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LETTER TO THE EDITOR

Discordance between quantum and classical correlation moments for chaotic systems

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Abstract. For systems whose classical orbits are chaotic, a set of quantum expectation values Q_r is constructed which vanish for all $\hbar$, unlike their classical counterparts C_r which are finite. This behaviour is not paradoxical because Q_r and C_r are moments of time correlation functions, which are dominated by the long-time limit where quantum and classical evolutions disagree.

According to the correspondence principle, quantum observables (expectations of Hermitian operators) should tend to their classical counterparts in the semiclassical limit, i.e. as Planck's constant $\hbar \to 0$. However, the semiclassical limit is highly singular (Berry 1991), and is vulnerable to disruption by any other limit with which it does not commute. An example is the long-time limit $t \to \infty$. In the combined semiclassical long-time limit, the correspondence principle need not apply, and very complicated behaviour can occur (see e.g. Berry 1988).

Here we give an example where the quantum–classical clash is extreme: the quantum observable is zero independently of $\hbar$, while if the orbits are chaotic its classical limit does not vanish. A related result was given by Kosloff and Rice (1980), who argued that the quantum mechanical value of a suitably defined Kolmogorov entropy vanishes, whereas the classical value does not. Another example has been presented by Ford *et al* (1991); they showed that the algorithmic complexity of computations for the quantum Arnold cat map always vanishes, while the classical complexity, reflecting the chaotic evolution, does not (of course, complexity is not the expectation of a Hermitian operator and so is not a quantum observable in any obvious way). In both the above examples, as with ours, the apparent breakdown of correspondence originates in the fact that the development of chaos involves the long-time limit. The example we give here has the virtue that the transcription from quantum to classical is particularly straightforward.

Let $\hat{A}$ and $\hat{B}$ be Hermitian operators that depend on the fundamental coordinate and momentum operators $\hat{q}$, $\hat{p}$ for a bound system whose evolution is governed by a time-independent Hamiltonian $\hat{H}$. Then we can define the quantum correlation function

$$Q(t) \equiv \tfrac{1}{2}\langle n|(\hat{A}_t\hat{B} - \hat{A}\hat{B}_t + \hat{B}\hat{A}_t - \hat{B}_t\hat{A})|n\rangle. \qquad (1)$$

This involves the nth eigenstate $|n\rangle$ of $\hat{H}$, and the Heisenberg (time-evolved) operators

$$\hat{A}_t \equiv \exp\{\mathrm{i}\hat{H}t/\hbar\}\hat{A}\exp\{-\mathrm{i}\hat{H}t/\hbar\} \qquad (2)$$

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and similarly for $\hat{B}_t$. $Q(t)$ is real because the operator in parentheses in (1) is Hermitian. The correlation moments, with which we will be concerned, are

$$Q_r \equiv \int_{-\infty}^{\infty} dt\, t^r Q(t). \tag{3}$$

Elementary arguments (involving independence of expectation value to a shift in the time at which Heisenberg operators are evaluated) show that $Q(t)$ is an odd function, so that all the even moments are zero. Now we show that the Q_r also vanish when r is odd. After introducing the resolution of the identity to separate the operators in (1), and the frequencies

$$\omega_{nm} \equiv \frac{E_n - E_m}{\hbar} \tag{4}$$

where E_n are the energy levels (discrete eigenvalues of $\hat{H}$), an elementary calculation gives

$$Q(t) = -2 \sum_m \sin\{\omega_{nm} t\}\, \mathrm{Im}\{\langle n|\hat{A}|m\rangle\langle m|\hat{B}|n\rangle\}. \tag{5}$$

Thus $Q(t)$ is an almost-periodic function. That its moments vanish can be seen by expressing them as derivatives of the Fourier transform of $Q(t)$ at the origin, and observing that (5) has no Fourier component at $\omega = 0$. Alternatively, we can use

$$\int_0^{\infty} dt\, t^r \sin\{\omega t\} = 0 \qquad \omega > 0,\ r \text{ odd} \tag{6}$$

whose truth can be established by a variety of arguments, for example expressing the integral as a derivative of a delta-function of ω, or introducing a convergence factor $\exp\{-\varepsilon t\}$ and taking the limit $\varepsilon \to 0$.

Let the classical counterpart of the quantum system have N (≥ 2) freedoms, and let

$$z \equiv (q, p) = (q_1, \ldots, q_N, p_1, \ldots, p_N) \tag{7}$$

denote position in the $2N$-dimensional phase space. Then corresponding to the quantum operators $\hat{A}$ and $\hat{B}$ are classical functions $A(z)$ and $B(z)$. The corresponding classical Hamiltonian $H(z)$ generates from the initial point z the orbit $Z_t(z)$ in time t, and the classical counterpart of the time-evolved operator (2) is

$$A_t(z) \equiv A(Z_t(z)). \tag{8}$$

To define the classical counterpart of the correlation function (1) we need to know what corresponds to the quantum expectation value in the state $|n\rangle$. This is a phase-space average over whatever classical invariant manifold corresponds to $|n\rangle$. By assumption, the classical systems we are considering are chaotic, so almost all orbits are ergodic on their energy surfaces. Thus the appropriate average is microcanonical, and the classical correlation function is

$$\begin{aligned} C(t) &= \langle A_t B - B_t A\rangle_E \\ &\equiv \frac{\int d^{2N}z\, \delta\{E - H(z)\}(A_t(z)B(z) - B_t(z)A(z))}{\int d^{2N}z\, \delta\{E - H(z)\}}. \end{aligned} \tag{9}$$

Of course this function is independent of $\hbar$. (There are also semiclassical 'scar' contributions to $Q(t)$ from each of the classical periodic orbits, but these are of order

$\hbar^{N-1}\exp\{i/\hbar\}$ (Berry 1991) and vanish in the classical limit, as the oscillations become infinitely fast and faint.) The classical correlation moments are

$$C_r \equiv \int_{-\infty}^{\infty} dt\, t^r C(t). \tag{10}$$

Again, elementary arguments (involving conservation of H and the fact that time evolution is a canonical transformation) show that $C(t)$ is an odd function, so that all the even moments vanish. But the odd moments need not vanish. To see why, we observe that the mixing property associated with chaos means that

$$C(t) \xrightarrow[t\to\infty]{} \langle A\rangle_E\langle B\rangle_E - \langle B\rangle_E\langle A\rangle_E = 0 \tag{11}$$

so that $C(t)$ rises from zero at $t=0$ and then decays to zero at infinity. Provided the decay is sufficiently fast, $C(t)$ has a continuous spectrum, and so is not an almost-periodic function. Therefore it can possess some non-zero moments, and typically will do so.

We can prove this for hyperbolic systems, for which it is known (Pollicott 1985, Ruelle 1986) that $\bar{C}(\omega)$, the Fourier transform of $C(t)$, is meromorphic in a strip including the real axis. But if all the moments of $C(t)$ are to vanish, then all derivatives of $\bar{C}(\omega)$ must vanish at $\omega=0$; by analytic continuation this implies that $\bar{C}(\omega)$, and hence $C(t)$, vanish identically. Thus any non-zero $C(t)$ must have non-zero moments.

We are unable to generalize this argument to arbitrary classical chaotic systems, because not enough is known about the analytic structure of their correlations. Therefore we cannot exclude cases such as

$$\bar{C}(\omega) = \int_{-\infty}^{\infty} dt\, C(t)\exp\{i\omega t\} = i\omega\exp\left\{-\frac{1}{4|\omega|} - A|\omega|\right\} \tag{12}$$

where, because of the essential singularity, all derivatives at $\omega=0$, and therefore all moments of $C(t)$, are zero. Moreover, $C(t)$, in addition to having a continuous spectrum, decays exponentially. This can be seen by Fourier inversion, which gives

$$C(t) = -\frac{1}{2\pi}\,\mathrm{Im}\,\frac{1}{\xi^2}K_2\{\xi\} \qquad \xi = \sqrt{t-iA}\exp\{i\pi/4\} = \sqrt{A+it} \tag{13}$$

where K denotes the modified Bessel function (Abramowitz and Stegun 1964), whose limiting forms are

$$C(t) \approx \begin{cases} \dfrac{t}{4\pi A^{5/2}}[4\sqrt{A}\,K_0\{\sqrt{A}\} + (8+A)K_1\{\sqrt{A}\}] & |t| \ll A \\ \dfrac{\mathrm{sgn}(t)}{|t|^{5/4}2\sqrt{2\pi}}\exp\{-\sqrt{\tfrac{1}{2}|t|}\}\cos\{\sqrt{\tfrac{1}{2}|t|}+\tfrac{1}{8}\pi\} & |t| \gg A. \end{cases} \tag{14}$$

We consider such cases as special, and unlikely to occur in any real classical system.

If the classical motion is integrable, the above arguments do not apply. For then the motion *is* almost periodic (indeed multiply periodic, since there are finitely many independent frequencies), and the quantum expectation value corresponds to averaging over the angles of the quantized invariant torus whose actions are associated with $|n\rangle$ (see e.g. Percival 1977). $C(t)$ is given by a formula similar to (5), in which the ω_{nm} are replaced by (non-zero) integer linear combinations of the N classical frequencies. It then follows from (6) that the moments are zero.

It seems paradoxical that a quantum expectation value can have zero moments while the moments of its classical limit are finite. But the moments we are calculating are constructed to exploit the clash of limits $\hbar \to 0$, $t \to \infty$, because they are dominated by the behaviour of $Q(t)$ and $C(t)$ at large t—precisely where the classical and quantum evolutions disagree. Specifically, for long times $t > \hbar/(\text{mean level spacing}) \sim 1/\hbar^{(N-1)}$, $Q(t)$ is dominated by oscillations associated with the discreteness of the spectrum, while $C(t)$ decays because of the mixing associated with chaos. The essence of *quantization is here incompatible with the essence of chaos.*

A purely mathematical example illustrating this curious behaviour is provided by the 'quantum' function

$$Q(t) = \hbar \sum_{m=-\infty}^{\infty} m \exp\{-\hbar^2 m^2\} \sin\{m\hbar t\} \tag{15}$$

and its 'classical' limit, in which the sum is replaced by an integral,

$$C(t) = \int_{-\infty}^{\infty} \mathrm{d}x\, x \exp\{-x^2\} \sin\{xt\} = \frac{\sqrt{\pi}}{2}\, t \exp\{-\tfrac{1}{4}t^2\}. \tag{16}$$

(Despite superficial appearances, this is not a model for any kind of harmonic oscillator.) Both are odd functions of t, whose moments are easily calculated to be

$$Q_r = 0 \qquad (\text{all } r)$$

$$C_r = \begin{cases} 0 & (r \text{ even}) \\ 2^{r+1}\sqrt{\pi}\,(\tfrac{1}{2}r)! & (r \text{ odd}) \end{cases} \tag{17}$$

showing the clash of limits.

In this example the mysterious classical appearance of the moments can be traced explicitly, by re-expressing (15) with the aid of the Poisson sum formula: without approximation, we have

$$\begin{aligned} Q(t) &= \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}x\, x \exp\{-x^2\} \sin\{xt\} \exp\left\{\frac{2\pi i n x}{\hbar}\right\} \\ &= \frac{\sqrt{\pi}}{2} \sum_{n=-\infty}^{\infty} \left(t - \frac{2\pi n}{\hbar}\right) \exp\left\{-\frac{1}{4}\left(t - \frac{2\pi n}{\hbar}\right)^2\right\}. \end{aligned} \tag{18}$$

Thus $Q(t)$ is here a series of copies of $C(t)$, displaced along the t axis by multiples of $2\pi/\hbar$. As $\hbar \to 0$ all these copies recede to $\pm\infty$, leaving $C(t)$ alone at finite t. The moments are derivatives of the Fourier transform of $Q(t)$ at zero frequency ω. Each copy generates a phase-shifted reproduction of the transform of $C(t)$, whose sum involves

$$\begin{aligned} \sum_{n=-\infty}^{\infty} \exp\{2\pi i n\omega/\hbar\} &= 1 + 2\,\mathrm{Re} \sum_{n=1}^{\infty} \exp\{2\pi i n\omega/\hbar\} \\ &= 1 + 2\,\mathrm{Re}\, \frac{\exp\{2\pi i\omega/\hbar\}}{1 - \exp\{2\pi i\omega/\hbar\}} \\ &= 1 - 1 = 0 \end{aligned} \tag{19}$$

(we ignore the delta-function at $\omega = 0$ because this is negated by a zero of the transform of $C(t)$ there). The -1 in (19) represents the contribution of all the copies to Q_r, and cancels C_r.

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