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Quantization ambiguity, ergodicity and semiclassics

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Abstract. It is well known that almost all eigenstates of a classically ergodic system are individually ergodic on coarse-grained scales. This has important implications for the quantization ambiguity in ergodic systems: the difference between alternative quantizations is suppressed compared with the $O(\hbar^2)$ ambiguity in the integrable or regular case. For two-dimensional ergodic systems in the high-energy regime, individual eigenstates are independent of the choice of quantization procedure, in contrast with the regular case, where even the ordering of eigenlevels is ambiguous. Surprisingly, semiclassical methods are shown to be much more precise in any dimension for chaotic than for integrable systems.

1. Introduction

For many years, it has been widely recognized that 'quantizing' a given classical system is inherently an ambiguous procedure, as a large family of quantum Hamiltonians may have the same classical limit [1]. For example, given the classical dynamics of a particle constrained to move on a closed loop, different choices of boundary condition give rise to different phases relating classical paths of different winding number. Knowledge of these Aharonov–Bohm phases is of course necessary to construct a semiclassical dynamics (which includes interference between classical paths), and thus many *semiclassical* theories correspond to the same *classical* dynamics. Physically, this $O(\hbar)$ or gauge ambiguity may be associated with the possibility of varying the magnetic flux enclosed by the loop.

This is not all, however: there are also many *quantum* theories, differing at $O(\hbar^2)$ or higher in the Hamiltonian, which all have the same *semiclassical* limit. There are many ways of seeing this $O(\hbar^2)$ ambiguity; one of the simplest is to imagine making a canonical transformation on the classical phase space, applying the canonical quantization prescription to the new coordinates,

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and then transforming back to the original coordinate system. Generically, one then obtains a new quantum Hamiltonian which differs from the original by $O(\hbar^2)$ plus higher-order terms:

$$\hat{H}' = \hat{H} + \hbar^2 \hat{A} + \cdots, \tag{1}$$

where the operator $\hat{A}$ has a well defined classical limit [2]. As classical dynamics is of course independent of the choice of coordinate system, this implies that quantization is inherently ambiguous at second order in $\hbar$.

An even more striking case is that of a particle constrained to move on a $d = 2$ surface embedded in $d = 3$ space. Here, the non-trivial metric contained in the kinetic term gives rise to obvious operator-ordering ambiguities in canonical quantization; this has led to much discussion in the literature over whether a term proportional to the local Gaussian curvature R of the surface should be added to the Hamiltonian and, if so, what the proportionality constant should be (different prescriptions suggest $\hbar^2 R/8$, $\hbar^2 R/6$, and $\hbar^2 R/12$ as the 'correct' answer) [3]–[5]. In the path integral approach, ambiguities at the same order arise in choosing how to incorporate the metric into the kernel and in deciding at what point in the infinitesimal time interval to evaluate functions of the metric [6].

Physically, one may define dynamics on a constraint surface through a limiting process, where the strength of restoring forces causing the particle to stay on the surface is taken to infinity. Classically, this procedure is known to give an unambiguous constrained dynamics [7], whereas in quantum mechanics, $O(\hbar^2)$ differences arise depending on the precise way in which the strength of the constraining potential is taken to infinity at various places along the surface [8]. The ambiguity here has a clear physical meaning: to determine the true quantum mechanics one needs to know the mechanism through which the particle is bound to the surface of constraint; it is not sufficient to know only the intrinsic properties of the surface itself. Similarly, there is no 'correct' answer to the problem of quantizing a classical double pendulum [4]: quantum dynamics at $O(\hbar^2)$ is determined by the precise way in which one takes to infinity the rigidity of the two rods.

In a $d = 2$ system, the energy spacing between adjacent levels is $O(\hbar^2)$, i.e. of the same order as the quantization ambiguity discussed above. It would then seem not to be possible to uniquely determine the eigenvalues and eigenstates of a $d = 2$ system given only the $d = 2$ classical dynamics. Furthermore, it should not be possible in general to compute semiclassically the levels and wavefunctions of a $d = 2$ quantum system, because a given semiclassical calculation has many quantum theories corresponding to it, with Hamiltonians related as in equation (1). Recently, however, it was shown theoretically using time evolution arguments, and numerically confirmed, that in strongly chaotic $d = 2$ systems long-time semiclassical methods can in fact be used to compute quantum properties to accuracy parametrically better than a level spacing, i.e. individual wavefunctions and eigenenergies can be semiclassically resolved [9]. This creates an apparent paradox, to be addressed in this paper.

We mention only briefly several important recent discussions of semiclassical accuracy, which offer different perspectives on this interesting subject. Vergini and coauthors [10] have investigated the accurate construction of quantum eigenstates and eigenvalues out of the semiclassical scar functions of short periodic orbits. The powerful harmonic inversion technique has been developed by Main and co-workers [11] for precise and efficient semiclassical calculations of energies, resonances, and matrix elements. Prosen and Robnik [12] have shown explicitly the failure of semiclassical torus quantization to reproduce the spectra of low-dimensional integrable systems, even when statistical properties are well described semiclassically. For a class of higher-dimensional integrable systems that are effectively $d = 2$ because of a high degree of symmetry, Rahav *et al* [13] have shown that the distribution of semiclassical errors in the spectrum is energy-independent. Primack and Smilansky have analysed semiclassical accuracy for $d = 3$ chaotic systems, focusing on including corrections to the state-counting function beyond the leading Weyl term [14]. Finally, Boasman [15] has investigated the accuracy of the boundary integral method in $d = 2$ billiards when the exact kernel is replaced by its semiclassical limit.

2. Wavefunctions in ergodic systems

Our answer to the above paradox is somewhat surprising: it is found that

(i) the quantization ambiguity is parametrically reduced in any dimension for classically ergodic as compared with regular systems;

(ii) in $d = 2$, the ambiguity for ergodic systems is small compared to a level spacing, in contrast with the integrable case where even the ordering of eigenlevels is ambiguous; and

(iii) in any dimension, semiclassical methods can be valid to much longer times in strongly chaotic as compared with integrable systems, allowing individual eigenenergies to be easily resolved for $d = 2$.

The key to these surprising results is the coarse-grained ergodicity of individual wavefunctions in classically ergodic systems. More precisely, in the classical limit, the quantum expectation value of any classically defined operator over individual eigenstates must approach the ergodic, microcanonical average of the operator, for almost all eigenstates. This behaviour has been proven mathematically under a variety of technical assumptions by Shnirelman *et al* [16], among others. Here we briefly present a simple physical argument that demonstrates the generality of the result.

Let $\hat{A}$ be an arbitrary quantum operator having the smooth phase space function $A(q,p)$ as its classical limit. For any energy E_0 we may choose a classically small energy window ΔE such that the microcanonical average $a(E)$ of the function $A(q,p)$ is as close as we like to a constant, a_0, for all $E \in [E_0, E_0 + \Delta E]$. Notice that in the $\hbar \to 0$ limit, the classically infinitesimal energy window will contain an arbitrarily large number of quantum eigenstates, $N \sim \hbar^{-d}$. We wish to show that for any ϵ, there exists $\hbar$ such that

$$\overline{(\langle n|\hat{A}|n\rangle - a_0)^2} < \epsilon^2, \tag{2}$$

where the average is taken over all wavefunctions $|n\rangle$ in the energy window $[E_0, E_0 + \Delta E]$.

Consider the quantum correlator

$$f(t) = \frac{1}{N}\mathrm{Tr}\,\hat{A}^\dagger \hat{A}(t) = \frac{1}{N}\mathrm{Tr}\,\hat{A}^\dagger \mathrm{e}^{\mathrm{i}\hat{H}t/\hbar}\hat{A}\mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}, \tag{3}$$

where the trace is over the N states in the energy window. Now define the time-averaged correlator:

$$F(T) = \frac{1}{\sqrt{2\pi T^2}}\int_{-\infty}^{\infty} \mathrm{d}t\,\mathrm{e}^{-t^2/2T^2} f(t) = \frac{1}{N}\sum_{n=1}^{N}\sum_{n'} |\langle n|\hat{A}|n'\rangle|^2 \mathrm{e}^{-(E_n - E_{n'})^2 T^2/2\hbar^2}. \tag{4}$$

$F_{\mathrm{cl}}(T)$, the time-averaged correlator of $A(q,p)$ and $A(q(t),p(t))$, is the classical counterpart of $F(T)$, and must by the definition of ergodicity tend to the ergodic value a_0^2 as $T \to \infty$. Now we simply choose T large enough so that $F_{\text{cl}}(T)$ is within $\mathrm{O}(\epsilon^2)$ of its long-time asymptotic value, and then choose $\hbar$ small enough so that the Ehrenfest time T_{Ehr}, at which classical–quantum correspondence breaks down, is large compared with T. (Notice that for a hard chaotic system, the breakdown time $T_{\text{Ehr}} \sim \lambda^{-1} \log S_{\text{typ}}/\hbar$ as $\hbar \to 0$, where λ is the Lyapunov exponent and S_{typ} is a typical action; however, here we make no specific assumption about the system apart from ergodicity.) We then have

$$\frac{1}{N} \sum_{n=1}^{N} |\langle n|\hat{A}|n\rangle|^2 \leq F(\infty) \leq F(T) \leq a_0^2 + \mathrm{O}(\epsilon^2). \tag{5}$$

Now a_0 is, of course, the mean value of the matrix elements $\langle n|\hat{A}|n\rangle$ (as can be seen formally by considering the correlation of $\hat{A}(t)$ with the identity operator), so equation (5) implies that the variance of the matrix elements is bounded above by ϵ^2, proving the statement of equation (2), and goes to zero in the $\hbar \to 0$ limit.

In the presence of degeneracies, the argument above clearly holds for *any* choice of orthonormal eigenbasis $|n\rangle$. Furthermore, the difference between the first two quantities in equation (5) is also bounded above by $\mathrm{O}(\epsilon^2)$; this implies

$$\langle n|\hat{A}|n'\rangle \to 0 \tag{6}$$

for almost all degenerate eigenstates $|n\rangle$ and $|n'\rangle$ in the $\hbar \to 0$ limit.

The above statistical argument leaves open the possibility of a zero-measure set of states grossly violating the ergodic condition $\langle n|\hat{A}|n\rangle \approx a_0$. This is not a deficiency in the argument: infinite sequences of highly non-ergodic states (namely, the bouncing-ball wavefunctions) have been shown to exist in chaotic systems with marginally stable classical orbits [17]. The fraction of such states does go to zero in the high-energy limit, in accordance with the predictions of the theorem [18].

We note again that no assumptions have been made in the argument about 'hard chaos' properties such as hyperbolicity or mixing; implications for the elimination of quantization ambiguity in two dimensions will thus hold for all classically ergodic systems.

Coarse-grained quantum ergodicity is a much weaker and more general result than the random wave hypothesis, which has been conjectured to be a statistical description of classically ergodic wavefunctions [19]. The latter conjecture suggests ergodic behaviour of quantum wavefunctions on single-wavelength or single-channel scales, and is violated by periodic orbit scars and other effects of short-time dynamics [20, 21]. For example, the quantum wavefunctions of the Sinai billiard, a paradigm of classical chaos, have been shown to have inverse participation ratios (IPRs) that diverge in the classical limit away from their ergodic and random wave values [21]. This strongly non-ergodic wavefunction behaviour on scales of size $\hbar$ is entirely consistent with ergodicity on coarse-grained scales as discussed above.

3. Implications for quantization ambiguity and semiclassical accuracy

Comparing the result of equation (2) with (1), we see that the leading effect of a change in the quantization prescription is to shift all energy levels classically close to E_0 by a constant displacement $\hbar^2 a_0$, comparable in size to a level spacing for $d = 2$; perturbation theory then gives

$$\delta E_n \equiv E'_n - E_n = \hbar^2 [a_0 \pm \mathrm{O}(\epsilon)] \tag{7}$$

with $\epsilon \ll 1$ for small $\hbar$ (high energy). In the special case of the random wave hypothesis or random matrix theory (RMT), we can use the fact that the energy hypersurface has $M \sim \hbar^{1-d}$ Planck-sized cells; since the deviations ϵ in the matrix elements $\langle n|\hat{A}|n\rangle$ arise from uncorrelated fluctuations in these cells, we obtain

$$\epsilon_{\mathrm{RMT}} \sim \frac{1}{\sqrt{M}} \sim \hbar^{(d-1)/2}. \tag{8}$$

The relative shift between *nearby* energy levels compared to a level spacing is therefore

$$\left(\frac{\delta E_n - \delta E_m}{\hbar^d}\right)^2 \sim \epsilon^2 \hbar^{4-2d} \overset{\mathrm{RMT}}{\sim} \hbar^{3-d}, \tag{9}$$

to be compared with $\hbar^{4-2d}$ (since $\epsilon_{\mathrm{reg}} \sim 1$) in the regular case. The $\hbar$-independent prefactor on the right-hand side of equation (9) may be shown semiclassically [22] to be proportional to the integral of a classical correlation function

$$\int_{-\infty}^{\infty} \mathrm{d}t\, [\overline{A(t)A(0)} - \overline{A}^2] \sim T_{\mathrm{corr}}[\overline{A^2} - \overline{A}^2], \tag{10}$$

where the average is over an energy hypersurface. Here T_{corr} is the timescale for decay of classical correlations. Clearly, the estimate (9) is valid only when the relative error is less than unity and perturbation theory holds.

The overall energy shift $\hbar^2 a_0$ in equation (7) is of course unphysical, corresponding simply to changing the Hamiltonian locally by a constant; only energy differences are measurable, and from the first relation in equation (9) we see that for $d = 2$ these become independent of one's choice of quantization in the $\hbar \to 0$ limit, i.e. for highly excited states, in any ergodic system. Energy splittings $E_n - E_m$ which are already classically large can of course change by $\mathrm{O}(\hbar^2)$ as one considers different quantum systems with the same semiclassical limit. However, the ratio $\delta(E_n - E_m)/(E_n - E_m) \to 0$ for almost all states $|n\rangle$, $|m\rangle$ in the semiclassical limit for $d = 2$, whether $|n\rangle$ and $|m\rangle$ are nearest-neighbour levels or are far apart in energy. Thus, in the classical limit of a $d = 2$ constrained surface, the way in which the particle is bound to the surface has no effect on any measurable quantity, *provided that motion on the constraint surface itself is ergodic*. (In the case of mixed phase space, states living on regular islands can move up or down relative to each other and to the rigid chaotic sea, as the quantization condition is varied.)

The result of equation (9) is consistent with the finding in [9] that in caustic-free chaotic $d = 2$ systems, long-time semiclassical dynamics approaches the quantum answer, and that the critical dimension for breakdown of the semiclassical approximation at the Heisenberg time is $d = 3$ for chaotic systems, as compared with $d = 2$ in the integrable case.

Transforming into the time domain, we find that for times t short compared to the Heisenberg time $T_H \sim \hbar^{1-d}$ at which individual eigenlevels get resolved but longer than the classical correlation time T_{corr}, the mean squared error in the time evolution of a wavepacket in a hard chaotic system grows (in any dimension) as

$$\hbar^2[\overline{A^2} - \overline{A}^2]T_{\mathrm{corr}}t, \tag{11}$$

while the same quantity grows quadratically with time, as

$$\hbar^2[\overline{A^2} - \overline{A}^2]t^2 \tag{12}$$

in the regular case. This implies that the break time after which quantum dynamics begins to depend strongly on details of the quantization prescription scales as

$$T_{\mathrm{break}} \sim \hbar^{-2} \tag{13}$$

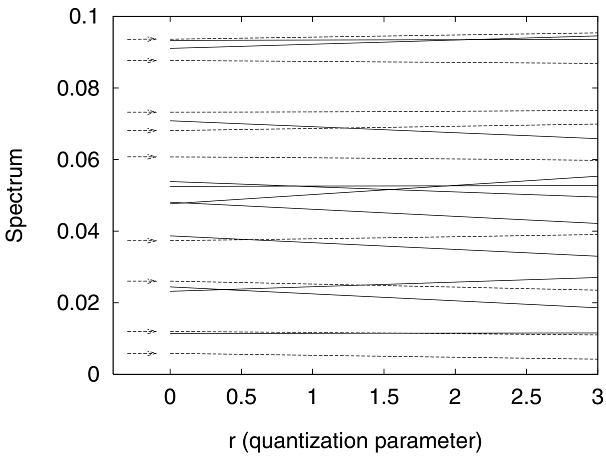

Figure 1. Sample spectrum as a quantization parameter is varied: solid lines represent the regular and dashed lines the chaotic case, both for $h = 1/512$. Arrows indicate eigenvalues of the long-time semiclassical chaotic dynamics.

for hard chaotic systems, in contrast with the much shorter break time $T_{\mathrm{break}} \sim \hbar^{-1}$ for regular systems. These scaling relations agree with results for the breakdown of the semiclassical approximation [9], indicating that equation (13) provides not only an upper bound on the timescale of validity of the semiclassical approximation, but a bound that can be saturated in the ideal case of caustic-free and diffraction-free dynamics.

For a simple numerical verification of the above results, we consider a discrete-time map on a two-dimensional toroidal phase space $(q, p) \in [0, 1) \times [0, 1)$ (notice that this scales with $\hbar$ equivalently to a $d = 2$ autonomous Hamiltonian system and can be thought of as a Poincaré section of the latter):

$$\begin{aligned} p \to \tilde{p} &= p - V'(q) \bmod 1 \\ q \to \tilde{q} &= q + \tilde{p} \bmod 1. \end{aligned} \tag{14}$$

The above equations of motion can be obtained from the time-periodic ('kicked') Hamiltonian

$$H = \frac{p^2}{2} + V(q) \sum_n \delta(t - n). \tag{15}$$

We let the potential be given by

$$V(q) = \pm \frac{q^2}{2} + \frac{0.4}{(2\pi)^2} \sin 2\pi q + r h^2 \cos 2\pi q, \tag{16}$$

where the $-$ sign gives completely chaotic dynamics [9, 23], while the $+$ sign leads to a (mostly) regular classical phase space. The $\sin 2\pi q$ term is added to break parity symmetries and make the dynamics nonlinear and generic in both cases, while r parametrizes a one-parameter family of possible quantizations.

Sample sections of the regular (solid curves) and chaotic (dashed curves) spectra are shown in figure 1, as a function of the quantization parameter r. We see in the regular case that the eigenvalues often cross each other as the quantization is varied, making impossible a semiclassical ordering of the spectrum, while in the chaotic case the eigenvalues never shift by an amount comparable to a mean level spacing (≈ 0.0117 in this calculation). We notice that in our example

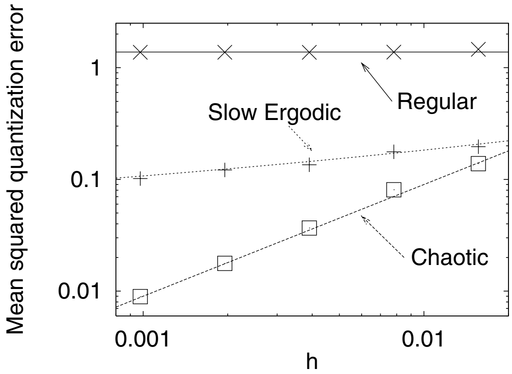

Figure 2. Mean-squared change in eigenvalues between two quantizations (in units where mean level spacing = 1), plotted as a function of the effective Planck constant.

the trace of $A(q,p) = r\cos 2\pi q$ is zero, so the overall spectral shift $\hbar^2 a_0$ of equation (7) vanishes as well. For $A(q,p)$ with nonzero average, there is a secular upward or downward trend in all the eigenvalues (regular and chaotic) as r increases, but no physical quantities are affected.

Despite the exponential proliferation of classical paths in the chaotic case, semiclassical calculations past the Heisenberg time can be performed to arbitrary precision with only a power-law amount of effort, using an iterative approach, and individual semiclassical eigenvalues and eigenstates can be extracted [9]. Semiclassically obtained eigenvalues for the chaotic system are indicated by arrows in figure 1 and are observed to agree well with the quantum results (independent of quantization). In the regular case, there is of course little meaning to semiclassically computed individual eigenvalues (since these depend on the basis in which the semiclassical calculation is performed), and these are not shown.

In figure 2 we show the mean-squared change in eigenlevel position, as a function of effective Planck constant (inverse momentum) $h = 1/64 \ldots 1/1028$, when the quantization parameter r is changed from 0.0 to 3.0. The $\times$ represent the regular case, and show that the quantization ambiguity there is large and energy-independent. The data points marked by squares correspond to the chaotic system, and clearly follow the linear law predicted by equation (9) (for $d = 2$). Finally, the pluses come from the 'slow ergodic' sawtooth potential map [20] defined by

$$V(q) = 0.3|q - \tfrac{1}{2}|, \tag{17}$$

where the quantization ambiguity is now put in the kinetic term: $H = \cdots + rh^2\cos 2\pi p$. Here we do not expect quantum wavefunctions to be ergodic on the scale of a single channel in momentum space [20], but they will be ergodic on scales $\sim 1/|\log\hbar|$ as $\hbar \to 0$. We then expect $\epsilon \sim 1/(\alpha + \beta\log\hbar)$ in equation (9), which behaviour is indeed observed in figure 2. We see that ergodicity without chaos is sufficient to obtain unambiguous quantization of $d = 2$ systems, though the error in the high-energy limit approaches zero more slowly in the slow ergodic than in the fully hyperbolic case.

4. Conclusions

Our finding of enhanced semiclassical accuracy in chaotic systems compared with the regular case is consistent with recent work by Prosen and collaborators on quantum fidelity [24], which shows that for a certain class of static perturbations the accuracy of quantum evolution decays more quickly in regular than in chaotic systems. Furthermore, quantum fidelity persists at longer and longer times as the correlation time of the classical dynamics is decreased. The explanation for this counterintuitive finding is completely analogous to the parallel findings for semiclassical accuracy [9]. In both situations, errors add coherently for regular systems because a given trajectory keeps revisiting the same regions of phases space, leading to a cumulative error growing linearly with time; for hard chaotic systems, each trajectory uniformly explores all of the energy hypersurface and the dominant part of the error adds incoherently, resulting in $\sqrt{t}$ growth with time.

As noted above, the quantization ambiguity provides only a lower bound for the typical error in semiclassical calculations, or alternatively an upper bound for the break time of semiclassical accuracy. We know that this bound is saturated only in the absence of diffraction [25] or caustics [26] in the dynamics, when by semiclassical evolution is meant pure Gutzwiller–Van-Vleck propagation [9]. One may conjecture that an improved semiclassics including a uniform approximation for caustics, if any exist in the chosen basis, and including diffractive scattering events to an order depending on the dimension, will restore semiclassical accuracy to the level given by the quantization ambiguity limit; for now this remains an open problem. We also note that equation (10) implies a limit on semiclassical accuracy that gets worse as the Lyapunov exponent of a hard chaotic system is reduced; this question, along with the energy-scale dependence of semiclassical accuracy and the connection with the Brownian motion model [2] is currently under investigation [27].

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