ensure orthonormality of the basis (18) in the new ''band index'' n, the coefficients $B_b^{(n)}(\mathbf{w})$ must form a unitary matrix. Obviously, the states (18) satisfy the BCs (3). In addition, it is natural to require that these states will satisfy quasiperiodicity conditions in $\mathbf{w}$, analogous to those of Eqs. (4) and (5), with well-defined Chern indices $\overline{\sigma}_n$. Clearly, this will be the case only if the matrix $B_b^{(n)}(\mathbf{w})$ in Eq. (18) satisfies these conditions with Chern indices $\sigma_{b,n}=\overline{\sigma}_n-\sigma_b$. The determinant of this matrix must be strictly periodic in $\mathbf{w}$; otherwise it will vanish at some $\mathbf{w}$ (see Sec. II and Ref. [32]), which cannot happen since the matrix is unitary. It follows from this that

$$\sigma_{\mathrm{GB}}\equiv\sum_{b=b_1}^{b_N}\sigma_b=\sum_{n=1}^{N}\overline{\sigma}_n. \tag{19}$$

In other words, the total Chern index σ_{GB} of the GB is ''conserved'' under the basis transformation in Eq. (18).

Another ''conservation'' law following from Eq. (18) is

$$\sum_{b=b_1}^{b_N}|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2=\sum_{n=1}^{N}|\overline{\Psi}_{n,\mathbf{w}}(\mathbf{R})|^2. \tag{20}$$

In particular, Eq. (20), when integrated over $\mathbf{w}$, implies that the generalized BHD (17) can be calculated using an arbitrary basis (18).

An important case is when one can find a new basis (18) whose Chern indices $\overline{\sigma}_n$ all vanish. Before discussing the meaning of this case, we first determine the conditions that need to be satisfied to make it possible. Because of Eq. (19), a necessary condition is clearly that $\sigma_{\mathrm{GB}}=0$. This condition is also sufficient, since if $\sigma_{\mathrm{GB}}=0$ one can always find a unitary matrix $B_b^{(n)}(\mathbf{w})$ with Chern indices $\sigma_{b,n}=-\sigma_b$ (implying that $\overline{\sigma}_n=0$ for all n). In fact, one can simply choose $B_b^{(n)}(\mathbf{w})$, $n=1,\ldots,N$, as the N orthonormal eigenvectors of an $N\times N$ Hermitian matrix that is strictly periodic in $\mathbf{w}$ and whose N homotopic invariants (Chern indices) are $-\sigma_b$, $b=b_1,\ldots,b_N$. Such a matrix can be explicitly constructed for any given set of integers σ_b with $\sigma_{\mathrm{GB}}=0$ [18]. It is worthwhile to stress here that due to the general Disphantine relation $p\sigma_b+q\mu_b=1$ [10,20] the condition $\sigma_{\mathrm{GB}}=0$ can be satisfied only if N is a multiple of q, i.e., the minimal N is $N=q$.

The fact that one can find a new basis (18) with $\overline{\sigma}_n=0$ for all n means that the GB can be viewed as ''weakly sensitive'' to variations in the BCs, despite the fact that the original Chern indices σ_b may be all different from zero. This can be expressed in a more precise way using Eq. (20). Since $\overline{\sigma}_n=0$, one can assume that $\overline{\Psi}_{n,\mathbf{w}}(\mathbf{R})$ has a finite localization domain (see Sec. II). Equation (20) then implies that the function $\Sigma_{b=b_1}^{b_N}|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$, characterizing the GB, has also a finite localization domain. In this sense, the GB exhibits weak sensitivity to variations in the BCs. Nonzero values of the Chern indices σ_b in this case only mask the true nature of the GB, which is best described in terms of the new basis. One can thus say that a GB consisting of q adjacent bands with $\sigma_{\mathrm{GB}}=0$ is analogous to a band with $\sigma_b=0$ in the case of $q=1$. In Sec. VI these ideas will be further developed in order to generalize the Chern-index characterization of the classical-quantum correspondence to the case of $q\neq 1$.

V. BHDs NEAR DEGENERACIES

In this section we show that the generalized BHD for two adjacent bands (to be denoted, for simplicity, by $b=1,2$) is approximately conserved as a nonintegrability parameter γ is slightly varied through a degeneracy point γ_0 of these bands, i.e., $\omega_1(\mathbf{w}_0)=\omega_2(\mathbf{w}_0)$ at $\gamma=\gamma_0$, where $\mathbf{w}_0$ is some isolated value of $\mathbf{w}$. This is despite the fact that the separate BHDs of the two bands usually change significantly under such variation.

Formally, the unitary evolution operator can be written as $\hat{U}=\exp[-i\hat{G}(\gamma)]$, where $\hat{G}(\gamma)$ is a Hermitian operator. The quasienergy states (6) are eigenstates of $\hat{G}(\gamma)$ with eigenvalues $\omega_b(\mathbf{w})$. Consider two values of γ, γ_1 and γ_2, very close to γ_0 and such that $\gamma_1<\gamma_0<\gamma_2$ and let us denote by $|\Psi_{b,\mathbf{w}}^{(j)}\rangle$, $j=1,2$, the eigenstates of $\hat{G}(\gamma_j)$. We assume that for γ in the interval $[\gamma_1,\gamma_2]$ (containing the degeneracy point) and for all $\mathbf{w}$, the distance between $\omega_1(\mathbf{w})$ and $\omega_2(\mathbf{w})$ is significantly smaller than the distance between any of these quasienergies and $\omega_b(\mathbf{w})$, $b\neq 1,2$. In this case, one can write, to a good approximation,

$$\Psi^{(2)}_{b',\mathbf{w}}(\mathbf{R}) \approx \sum_{b=1}^{2} B_b^{(b')}(\mathbf{w}) \Psi^{(1)}_{b,\mathbf{w}}(\mathbf{R}), \tag{21}$$

where the expansion coefficients $B_b^{(b')}(\mathbf{w})$, $b,b'=1,2$, form a 2×2 unitary matrix built from the normalized eigenvectors of the 2×2 Hermitian matrix $G_{b,b'}(\mathbf{w}) = \langle \Psi^{(1)}_{b,\mathbf{w}} | \hat{G}(\gamma_2) | \Psi^{(1)}_{b',\mathbf{w}} \rangle$. Equation (21) is thus an approximate special case of Eq. (18). Nevertheless, the general relation (19) holds exactly in this case as well. It expresses the well known conservation of the total Chern index $\sigma_1+\sigma_2$ in the passage through a degeneracy point [19,26].

From Eq. (21) we get the relation

$$|\Psi^{(1)}_{1,\mathbf{w}}(\mathbf{R})|^2 + |\Psi^{(1)}_{2,\mathbf{w}}(\mathbf{R})|^2 \approx |\Psi^{(2)}_{1,\mathbf{w}}(\mathbf{R})|^2 + |\Psi^{(2)}_{2,\mathbf{w}}(\mathbf{R})|^2, \tag{22}$$

which is an approximate special case of Eq. (20). After integrating Eq. (22) over the entire BZ, we obtain the approximate conservation law for the generalized BHD of the two bands:

$$P^{(1)}_{1,2}(\mathbf{R}) \approx P^{(2)}_{1,2}(\mathbf{R}).$$

As a first, instructive example, we consider the degeneracy between bands $b=3,4$ in the KH model with $\rho=1/11$ for $\gamma=\gamma_0\approx 0.264$ (see Ref. [9]). For $\gamma=\gamma_1=0.26<\gamma_0$, the Chern indices of the two bands are, respectively, $\sigma_3=\sigma_4=0$, while for $\gamma=\gamma_2=0.2645>\gamma_0$ they change to $\sigma_3=-\sigma_4=2$ [35]. For $\gamma=\gamma_3\approx 0.2653$, the Chern indices reassume the values $\sigma_3=\sigma_4=0$ due to a second degeneracy between the two bands. Thus, for both $\gamma=\gamma_1$ and $\gamma=\gamma_3$, one can associate Wannier functions $\langle \mathbf{R}|\varphi_b\rangle$ with these bands, as in Eq. (15). These functions are expected to be localized on classical regular orbits (tori), such as those shown in Fig. 1(b). Our numerical results indicate that $\langle \mathbf{R}|\varphi_b\rangle$ for $b=3$ ($b=4$) at $\gamma=\gamma_3$ is essentially the same as $\langle \mathbf{R}|\varphi_b\rangle$ for $b=4$ ($b=3$) at $\gamma=\gamma_1$. This ''exchange'' of Wannier functions in the passage through the degeneracy can be understood as follows. Sufficiently far from the degeneracy region the bands vary almost linearly as a function of γ (see Fig. 11 in Ref. [9]) and are well approximated by a primitive semiclassical quantization of the two tori on which the functions $\langle \mathbf{R}|\varphi_b\rangle$, $b=3,4$, are localized. Near the degeneracy region, however, the actual band structure results from an ''avoided crossing'' between the two bands [see Fig. 12(a) in Ref. [9]], leading to the exchange phenomenon. In Fig. 6(a) we plot the BHDs for the two bands along the symmetry line $u=v$ for $\gamma=\gamma_1$. These BHDs exhibit, essentially, the profiles of the two Wannier functions. A similar plot for $\gamma=\gamma_2$ (between the two degeneracies) is shown in Fig. 6(b). It is evident that the BHDs have changed significantly following the small variation in γ from γ_1 to γ_2. However, Fig. 6(c) shows that the generalized BHD for the two bands is conserved to high accuracy under this variation. This BHD, associated with a GB having a total Chern index $\sigma_{\mathrm{GB}}=0$ (see Sec. IV), corresponds essentially to a ''superposition'' of the two Wannier functions. Between the two degeneracies, the GB can be still described by Wannier functions, associated with a new basis (18) with $\bar{\sigma}_n=0$.

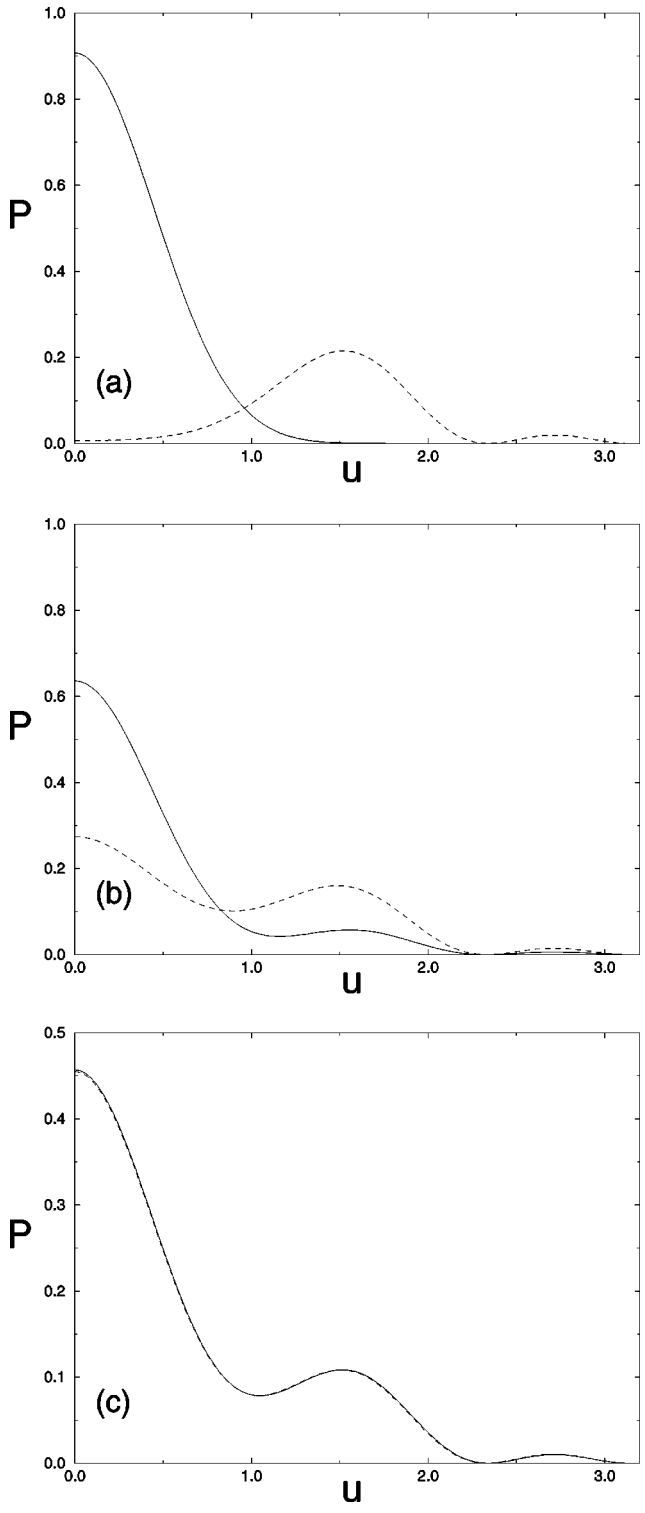

FIG. 6. (a) BHDs along the symmetry line $u=v$ for bands $b=3$ (solid line) and $b=4$ (dashed line) in the case of the KH model with parameters $\gamma=0.26$ and $\rho=1/11$. The BHDs were calculated by averaging $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$ over 100×100 values of $\mathbf{w}$ uniformly distributed in the BZ. (b) Similar to (a), but for $\gamma=0.2645>\gamma_0\approx 0.264$, where γ_0 is a degeneracy point for bands $b=3,4$. Notice the dramatic change of the BHDs relative to those of case (a), despite the small variation in γ through the degeneracy point. (c) Generalized BHD for bands $b=3,4$, obtained by averaging the results for the two bands in case (a) (solid line) and in case (b) (dashed line).

As a second example we consider a GB with $\sigma_{GB} \neq 0$ in the same model ($\rho = 1/11$). For $\gamma = \gamma_0 \approx 0.3387$, a degeneracy between the bands $b = 5$ and $b = 6$ takes place. Due to the special symmetries of the KH model [8], a degeneracy between bands $b = 6$ and $b = 7$ must occur at precisely the same value of γ_0 but at a different value of $\mathbf{w}_0$. As γ is varied through γ_0, the Chern indices of bands $b = 5,7$ both change from $\sigma_b = 0$ to $\sigma_b = -1$, while σ_6 changes from $\sigma_6 = 1$ to $\sigma_6 = 3$. The BHDs for all these bands are shown in Figs. 7(a) (for $\gamma < \gamma_0$) and 7(b) (for $\gamma > \gamma_0$). Since the bands $b = 5,6,7$ degenerate at the same value of γ_0, it is clear from our previous analysis that only the generalized BHD of all these three bands can be expected to be approximately conserved in the passage through the degeneracy point. In fact, Fig. 7(c) shows that this BHD, associated with a GB having $\sigma_{GB} = 1$, is conserved with significantly better accuracy than in the case of Fig. 6(c).

VI. BHDs UNDER SMALL VARIATIONS OF ρ

In this section we show how to define generalized BHDs for $q \neq 1$ that are continuous under small variations of ρ on the rational numbers. The topological characterization of the classical-quantum correspondence in the torus is then generalized to $q \neq 1$. We shall use the renormalization-group approach of Wilkinson [23,24], which was applied to the investigation of the spectrum of a general class of time-independent Hamiltonians on the torus. In what follows we assume that the generator $\hat{G}$ of the evolution operator $\hat{U} = \exp(-i\hat{G})$ belongs to this class of Hamiltonians.

We first briefly summarize the main results of Refs. [23,24]. Let $\rho' = q'/p'$ be a rational number sufficiently close to $\rho = q/p$ and such that $p' \gg p$. The p' bands for $\rho' = q'/p'$ can then be grouped into p ''clusters'' of adjacent bands, where each cluster is associated in a natural way with a band b for $\rho = q/p$. Namely, the energy or quasienergy interval covered by the bands in the cluster is relatively close to that covered by band b; in addition, the total Chern index of the cluster is equal to σ_b,

$$\sigma(C_b) \equiv \sum_{b'=d(b)}^{d(b)+N_b-1} \sigma'_{b'} = \sigma_b , \tag{23}$$

where C_b denotes the cluster corresponding to band b, $d(b)$ is the label of the lowest band in the cluster, N_b is the number of bands in the cluster, and $\sigma'_{b'}$ is a Chern index for $\rho' = q'/p'$. The spectrum and eigenstates in cluster C_b can be approximately calculated from an effective Hamiltonian H_{eff} obtained by properly quantizing the band function $\omega_b(\mathbf{w})$. The effective scaled $\hbar$ in this quantization turns out to be

$$\rho_{\text{eff}} = \frac{q_{\text{eff}}}{p_{\text{eff}}} = \frac{pq' - p'q}{p'\sigma_b + q'\mu_b} , \tag{24}$$

where μ_b is the integer uniquely determined from the Diophantine equation $p\sigma_b + q\mu_b = 1$. It is easy to show that the numerator and denominator in the last fraction in Eq. (24) are relatively prime integers. Equation (24) then implies a simple formula for the number of bands in the cluster, $N_b = p_{\text{eff}}$,

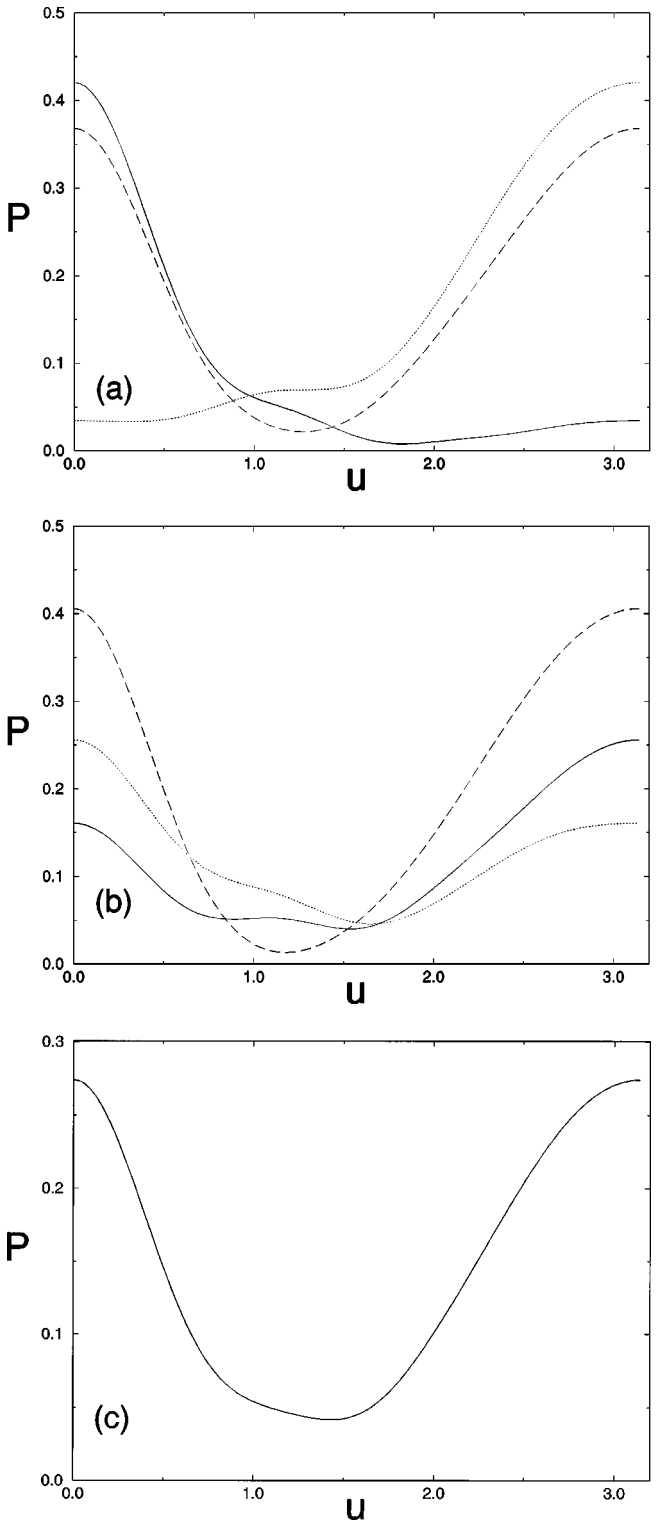

FIG. 7. (a) Similar to Fig. 6(a), but for the bands $b = 5$ (solid line), $b = 6$ (dashed line), and $b = 7$ (dotted line) in the case of $\gamma = 0.3385 < \gamma_0 \approx 0.3387$, where γ_0 is a degeneracy point of all the three bands. (b) Similar to (a), but for $\gamma = 0.339 > \gamma_0$. (c) Generalized BHD for bands $b = 5,6,7$, obtained by averaging the results for the three bands in case (a) (solid line) and in case (b) (dashed line, essentially indistinguishable from the solid line).

$$N_b = p'\sigma_b + q'\mu_b . \tag{25}$$

Now, the existence of an approximate effective Hamiltonian $H_{\rm eff}$ for a cluster means that the space of states in band b approximately coincides with the space of states in the N_b bands of cluster C_b. Provided ρ' is sufficiently close to ρ, any state in the cluster is well approximated by a linear combination of states that belong only to band b. This fact is expressed concisely by the statement that the projection operator for band b is approximately equal to that for cluster C_b:

$$\frac{1}{|T_{\rm BZ}|}\int_{T_{\rm BZ}} d\mathbf{w}|\Psi_{b,\mathbf{w}}\rangle\langle\Psi_{b,\mathbf{w}}| \approx \mathcal{N}\sum_{b'=d(b)}^{d(b)+N_b-1}\frac{1}{|T'_{\rm BZ}|}\int_{T'_{\rm BZ}} d\mathbf{w}'|\Psi'_{b',\mathbf{w}'}\rangle\langle\Psi'_{b',\mathbf{w}'}|, \tag{26}$$

where all the primed quantities refer to ρ' and $\mathcal{N}$ is a normalization constant that remains to be determined. Let us assume, for simplicity, that the phase-space variables $\mathbf{R}'=(u',v')$ for ρ' ($[\hat{u}',\hat{v}']=2\pi i\rho'$) are related to the variables $\mathbf{R}=(u,v)$ for ρ by $\mathbf{R}'=\sqrt{\rho/\rho'}\,\mathbf{R}$. Using then the expressions in Eqs. (6) and (8) for both ρ and ρ', we immediately obtain from Eq. (26) that

$$\begin{aligned} P_b(\mathbf{R}) &= \frac{1}{|T_{\rm BZ}|}\int_{T_{\rm BZ}} d\mathbf{w}|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2 \\ &\approx \frac{1}{N_b}\sum_{b'=d(b)}^{d(b)+N_b-1}\frac{1}{|T'_{\rm BZ}|}\int_{T'_{\rm BZ}} d\mathbf{w}'|\Psi'_{b',\mathbf{w}'}(\mathbf{R}')|^2 \\ &= P'_{C_b}(\mathbf{R}'), \end{aligned} \tag{27}$$

where the constant $\mathcal{N}$ in Eq. (26) has been determined as $\mathcal{N}=1/N_b$ from the normalization condition (14). Equation (27) shows that the BHD $P_b(\mathbf{R})$ for band b is approximately equal to the generalized BHD $P'_{C_b}(\mathbf{R}')$ for the cluster C_b. In the limit $\rho'\to\rho$, the space of the cluster becomes identical to that of band b [the approximate equality in Eq. (26) is replaced by an equality] and $P'_{C_b}(\mathbf{R}')\to P_b(\mathbf{R})$. This expresses the continuity of the generalized BHD, associated with clusters C_b, under small variations of ρ on the rationals.

The most important reference values of ρ are, of course, those with $q=1$ (i.e., $\rho=1/p$), for which the topological characterization of the classical-quantum correspondence on the torus is well established [8–10]. Using the analysis in the preceding paragraph, this characterization can be easily extended to rational values $\rho'=q'/p'$ ($q'\neq 1$) sufficiently close to $\rho=1/p$. Consider first the case of $\sigma_b=0$, with eigenstates localized on a regular classical orbit and exhibiting weak sensitivity to variations in the BCs. Here the Diophantine equation $p\sigma_b+q\mu_b=1$ ($q=1$) implies that $\mu_b=1$. Then, from Eq. (25), the corresponding cluster C_b consists simply of $N_b=q'$ bands with total Chern index $\sigma(C_b)=0$ [see Eq. (23)]. As shown in Sec. IV, one can find for such a cluster (or generalized band) a new basis (18) whose effective Chern indices all vanish. The cluster can then be viewed as exhibiting weak sensitivity to variations in the BCs, in analogy to the single band b. In addition, because of Eq. (27), the generalized BHD for the cluster is approximately equal to the BHD for band b and is therefore localized on the same classical regular orbit. In the case of $\sigma_b\neq 0$, the number N_b of bands in the cluster is generally different from q' and varies with b. However, the Chern index $\sigma(C_b)$ of the cluster is still equal to σ_b [Eq. (23)] and, like the single band b, the cluster exhibits strong sensitivity to variations in the BCs, in the sense that a new basis (18) whose effective Chern indices all vanish does not exist (see Sec. IV). If the BHD for band b is spread over the classically chaotic region, the same will be true for the generalized BHD of the cluster. The topological characterization of the classical-quantum correspondence on the torus is thus generalized to ρ' sufficiently close to $\rho=1/p$ by replacing single bands b with the corresponding clusters C_b.

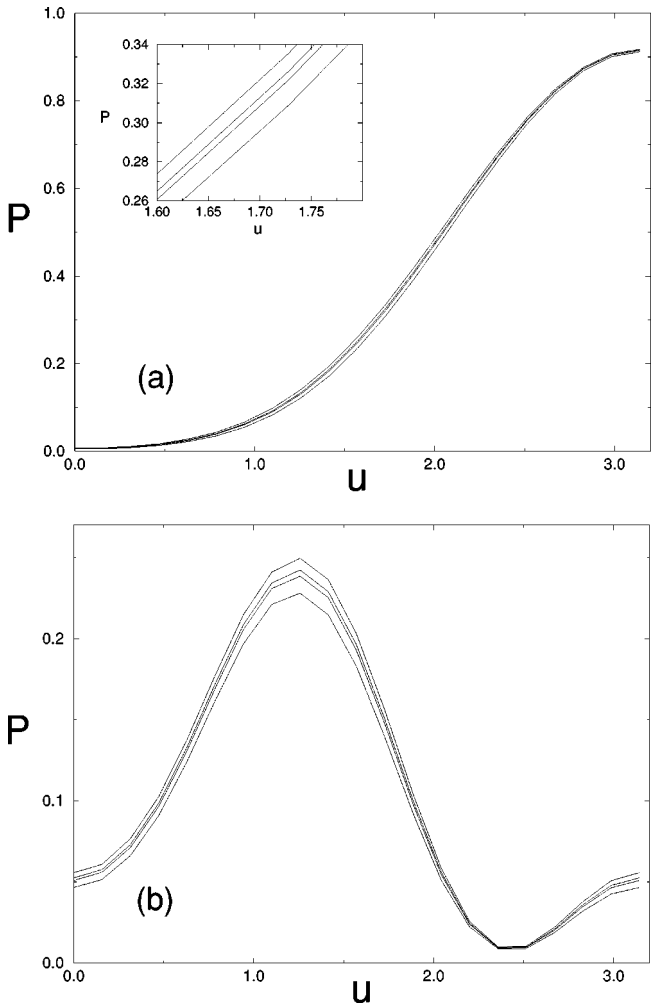

FIG. 8. BHDs along the symmetry line $u=v$ for bands and clusters of bands in the KH model with nonintegrability parameter $\gamma=0.3$. (a) The upper curve (see a magnification in the inset) is the BHD for band $b=1$ in the case of $\rho=1/5$. The other three curves are the generalized BHDs for the corresponding cluster C_b in the cases of $\rho=6/31,4/21,2/11$, in order of descending curves (see also the inset). (b) Similar to (a), but for the central band $b=3$. In both cases, the BHDs were calculated by averaging $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$ over 400×400 values of $\mathbf{w}$ uniformly distributed in the BZ.

As an example, we consider the case of $\rho=1/5$ for the KH model with $\gamma=0.3$. While for this value of γ the chaotic region occupies a significant portion of the phase space (see Fig. 1), the Chern indices turn out to be the same as in the

integrable limit (Harper model), i.e., $\sigma_b=0$ for $b=1,2,4,5$ (''regular-motion'' bands) and $\sigma_3=1$ (''chaotic-motion'' band). Similarly, for three rational approximants ρ' of ρ, $\rho'=2/11,4/21,6/31$, the Chern indices are the same as those in the Harper model [17] (however, the quasienergy spectra and states are, of course, completely different from those in the integrable limit). Using then formula (25), we find for these values of ρ' that $N_b=q'$ for $b=1,2,4,5$ while $N_b=q'+1$ for $b=3$. Figure 8(a) shows the BHD $P_b(\mathbf{R})$ for $b=1$ and the corresponding generalized BHDs $P'_{C_b}(\mathbf{R}')$, calculated using Eq. (27), along the symmetry line $u=v$. Similar results for $b=3$ are shown in Fig. 8(b). The convergence of $P'_{C_b}(\mathbf{R}')$ to $P_b(\mathbf{R})$ as ρ' approaches ρ is clear in both cases.

VII. CONCLUSIONS

The framework of quantum dynamics on a toral phase space offers the possibility of classifying the eigenstates as regular or chaotic according to their sensitivity to variations in the boundary conditions, i.e., variations of the quasicoordinate $\mathbf{w}$ in the Brillouin zone. A measure of this sensitivity for a given band b is the Chern index σ_b, which determines the quasiperiodicity conditions (4) and (5) satisfied by the band eigenstates. Provided ρ (the scaled $\hbar$) assumes a rational value of the form $1/p$ (p being a sufficiently large integer), eigenstates well localized on regular classical orbits belong to bands with $\sigma_b=0$. On the other hand, eigenstates concentrated in chaotic regions of the phase space usually belong to bands with $\sigma_b\neq 0$.

By definition, σ_b characterizes the entire band b, rather than individual eigenstates. The Chern-index classification into regular or chaotic refers then to bands and not to eigenstates. It is also well known [8,10] that σ_b can be expressed as a uniform average over $\mathbf{w}$ in the BZ:

$$\sigma_b=\frac{i}{2\pi}\int_{T_{\mathrm{BZ}}} d\mathbf{w}\int_{T_Q^2} d^2\mathbf{R}\left[\frac{\partial\Psi^*_{b,\mathbf{w}}(\mathbf{R})}{\partial w_1}\,\frac{\partial\Psi_{b,\mathbf{w}}(\mathbf{R})}{\partial w_2}-\frac{\partial\Psi^*_{b,\mathbf{w}}(\mathbf{R})}{\partial w_2}\,\frac{\partial\Psi_{b,\mathbf{w}}(\mathbf{R})}{\partial w_1}\right], \tag{28}$$

where $\Psi_{b,\mathbf{w}}(\mathbf{R})$ is the coherent-state representation of the eigenstate $|\Psi_{b,\mathbf{w}}\rangle$. These observations motivate one to introduce other global characterizations of the bands that take into account all the BCs only in an average sense, thus resolving the ambiguity in the choice of a particular BC. These additional characterizations should provide a more detailed description of the classical-quantum correspondence on the torus without referring to the individual, nonclassical BCs.

In this paper we have introduced and studied one such characterization, the band Husimi distribution, given by the uniform average of $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$ over $\mathbf{w}$. The BHD may be viewed as the representative Husimi distribution for ''level'' b and is expected to be closer to a classical probability density than $|\Psi_{b,\mathbf{w}}(\mathbf{R})|^2$. This expectation was shown to be fulfilled in several aspects in Sec. III. The BHD concept plays an important role in extending the Chern-index characterization of the classical-quantum correspondence to rational values of ρ with numerators larger than 1 (see Sec. VI). In this case, a generalized version of the BHD has to be introduced (see Sec. IV), given by the average of the BHDs associated with a cluster of adjacent bands for $\rho'=q'/p'\approx 1/p$.

Smoothing a quantum probability distribution over a range of energy levels is important in the theoretical study of scars using the semiclassical periodic-orbit theory [5,6]. In the case of the BHD, this smoothing is performed over the continuous range of one band, corresponding essentially to a single level in the framework of a toral phase space. Using the adaptation of periodic-orbit theory to this framework [12], it may be possible to achieve a better understanding of the nature of BHDs and generalized BHDs in the semiclassical limit.

An important question is to what extent information about the individual band eigenstates can be recovered from the BHD. We recall here the well known fact in solid-state physics that all the Bloch eigenstates in a band can be simply reproduced from the corresponding Wannier function. Thus, in this case, no information about the individual eigenstates is lost by averaging over them (the average being the Wannier function). The relation (15), valid only for $\sigma_b=0$, is analogous to the formula expressing the Bloch eigenstates in terms of the Wannier function. In this case, the relation (16) shows that the BHD is closely related to the absolute value squared of a Wannier function. This relation may be extended to $\sigma_b\neq 0$ using results from Ref. [24]. It was also shown recently [38] that the Wigner functions of all of the band eigenstates can be reproduced from the Wigner analog of the BHD. On the basis of these observations, we expect that it should be possible to recover, at least partially, relevant information about the individual eigenstates from the BHDs. This will be investigated in future works.

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