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Quantum Mechanical Cumulant Dynamics near Stable Periodic Orbits in Phase Space

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We formulate a general method for the study of semiclassical-like dynamics in stable regions of a mixed phase-space. In the simplest case, this involves determining stable Gaussian wavepacket solutions, and then propagating them using a cumulant-based formalism. We apply our method to the problem of quantum accelerator modes, determining their relative longevity under different parameter regimes, and obtaining good qualitative agreement with exact wavefunction dynamics.

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Semiclassical approaches in quantum chaotic dynamics have proved very successful in forging conceptual links between classically chaotic systems and their quantum mechanical counterparts [1]. When trying to include quantum mechanical effects, an obvious step beyond point-particle dynamics is to consider the evolution of Gaussian wavepackets. Straightforward semiclassical Gaussian wavepacket dynamics are limited in that, e.g., the wavepacket is unrealistically forced to maintain its Gaussian form. Pioneering work by Huber, Heller, and Littlejohn [2] proposed remedying this by allowing complex classical trajectories. These also permit the study of a wider range of classically forbidden processes, and the propagation of superpositions of Gaussians. We propose an alternative approach, which, most simply, is to follow the dynamics of the cumulants of initially Gaussian wavepackets. When taken to second order, the dynamics are described purely in terms of means and variances, as in a Gaussian wavepacket, but evolution into non-Gaussian wavepackets is not proscribed. After developing the formalism, we apply it to an exciting development in atom-optical studies of quantum-nonlinear phenomena: quantum accelerator modes (QAM) [3, 4, 5, 6, 7, 8, 9]. Quantum accelerator modes have proved to be a fascinating example of a robust quantum resonance effect, and the demonstrated coherence of their formation [6] promises important applications in coherent atom optics [4, 10]. In a configuration consisting of a laser cooled cloud of freely falling cesium atoms subjected to periodic δ -like kicks from a vertically oriented off-resonant laser standing wave [3, 4, 5, 6, 7, 8], QAM are characterized experimentally by a momentum transfer, linear with kick number, to a substantial fraction (up to $\sim 20\%$) of the initial cloud of atoms. This system is also attractive in that it is possible to tune its effective classicality in an accessible regime far from the true semiclassical limit, making it an ideal testing ground for semiclassical theories. We use our approach to obtain insight into the relative longevity of QAM, and present very encouraging results on its utility.

We consider two conjugate self-adjoint operators: $\hat{\xi}$ and $\hat{\zeta}$, such that $[\hat{\xi}, \hat{\zeta}] = i\eta$, and a Hamiltonian $\hat{H}(\hat{\xi}, \hat{\zeta})$. The dynamics of these operators can be fully described by the expectation

values $\mu_\xi = \langle \hat{\xi} \rangle$ and $\mu_\zeta = \langle \hat{\zeta} \rangle$ only as $\eta \rightarrow 0$. In this limit there is a well-defined $\{\xi, \zeta\}$ phase space, which generally consists of a mixture of stable islands based around stable periodic orbits, and a chaotic sea. This is the case for our model example, the δ -kicked accelerator (see Fig. 1) [5].

When considering dynamics near a stable periodic orbit in phase space, we use that: local dynamics approximate those of a harmonic oscillator [11], and Gaussian wavepackets remain Gaussian when experiencing harmonic dynamics. This motivates the initial use of a Gaussian ansatz of the form [2, 12]

$$\psi(\xi) = (2\pi\sigma_\xi^2)^{-1/4} \times \exp\left(-\frac{[1 - i2\sigma_{\xi\zeta}^2/\eta][\xi - \mu_\xi]^2}{4\sigma_\xi^2} + \frac{i\mu_\zeta[\xi - \mu_\xi]}{\eta}\right), \quad (1)$$

where $\sigma_\xi^2 = \langle \hat{\xi}^2 \rangle - \langle \hat{\xi} \rangle^2$ is the variance in $\hat{\xi}$, and $\sigma_{\xi\zeta}^2 = \langle \hat{\xi}\hat{\zeta} + \hat{\zeta}\hat{\xi} \rangle/2 - \langle \hat{\xi} \rangle \langle \hat{\zeta} \rangle$ is the symmetrized covariance in $\hat{\xi}$ and $\hat{\zeta}$. As Eq. (1) describes a minimum uncertainty wavepacket, the $\hat{\zeta}$ variance, $\sigma_\zeta^2 = \langle \hat{\zeta}^2 \rangle - \langle \hat{\zeta} \rangle^2$, can be deduced from the general uncertainty relation $\sigma_\xi^2 \sigma_\zeta^2 - (\sigma_{\xi\zeta}^2)^2 = \eta^2/4$ [this can be seen from Eq. (1), using $-i\eta\partial/\partial\xi$ as the $\hat{\zeta}$ representation of $\hat{\zeta}$]. If the stable islands around the periodic orbits of interest are significant compared to the size of a minimum uncertainty wavepacket, we find stable periodic orbits in $\{\mu_\xi, \mu_\zeta, \sigma_\xi^2, \sigma_{\xi\zeta}^2\}$ when such a Gaussian ansatz is enforced. In reality this stability is only approximate, but we will nevertheless utilize such solutions, as they are good estimates to maximally stable Gaussian wavepackets.

A complete picture of the observable dynamics can only be determined from the time-evolution of all possible expectation values of products of the dynamical variables. Except for very simple systems, this produces a complicated hierarchy of coupled equations. In order to gain any insight we must determine a truncation scheme to reduce this to a manageable description. This is in a sense achieved by the Gaussian ansatz, which considers only means and variances. Means and variances are the first two orders of an infinite hierarchy of cumulants [13], which we denote by double angle brackets to distinguish

them from expectation values. The non-commutative cumulants can be obtained directly in terms of operator expectation values through [14]

$$\langle\langle \hat{q}_1 \cdots \hat{q}_n \rangle\rangle = \frac{\partial}{\partial \tau_1} \cdots \frac{\partial}{\partial \tau_n} \ln \langle e^{\tau_1 \hat{q}_1} \cdots e^{\tau_n \hat{q}_n} \rangle |_{\tau_1=0, \dots, \tau_n=0}, \quad (2)$$

where $\hat{q}_i \in \{\hat{\xi}, \hat{\zeta}\}$. More conveniently, the expectation values can be expressed in terms of cumulants:

$$\begin{aligned} \langle \hat{q}_1 \rangle &= \langle\langle \hat{q}_1 \rangle\rangle, \\ \langle \hat{q}_1 \hat{q}_2 \rangle &= \langle\langle \hat{q}_1 \hat{q}_2 \rangle\rangle + \langle\langle \hat{q}_1 \rangle\rangle \langle\langle \hat{q}_2 \rangle\rangle, \\ \langle \hat{q}_1 \hat{q}_2 \hat{q}_3 \rangle &= \langle\langle \hat{q}_1 \hat{q}_2 \hat{q}_3 \rangle\rangle + \langle\langle \hat{q}_1 \rangle\rangle \langle\langle \hat{q}_2 \hat{q}_3 \rangle\rangle + \langle\langle \hat{q}_2 \rangle\rangle \langle\langle \hat{q}_1 \hat{q}_3 \rangle\rangle \\ &\quad + \langle\langle \hat{q}_3 \rangle\rangle \langle\langle \hat{q}_1 \hat{q}_2 \rangle\rangle + \langle\langle \hat{q}_1 \rangle\rangle \langle\langle \hat{q}_2 \rangle\rangle \langle\langle \hat{q}_3 \rangle\rangle, \dots, \end{aligned} \quad (3)$$

where the ordered observables have been partitioned in all possible ways into products of cumulants. Cumulants tend to become smaller with increasing order, unlike expectation values; intuitively, higher-order cumulants encode only an ‘extra bit’ of information that lower-order cumulants have not yet provided. It is therefore often possible to provide a good description by systematically truncating, expressing moments of all orders in terms of cumulants up to some finite order [14]. Truncating at first order is equivalent to considering only mean values, and thus reproduces the corresponding Hamilton’s equations of motion. It is tempting to think that truncating at second order is equivalent to enforcing the Gaussian ansatz. This will not in general reproduce the dynamics given by enforcing the Gaussian ansatz. Gaussian wavepacket dynamics are unitary, meaning that the uncertainty relation is always exactly observed, and that one need consider only two of $\{\sigma_\xi^2, \sigma_\zeta^2, \sigma_{\xi\zeta}^2\}$. This is only true when no terms in the Hamiltonian are of greater than quadratic order in $\{\hat{\xi}, \hat{\zeta}\}$ [2]. Furthermore, finding a fixed point of $\{\mu_\xi, \mu_\zeta, \sigma_\xi^2, \sigma_{\xi\zeta}^2\}$ is equivalent to finding a perfectly Gaussian eigenstate of the system, which is only true for the harmonic oscillator.

When propagating the second-order truncated equations of motion for the first and second order cumulants, it is necessary to consider the dynamics of each of $\{\sigma_\xi^2, \sigma_\zeta^2, \sigma_{\xi\zeta}^2\}$ explicitly, as, unlike for the Gaussian ansatz [Eq. (1)], the uncertainty relation is not hard-wired into the formalism. This implies that the evolution described solely in terms of the first and second order cumulants is not unitary. This feature of our approach more accurately reflects the fact that truncating generally leaves us with an incomplete description of the dynamics, with a correspondingly inevitable loss of information about the state of the system. We are also not restricted to initially pure states, although this flexibility is not exploited here.

Nonetheless, when situated inside a stable island in $\{\xi, \zeta\}$ phase space, such a ‘stable’ Gaussian wavepacket should be long-lived due to the harmonic nature of the local dynamics [15]. We then use the equations of motion appropriate to second-order cumulant dynamics to get an idea of how long-lived the initial wavepacket actually is, as physically sensible imperfections are included in the dynamics in a straightforward manner.

The approach we have described is most obviously applicable in the standard semiclassical regime, but is not restricted to it. We will illustrate our method by applying it to a very interesting and experimentally relevant system, the quantum δ -kicked accelerator [5], outside the semiclassical regime. Our approach provides useful insights on the longevity of QAM in this system, essential for their possible application in coherent atom optics [4, 10].

The dynamics of the atoms in the Oxford QAM experiment [3, 4, 5, 6, 7, 8] are well modelled by the one-dimensional δ -kicked accelerator Hamiltonian:

$$\hat{H} = \frac{\hat{p}^2}{2m} + mg\hat{z} - \hbar\phi_d [1 + \cos(G\hat{z})] \sum_{n=-\infty}^{\infty} \delta(t - nT). \quad (4)$$

Here \hat{z} is the position, \hat{p} the momentum, m the particle mass, g the gravitational acceleration, t the time, T denotes the pulse period, $G = 2\pi/\lambda_{\text{spat}}$ where λ_{spat} is the spatial period of the potential applied to the atoms, and $\hbar\phi_d$ quantifies the depth of this potential.

The near-fulfilment of the quantum resonance condition (closeness to particular resonant pulse periodicities [4, 9, 16]) means the free evolution of a wavefunction, e.g., initially well localized in momentum and (periodic) position space immediately after it experiences a kick, causes it to rephase to close to its initial condition just before each subsequent kick. The treatment due to Fishman, Guarneri, and Rebuzzini accounts for this in terms of a so-called ϵ -classical limit [9], where a kind of kick-to-kick classical point dynamics is regained in the limit of the pulse periodicity approaching integer multiples of the half-Talbot time $T_{1/2} = 2\pi m/\hbar G^2$ [4], i.e., as $\epsilon = 2\pi(T/T_{1/2} - \ell) \rightarrow 0$, where $\ell \in \mathbb{Z}$. This accurately accounts for the observed acceleration for up to ~ 100 kicks, as well as predicting numerous experimentally observed high-order accelerator modes [7]. It is this ϵ , whose smallness indicates nearness to special resonant kicking frequencies, leading to the production of QAM [9], and not \hbar , which takes the place of η in our cumulant-based approach. We now sketch the treatment of Refs. [9] to justify the appropriate phase-space which is the starting point of our analysis, providing enough detail for the explanation to be self-contained.

Moving to a frame comoving with the gravitational acceleration [$\hat{U} = \exp(img\hat{z}t/\hbar)$], Eq. (4) transforms to:

$$H = \frac{(\hat{p} - \gamma\hat{t})^2}{2} - \kappa(1 + \cos\hat{\chi}) \sum_{n=-\infty}^{\infty} \delta(\tilde{t} - n). \quad (5)$$

We have used scaled units: $\hat{\chi} = G\hat{z}$, $\hat{p} = GT\hat{p}/m$, and $\tilde{t} = t/T$. The parameters are: the rescaled effect of gravity $\gamma = gGT^2$, and the stochasticity parameter $\kappa = \hbar\phi_d G^2 T/m = \hbar\phi_d$, where $\hbar k = \hbar G^2 T/m = 2\pi T/T_{1/2} = -i[\hat{\chi}, \hat{p}]$ is a rescaled Planck constant. As the transformed Hamiltonian is spatially periodic, we parametrize the momentum in terms of the *quasi-momentum* (in the lab frame, the *initial* quasimomentum) β , i.e., $|\rho\rangle = |(n + \beta)\hbar k\rangle$, where $n \in \mathbb{Z}$ and $\beta \in [0, 1)$. The corresponding time-dependent kick-to-kick time-evolution operator $\hat{F}_n = \int d\beta \hat{F}_n(\beta) \hat{P}(\beta)$. Here $\hat{P}(\beta)$ is a projection oper-

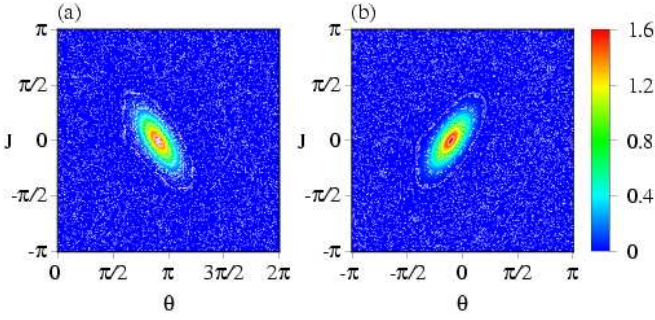


FIG. 1: (color online). Poincaré sections determined by ϵ -classical versions of Eq. (7) (white dots), superimposed on Wigner functions corresponding to single wavepackets of the form given in Eq. (1) (color density plots). Means and variances determined by Eq. (8), for $\tilde{k} = 2$ and (a) $\epsilon = -0.2$, (b) $\epsilon = 0.2$. Units are dimensionless.

ator ensuring that $\hat{F}_n(\beta)$ acts on a subspace of one value of β only, and the time-evolution of the transformed wavevector $|\psi\rangle$ is given by $|\psi(\tilde{t} = n')\rangle = \prod_{n=1}^{n'} \hat{F}_n |\psi(0)\rangle$. Substituting $\epsilon = 2\pi(T/T_{1/2} - \ell) = \tilde{k} - 2\pi\ell$,

$$\hat{F}_n(\beta) = \exp(-i[\hat{I} + \text{sgn}(\epsilon)[\pi\ell + \tilde{k}\beta - \gamma(n - 1/2)]]^2/2\epsilon) \times \exp(i\tilde{k} \cos \hat{\theta}/|\epsilon|). \quad (6)$$

Subspaces of different β are decoupled. A wavefunction contained within any such subspace is periodic, multiplied by a phase $e^{-i\beta\hat{x}}$, and can be equivalently represented by a rotor wavefunction [9]. We have therefore introduced the angle variable $\hat{\theta} = \hat{x} \text{mod}(2\pi)$ and its discrete conjugate momentum \hat{I} ($\propto \hat{p}|\epsilon|/\tilde{k}$ with a discrete spectrum of integer multiples of $|\epsilon|$), where $[\hat{\theta}, \hat{I}] = i|\epsilon|$ and $\tilde{k} = \kappa|\epsilon|/\tilde{k} = \phi_d|\epsilon|$.

The kick-to-kick Heisenberg map corresponding to the time-evolution operator of Eq. (6) is given by

$$\hat{\theta}_{n+1} = \hat{\theta}_n + \text{sgn}(\epsilon)\hat{J}_{n+1}, \quad (7a)$$

$$\hat{J}_{n+1} = \hat{J}_n - \tilde{k} \sin \hat{\theta}_n - \text{sgn}(\epsilon)\gamma, \quad (7b)$$

where we have introduced $\hat{J}_n = \hat{I}_n + \text{sgn}(\epsilon)[\pi\ell + \tilde{k}\beta - \gamma(n - 1/2)]$. We thus reduce the dynamics of each of the decoupled β -rotor subspaces to a mapping [Eq. (7)] plus a simple transformation, where the overall dynamics can be recovered by the superposition principle [9]. The general relation $[\hat{\xi}, \hat{\zeta}] = i\eta$, which we use for this specific example replaced by $[\hat{\theta}, \hat{J}] = i|\epsilon|$. Quantum accelerator modes are explained by stable periodic orbits in the $\{\theta, J\}$ phase space obtained by taking the pseudoclassical limit ($|\epsilon| \rightarrow 0$) [9], independent of what the phase space structure in the semiclassical limit ($\tilde{k} \rightarrow 0$) might be. We consider the originally discovered (1,0) accelerator modes around $T = T_{1/2}$ [3], corresponding to a fixed point of order 1 and jumping index 0 in the ϵ -classical mapping produced by replacing the operators in Eq. (7) with their mean values [9].

The quantities we consider are the mean position θ , the mean momentum J , the position variance σ^2 , the momentum

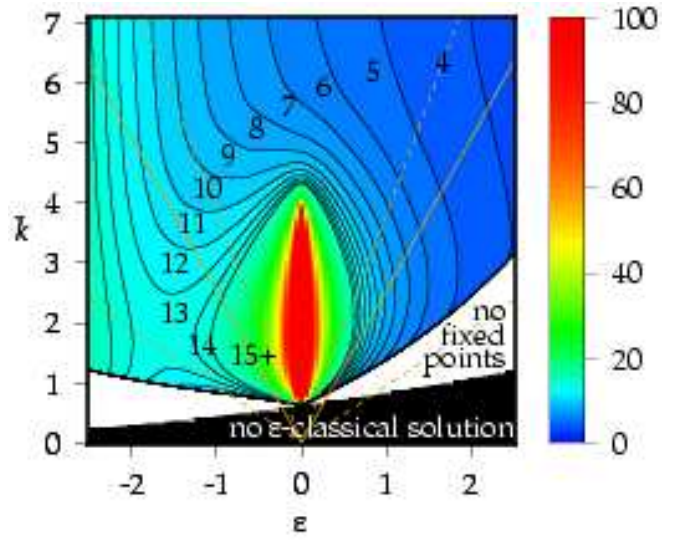


FIG. 2: (color online). Number of iterations of Eq. (9) evolved by a Gaussian stable fixed point such that $|\mathcal{J}| < \pi$. Black indicates absence of ϵ -classical stable solutions [9], white absence of Gaussian stable solutions. Numbers label the contours where $|\mathcal{J}| < \pi$ for that number of iterations (the number of iterations is capped at 100). The solid line marks the average experimental laser intensity $\phi_d = 0.8\pi$, dashes demarcate its experimental range (0.3 π –1.2 π) [6]. Units are dimensionless.

variance S^2 , and the symmetrized covariance Υ , corresponding to the general quantities $\{\mu_\xi, \mu_\zeta, \sigma_\xi^2, \sigma_\zeta^2, \sigma_{\xi\zeta}^2\}$. Enforcing the Gaussian ansatz of Eq. (1) and implicitly assuming $\sqrt{\sigma^2}$ to be small compared to 2π , the resulting kick-to-kick Gaussian mapping is given by

$$\theta_{n+1} = \theta_n + \text{sgn}(\epsilon)\mathcal{J}_{n+1}, \quad (8a)$$

$$\mathcal{J}_{n+1} = \mathcal{J}_n - \tilde{k}e^{-\sigma_n^2/2} \sin \theta_n - \text{sgn}(\epsilon)\gamma, \quad (8b)$$

$$\sigma_{n+1}^2 = \sigma_n^2 + 2\text{sgn}(\epsilon)(\Upsilon_n - \tilde{k}e^{-\sigma_n^2/2} \sigma_n^2 \cos \theta_n) + [2(\Upsilon_n - \tilde{k}e^{-\sigma_n^2/2} \sigma_n^2 \cos \theta_n)^2 + \epsilon^2]/4\sigma_n^2, \quad (8c)$$

$$\Upsilon_{n+1} = \Upsilon_n - \tilde{k}e^{-\sigma_n^2/2} \sigma_n^2 \cos \theta_n + \text{sgn}(\epsilon)[2(\Upsilon_n - \tilde{k}e^{-\sigma_n^2/2} \sigma_n^2 \cos \theta_n)^2 + \epsilon^2]/4\sigma_n^2, \quad (8d)$$

where S_{n+1}^2 can be deduced from $\sigma_{n+1}^2 S_{n+1}^2 - \Upsilon_{n+1}^2 = \epsilon^2/4$. In our search for ‘stable’ Gaussian wavepackets, we search for solutions extending the conditions $\theta_{n+1} = \theta_n$ and $\mathcal{J}_{n+1} = \mathcal{J}_n$, appropriate to an ϵ -classical fixed point, to $\sigma_{n+1}^2 = \sigma_n^2$, $S_{n+1}^2 = S_n^2$ and $\Upsilon_{n+1} = \Upsilon_n$. A Gaussian solution is thus dependent on ϵ as well as \tilde{k} and γ . We consider situations which correspond experimentally to freely varying the kicking periodicity and the laser intensity, with $\gamma = gGT^2$ determined by $T = (\epsilon + 2\pi)T_{1/2}/2\pi$, $g = 9.8 \text{ ms}^{-2}$, and $G = 2\pi/(447 \text{ nm})$. Wigner representations [13] of such ‘stable’ Gaussian wavepackets, overlaid by Poincaré sections of the ϵ -classical phase space [9], are shown in Fig. 1. We see that the Wigner functions closely match the shape of the stable island.

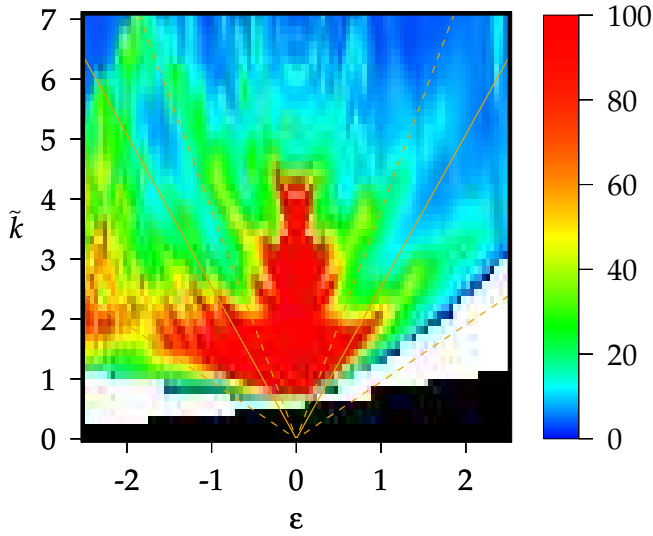


FIG. 3: (color online). As in Fig. 2, but for exact wavepacket evolutions, propagating initial conditions from Eq. (10) with the time evolution operator of Eq. (6) ($\beta = 0$). Units are dimensionless.

We now come to the central point of our analysis, propagating Gaussian fixed point solutions using the full second-order cumulant mapping, where all variances must be considered explicitly:

$$\theta_{n+1} = \theta_n + \text{sgn}(\epsilon)\mathcal{J}_{n+1}, \quad (9a)$$

$$\mathcal{J}_{n+1} = \mathcal{J}_n - \tilde{k}e^{-\sigma_n^2/2} \sin \theta_n - \text{sgn}(\epsilon)\gamma, \quad (9b)$$

$$\sigma_{n+1}^2 = \sigma_n^2 + S_{n+1}^2 + 2\text{sgn}(\epsilon)(\Upsilon_n - \tilde{k}e^{-\sigma_n^2/2}\sigma_n^2 \cos \theta_n), \quad (9c)$$

$$S_{n+1}^2 = S_n^2 - 2\tilde{k}e^{-\sigma_n^2/2}\Upsilon_n^* \cos \theta_n + \tilde{k}^2(1 - e^{-\sigma_n^2})[1 + e^{-\sigma_n^2} \cos(2\theta_n)]/2, \quad (9d)$$

$$\Upsilon_{n+1} = \Upsilon_n - \tilde{k}e^{-\sigma_n^2/2}\sigma_n^2 \cos \theta_n + \text{sgn}(\epsilon)S_{n+1}^2. \quad (9e)$$

This mapping has no fixed points. In Fig. 2, we display the time for which the center of mass momentum remains inside its initial phase space cell ($|\mathcal{J}_n| < \pi$), using this as a rule-of-thumb measure of relative longevity (for a genuine fixed point this would be forever). We see that there is a sizable region where there are no stable Gaussian fixed points, in addition to the region where there are no ϵ -classical solutions, and that QAM for $\epsilon < 0$ are generally more long-lived. These observations are broadly born out by experiment [3].

We have also computed for how long $|\mathcal{J}_n| < \pi$ when integrating the exact evolution described by Eq. (6) [5]. The computationally more convenient \mathcal{I} representation of the initial state determined by Eqs. (8a)–(8d) is then $|\psi\rangle \propto \sum_{n=-\infty}^{\infty} c_n |\mathcal{I} = n|\epsilon\rangle$, where [17]

$$c_n = \left[\frac{\sigma^2}{2\pi(\epsilon^2/4 + \Upsilon^2)} \right]^{1/4} \times \exp\left(-\frac{\sigma^2/\epsilon^2[n|\epsilon| - \mathcal{I}_0]^2}{1 - i2\Upsilon/|\epsilon|} - \frac{i\theta_0[n|\epsilon| - \mathcal{I}_0]}{|\epsilon|} \right). \quad (10)$$

This corresponds to a spatially periodic train of shifted Gaussians. Figure 3 shows the results of these integrations. We see that Fig. 2 reproduces its qualitative features quite well, especially for smaller values of ϵ and \tilde{k} . More surprising is the replication of a saddle-point feature at around $\{\epsilon = -1.5, \tilde{k} = 2\}$, indicating a resurgence of stability for large ϵ that is clearly not an artefact of our approximations.

In conclusion, we have developed a general method for using second order cumulants to study semiclassical-like dynamics near stable periodic orbits in phase space. We have successfully applied this method to quantum accelerator mode dynamics, which operate in an unusual ϵ -semiclassical regime, thus gaining insight into the longevity of quantum accelerator modes in different parameter regimes.

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