Universal turning point behavior for Gaussian-Klauder states and an application for maximally eccentric Rydberg atoms

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Universal behavior of Gaussian-Klauder states emerges near soft classical turning points, as expressed through a complex-valued Airy transformation that approximates the wave function. Study of these classical turning points provides analytic evidence that Gaussian-Klauder states generally display recurrent localization for many classical orbital periods. Analytic position and momentum moments of the wave function are determined from this approximation, leading in part to connections with the traditionally chosen positional Gaussian wave functions as the limit of large energy uncertainty. Application of this procedure to hydrogenic states of maximal eccentricity leads to the classical limit of recurrent collisional bouncing in the Kepler problem, via the explicit construction of states that maintain phase space localization for many orbital periods.

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Harmonic oscillator coherent states represent the ideal when considering classical correspondence of a quantum system. These coherent states form an overcomplete set of nondispersive, minimum uncertainty wave functions, whose position and momentum expectation values forever follow their classical trajectories [1]. Other useful properties include alternative representations of operators in coherent state space and the creation of Husimi-Wigner distributions [2–5]. Generalization of the harmonic oscillator coherent states to other systems is motivated by the promise of such properties, but typically only a subset of these properties may be self-consistently preserved. Thus, various approaches to generalized coherent states have been developed on different lines of generalization. At least two such approaches have been explored: group-theoretic and Gaussian-Klauder coherent states.

Generalized coherent states were early considered a property of the simple group structure underlying the harmonic oscillator [1], with particular applications desired for the SO(4) symmetry of the hydrogen atom. However, though the group-theoretic coherent states for hydrogen possess the useful properties of being nondispersive and localized in both eccentricity and angular momentum, they are completely delocalized along the azimuthal angle (i.e., along the classical orbit) [6]. This group-theoretic approach for hydrogen is then insufficient to construct states that share the localization properties of harmonic oscillator coherent states. Lack of localization in phase space prohibits the investigation of many questions in classical correspondence that a coherent state picture might otherwise provide.

A solution to the localization problem was realized with the Gaussian-Klauder (GK) construction [6] [to be defined in Eq. (1)]. At the expense of allowing *eventual* delocalization at some presumably distant time, the GK approach routinely provides a means for an overcomplete set of long-lived, localized states that are suitable for classical correspondence. Low dispersiveness of a state in time is ensured by an emphasis on energy localization as primary to phase space localization, a point revisited quantitatively later in this Brief Report. In its original application to the hydrogen system, this approach reduces to a straightforward superposition of the group-theoretic states to ensure localization of the wave function along the azimuthal angle [6]. GK states have since been applied to a wide variety of systems, both with and without strong group symmetry, to provide evidence that the GK coherent states are a viable means to establish classical correspondence for systems with regular spectra [7–9].

To date, the study of GK states has largely focused on these results of particular systems as a means to understand GK states in general. The present report rather establishes universal properties for a set of one-dimensional (or effectively one-dimensional) quantum systems that possess at least one soft classical turning point and need not contain any special group symmetry. By examining the evolution of the wave function near a turning point, the following text builds an analytic Airy-transform approximation that is based on linearity of the potential near this turning point. The Airy transform approximation predicts a polynomial growth in time for position and momentum variances and also predicts the appearance of Gaussians in position for increasing energy uncertainty. The report concludes with a brief example for the hydrogen atom: Rydberg coherent states of maximal eccentricity, i.e., "bouncing" Rydberg states (these were all but explicitly written in Ref. [6]). This system is effectively one-dimensional with a soft classical turning point at the classical apoapsis, such that turning point behavior may be analyzed as in the rest of this report.

The simplest definition of a Gaussian-Klauder state, with an energy eigenstate basis set $\{|n\rangle\}$ and with nondegenerate energies $E_n=\hbar\omega_n$, is

$$|\psi_{\mathrm{GK}}(t)\rangle = Z^{-1/2}\sum_n e^{-\Delta n^2/4\sigma^2}e^{-i\omega_n t}|n\rangle,$$

$$Z=\sum_n e^{-\Delta n^2/2\sigma^2}, \tag{1}$$

where n_0 is the mean quantum number of the state and $\Delta n=n-n_0$ is the relative quantum number. σ is a real parameter related to the energy uncertainty.

In analogy to the evenly spaced harmonic oscillator spectrum, which ensures exact periodicity in time for the wave

function (up to a global phase), a sufficiently narrow portion of a regular energy spectrum is also linear and exhibits approximate periodic evolution for states restricted to this energy window. Long-lived phase space localization for GK states then relies on energy localization, as expressed through the parameter σ.

Regular spectra are assumed for this paper, such that a Taylor series is assumed to exist for the energy eigenvalues around a given mean quantum number n_0:

$$\omega_n = \omega_{n_0} + \frac{2\pi}{T_1}\Delta n + \frac{2\pi}{T_2}\Delta n^2 + \cdots, \tag{2}$$

where T_1 and T_2 are the (signed) period and revival times, respectively [10]. These times are well separated in the classical limit, i.e., $T_1 \ll T_2$. Higher order terms in Eq. (2) are ignored for the purposes of this Brief Report, which is consistent with our focus on initial times of the evolution. A GK state $|\psi_{\mathrm{GK}}(t)\rangle$ in this approximation may be written in terms of the slowly varying complex parameter κ^2:

$$1/\kappa^2 = 1/\sigma^2 + \frac{8i\pi t}{T_2},$$

$$|\psi_{\mathrm{GK}}(t)\rangle \approx Z^{-1/2} e^{-i\omega_{n_0} t} \sum_n e^{-\Delta n^2/4\kappa^2} e^{-2\pi i \Delta n t/T_1} |n\rangle. \tag{3}$$

The time dependence of κ then characterizes the nonperiodic portion of an initial evolution.

At this level of detail, a simple measure of the delocalization of an evolving GK state is the autocorrelation function [11,12]

$$\langle \psi_{\mathrm{GK}} | e^{-i\hat{H}t/\hbar} | \psi_{\mathrm{GK}} \rangle = Z^{-1} \sum_n e^{-\Delta n^2/2\sigma^2} e^{-i\omega_n t}. \tag{4}$$

Equation (4) has been analyzed both for initial behavior and fractional revival behavior [10]. From such an analysis, the initial time before the onset of revival behavior is estimated:

$$\tau_{\mathrm{initial}} \sim \frac{|T_2|}{4\sqrt{2}\sigma}. \tag{5}$$

The dependence of Eq. (5) on σ suggests an inverse relationship between energy uncertainty and the time before the first complete delocalization of the state in phase space (considerations of Eq. (11) to come will further support this). Unfortunately, the autocorrelation function generally provides limited detailed information on this matter. For example, Eq. (4) is completely insensitive to initial phases of the energy eigenstate expansion coefficients.

Explicit construction of wave functions is a much more satisfactory measure of delocalization than the autocorrelation function. Specifically for this report, GK states are considered for the one-dimensional Schrödinger equation with position variable x and potential $V(x)$. Assuming $V(x)$ is a smooth function in x, energy eigenstates of the Schrödinger equation may be approximated by means of the Airy uniform approximation, which supplies a solution both near and far away from a single given turning point [13]. Near the turning point, this solution reduces to the usual Airy approximation

$$\psi_n(x) \approx N_n^{-1/2} \mathrm{Ai}\left[\frac{x - x_n}{\alpha_n}\right],$$

$$\alpha_n \equiv [2m|V'(x_n)|/\hbar^2]^{-1/3} \tag{6}$$

with x_n the turning point position at eigenenergy E_n, N_n a scaling constant to match the Airy approximation to the exact normalized eigenfunction, and α_n the characteristic Airy length of the turning point.

The key approximation in this paper is related to the relative constancy of $N_n^{-1/2}$ and α_n compared to x_n as n is varied. As such, these variables are set to the constants $N=N_{n_0}$ and $\alpha=\alpha_{n_0}$. The variation of x_n is only taken to first order:

$$x_n \approx x_{n_0} + \delta \Delta n \tag{7}$$

with $\delta = \frac{\partial x_n}{\partial n}|_{n_0}$. These approximations may appear restrictive, but several examples exist where the following analysis leads to meaningful results (e.g., many power law potentials and the Rydberg atom example in the latter part of this Brief Report).

With these assumptions, and with time evaluated at multiples of the fundamental period T_1, the GK positional wave function near the turning point is (ignoring the overall phase $e^{-i\omega_{n_0} t}$)

$$\psi_{\mathrm{GK}}(y,t) \approx N^{-1/2} \sum_{\Delta n} e^{-\Delta n^2/4\kappa^2} \mathrm{Ai}\left[\frac{y - \delta \Delta n}{\alpha}\right], \tag{8}$$

where $y = x - x_{n_0}$, and κ has the implicit time dependence of Eq. (3). Equation (8) is a discrete sum approximation to the Airy transform of a Gaussian, which may be written as the identity [13]

$$\frac{1}{\sqrt{4\pi\lambda^2}} \int e^{-x^2/4\lambda^2} \mathrm{Ai}\left(\frac{y - x}{\alpha}\right) dx = \exp\left(\beta^2 \phi + \frac{2}{3}\beta^6\right) \mathrm{Ai}(\phi + \beta^4), \tag{9}$$

where $\phi = y/\alpha$ and $\beta^2 = \lambda^2/\alpha^2$, and λ^2 may be complex. Up to a multiplicative constant, Eq. (9) approximates the turning point wave function with the choice of complex parameter $\beta^2 = \kappa^2 \delta^2/\alpha^2$.

The accuracy of Eq. (9) in approximating Eq. (8) for a given ϕ may be determined through treatment of Eq. (8) with the Poisson summation formula [14], though this is not done here. Of note is that while the result in Eq. (9) is typically square integrable over ϕ, Eq. (8) is not square integrable over all of y. This peculiarity is related to the failure for the oscillating portion of Airy functions to represent the exact orthonormal eigenfunctions far from the turning point. For reasons of square-integrability and analyticity, Eq. (9) will be understood as the approximate wave function of choice, from which calculations will be derived.

The momentum space representation of Eq. (9) [notice this representation involves Fourier transforming the convolution on the left hand side of Eq. (9)] straightforwardly leads to the computation of a moment generating function.

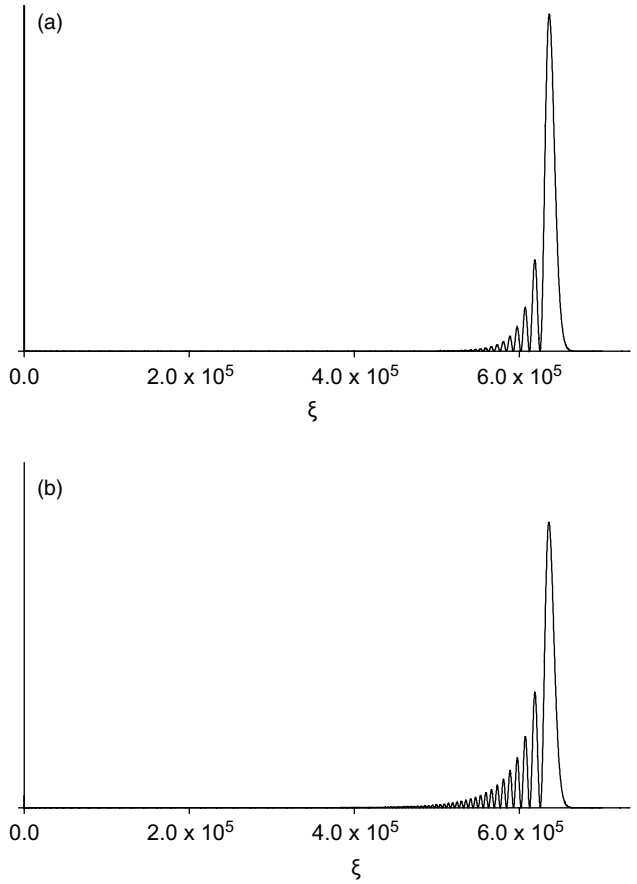

FIG. 1. A maximally eccentric GK Rydberg state, with mean quantum number $k_0=400$ and quantum number uncertainty $\sigma^2=1$, given at (a) initial time and (b) at 10 periods. Plots display the probability density $|\psi|^2$ (with arbitrary scale, fixed by normalization) against the parabolic coordinate ξ (in atomic units). Relatively small changes between the wave functions in (a) and (b) are a consequence of a small energy uncertainty leading to increased temporal stability.

Defining $p_\phi=-i\partial_\phi$, $A=\mathrm{Re}(\beta^2)$, and $B=\mathrm{Im}(\beta^2)$, then the leading moments of the normalized turning point GK state in Eq. (9) are

$$\langle\phi\rangle=-\frac{1}{4A},$$

$$\langle\Delta\phi^2\rangle=\frac{1}{8A^2}+\frac{B^2}{A}+A,$$

$$\langle p_\phi\rangle=0,$$

$$\langle\Delta p_\phi^2\rangle=\frac{1}{4A},$$

$$\langle\Delta\phi^2\rangle\langle\Delta p_\phi^2\rangle=\frac{1}{32A^3}+\frac{B^2}{4A^2}+\frac{1}{4} \tag{10}$$

with an again implicit time dependence. Strong dependence of the variances on A indicates that the primary factor in delocalization of a GK state is the smallness of $\mathrm{Re}(\beta^2)$. Indeed, $\mathrm{Re}(\beta^2)$ becomes vanishingly small with increasing time [Eq. (3)].

The time dependence of Eq. (10) may be given explicitly as expressions that are polynomial in time:

$$\langle\Delta\phi^2\rangle(t)=\left(\frac{1}{8g^2\sigma^4}+g\sigma^2\right)+\frac{16\pi^2}{g^2}\left(\frac{t}{T_2}\right)^2+\frac{512\pi^4\sigma^4}{g^2}\left(\frac{t}{T_2}\right)^4,$$

$$\langle\Delta p_\phi^2\rangle(t)=\frac{1}{4g\sigma^2}+\frac{16\pi^2\sigma^2}{g}\left(\frac{t}{T_2}\right)^2 \tag{11}$$

with $g=\delta^2/\alpha^2$ a dimensionless ratio. Estimates of the packet delocalization time τ may be determined through Eq. (11). For instance, if attaining some large positional uncertainty $\Delta\phi_0^2$ at some time τ defines delocalization, and additionally $\langle\Delta\phi^2\rangle(t)$ is assumed to be dominated by the t^4 term, then the $\tau\propto|T_2|/\sigma$ dependence in the autocorrelation estimate (5) is recovered. Delocalization in the classical limit is again demonstrated to be slow relative to the orbital period, as a consequence of the large ratio $|T_2|/|T_1|$.

Equation (10) predicts that for large $\mathrm{Re}(\beta^2)$, the total uncertainty $\langle\Delta\phi^2\rangle\langle\Delta p_\phi^2\rangle$ of the state approaches the minimal 1/4, indicating that the state is a Gaussian in position and momentum space. Thus, the positional Gaussian states that have been often used in the investigation of quantum dynamics may be represented by GK states with large energy uncertainties (but not so large that the assumptions of this paper are violated).

Also found are minimum positional uncertainty states, as determined at initial times $[\mathrm{Im}(\beta^2)=0]$. By Eq. (10), such states arise for the turning point system when $\mathrm{Re}(\beta^2)_{\min}=2^{-2/3}\approx0.63$ to give a minimum width $\langle\Delta\phi^2\rangle_{\min}=(3/2)2^{-2/3}\approx0.94$. This is a sensible result: the minimum initial positional width for a GK state at the turning point is on the same order as the local Airy natural length α. The minimum width states separate initial conditions into those that tend to represent either Gaussians $[\mathrm{Re}(\beta^2)>\mathrm{Re}(\beta^2)_{\min}]$ or Airy functions with exponential damping $[\mathrm{Re}(\beta^2)<\mathrm{Re}(\beta^2)_{\min}]$.

Application of turning point dynamics to maximally eccentric Rydberg atoms provides an interesting example (maximally eccentric eigenstates have a prominent role in the theory of Rydberg molecules [15]). Maximally eccentric Rydberg states are constructed by the same procedure as the generalized GK coherent states of the hydrogen atom [6], existing as the opposite limit to circular states. The set of maximally eccentric eigenstates derive from the $\mathrm{SO}(3)\otimes\mathrm{SO}(3)$ decomposition of hydrogen's SO(4) dynamical group [6,16], though expression of these states in coordinate form is often best given in parabolic coordinates $\xi=r(1+\cos\theta)$ and $\eta=r(1-\cos\theta)$, with r and θ the usual radius and polar angle, respectively [17]. Attention is directed to the differential equation satisfied by the ξ part of the maximally eccentric eigenfunctions [17]

$$\frac{\partial^2\psi}{\partial\xi^2}+\frac{1}{\xi}\frac{\partial\psi}{\partial\xi}+\left(-\frac{1}{4(k+1)^2}+\frac{1}{\xi}\frac{2k+1}{2k+2}\right)\psi=0 \qquad (12)$$

with integers $k\geqslant 0$, and the usual energy quantum number equal to $n=k+1$. If the $\frac{\partial\psi}{\partial\xi}$ term is ignored for the large ξ associated with the classical turning point (this can be done consistently for large energies), then the GK state at this turning point follows from the Airy transform principles earlier in this report. These maximally eccentric "bouncing" states may then be analyzed at the turning point as a one-dimensional problem. With a few short calculations, good localization in position space relative to the semimajor axis may be demonstrated (the large-k asymptotic limit for the ratio of minimum initial width $\sqrt{\langle\Delta\xi^2\rangle_{\min}}$ to the semimajor axis is proportional to $k^{-2/3}$, which becomes small in the limit of large k). This localization in ξ can also be demonstrated to ensure localization in the full phase space, as a result of the factor $e^{-\eta/2(k+1)}$ that multiplies maximally eccentric eigenstates [17]. Figure 1 illustrates one example of a maximally eccentric GK state.

Estimates of the time before delocalization of the maximally eccentric GK states follow from Eq. (5), which depends only on the local details of the spectrum around a given quantum number. Due to the degeneracy of the hydrogen atom, these estimates then correspond exactly to circular GK states of the same energy uncertainty and mean quantum number (covered earlier in Ref. [6]).

Experimental realization of these bouncing states may be impractical, due to the rapid decay of eccentric states into circular states [18]. Theoretical implications include, however, a classical limit of Keplarian orbits with eccentricity very near 1. This limit is not entirely obvious, since permanent polarization of the state along a given direction follows from the SO(4) symmetry of the Coulomb system (classically, from the conservation of the Runge-Lenz vector and angular momentum). The situation is in contrast to circular coherent states, which may be formed for a wide variety of central potentials.

In summary, application of Gaussian-Klauder states to integrable quantum systems has been demonstrated here and elsewhere to be a viable means of addressing generalized coherent states. In particular, the simplicity of the problem near soft classical turning points provides an analytical handle on the phase space localization (and packet shape) of GK states. The turning point formalism in this way lends credence to the estimates derived from the autocorrelation function in Eq. (4), e.g., the estimates of localization lifetimes. Relevance of this machinery to the hydrogen problem occurs in the examination of maximally eccentric "bouncing" states, whose classical limit is the recurrent radial collisions of a localized classical ensemble with the force center.

Such success has been based entirely on integrable quantum systems, where energy spectra and eigenfunctions remain well behaved. However, the usefulness of GK states applied to near-integrable systems is unclear. Our preliminary studies of this problem for the periodically time-perturbed case have offered an interesting analogy to classical adiabatic theory: find a given order adiabatically-approximated Hamiltonian H_{ad} and use the GK states of this smoothed problem as a coherent state approximation for the exact problem. This would seem a fitting answer to the coherent states of a near-integrable system.

[1] W. M. Zhang, D. H. Feng, and R. Gilmore, Rev. Mod. Phys. **62**, 867 (1990).
[2] S. J. Chang and K. J. Shi, Phys. Rev. A **34**, 7 (1986).
[3] K. Nakamura, A. R. Bishop, and A. Shudo, Phys. Rev. B **39**, 12422 (1989).
[4] R. F. Fox and T. C. Elston, Phys. Rev. E **50**, 2553 (1994).
[5] R. F. Fox and T. C. Elston, Phys. Rev. E **49**, 3683 (1994).
[6] R. F. Fox, Phys. Rev. A **59**, 3241 (1999).
[7] R. F. Fox and M. H. Choi, Phys. Rev. A **61**, 032107 (2000).
[8] R. F. Fox and M. H. Choi, Phys. Rev. A **64**, 042104 (2001).
[9] W. H. Mather and R. F. Fox, Phys. Rev. A **73**, 032109 (2006).
[10] C. Leichtle, I. S. Averbukh, and W. P. Schleich, Phys. Rev. A **54**, 5299 (1996).
[11] M. Nauenberg, J. Phys. B **23**, L385 (1990).
[12] P. Bellomo and C. R. Stroud, Phys. Rev. A **59**, 900 (1999).
[13] O. Vallée, *Airy Functions And Applications To Physics/Olivier Vallée, Manuel Soares* (World Scientific, Hackensack, NJ, 2004).
[14] R. Courant and D. Hilbert, *Methods of Mathematical Physics* (Interscience Publishers, New York, 1953).
[15] M. R. Flannery, D. Vrinceanu, and V. N. Ostrovsky, J. Phys. B **38**, S279 (2005).
[16] D. Vrinceanu and M. R. Flannery, Phys. Rev. A **63**, 032701 (2001).
[17] H. Bethe and E. Salpeter, *Quantum Mechanics of One-and-Two-Electron Atoms* (Plenum, New York, 1977).
[18] M. R. Flannery and D. Vrinceanu, Phys. Rev. A **68**, 030502(R) (2003).