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Semiclassical level spacings when regular and chaotic orbits coexist

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Abstract. We calculate semiclassical limiting level spacing distributions $P(S)$ for systems whose classical energy surface is divided into a number of separate regions in which motion is regular or chaotic. In the calculation it is assumed that the spectrum is the superposition of statistically independent sequences of levels from each of the classical phase-space regions, sequences from regular regions having Poisson distributions and those from irregular regions having Wigner distributions. The formulae for $P(S)$ depend on the sum of the Liouville measures of all the classical regular regions, and on the separate Liouville measures of the significant chaotic regions.

1. Introduction

For a bound quantum system with f freedoms, the number of energy levels in any narrow interval E to $E+\Delta E$ diverges as $\Delta E/\hbar^f$ in the semiclassical limit $\hbar \to 0$. It is then possible to define the probability distribution $P(S)$ of the spacings S between successive levels in the interval, and regard $P(S)$ as one way of characterising the semiclassical spectrum at energy E. A natural question is: how is $P(S)$ related to the classical motion on the energy surface E? Three special cases have been studied before; in each of them, $P(S)$ takes universal functional forms parametrised by the mean level density ρ which, for a system with Hamiltonian $H(q_1 \ldots q_f, p_1 \ldots p_f)$, is given by

$$\rho = (2\pi\hbar)^{-f} \int \mathrm{d}q_1 \ldots \int \mathrm{d}q_f \int \mathrm{d}p_1 \ldots \mathrm{d}p_f \, \delta(E - H(q_1 \ldots p_f)). \tag{1}$$

The first special case is that of one-dimensional systems, such as particles moving in single potential wells, where the phase-plane contours are simple closed curves. The levels form, locally, a perfectly regular sequence of WKB type, and

$$P(S) = \delta(S - \rho^{-1}). \tag{2}$$

This trivial situation will not be considered further.

The second special case is that of multidimensional integrable systems, where trajectories wind smoothly round f-dimensional tori in the $2f$-dimensional phase space. Berry and Tabor (1977) showed that the levels are uncorrelated and so form a Poisson process whose level spacing distribution is

$$P(S) = \rho \, \mathrm{e}^{-\rho S}. \tag{3}$$

The third special case is that of chaotic motion, where systems are ergodic and almost all orbits densely and unpredictably explore the $(2f-1)$-dimensional energy surface. Growing numerical evidence (most recently by Bohigas *et al* (1984) and earlier by McDonald and Kaufman (1979), Berry (1981a) and Casati *et al* (1980)) and a persuasive theoretical argument (Pechukas 1983) suggest that the statistics of energies of these semiclassical irregular states are the same as those of ensembles of real symmetric matrices whose elements are Gaussian distributed (Porter 1965). For such systems, $P(S)$ is closely approximated by the Wigner distribution

$$P(S)=\tfrac{1}{2}\pi\rho^2 S\exp(-\tfrac{1}{4}\pi\rho^2 S^2). \tag{4}$$

Generic systems do not conform to these special cases: their phase space is mixed, in the sense that some orbits with energy E wind regularly round f-dimensional tori and others explore $(2f-1)$-dimensional regions chaotically. Our purpose in this paper is to obtain corresponding expressions for $P(S)$ which provide a natural interpolation between the Poisson formula (3) and the Wigner formula (4).

Underlying our calculation is the idea that each connected regular or irregular classical phase-space region in ΔE gives rise to its own sequence of regular or irregular levels. For the ith such region, the level density ρ_i is proportional to the Liouville measure of the region and is given by an expression of the form (1) with the integration correspondingly restricted, and the level spacing distribution $P_i(S)$ has the form (3) for a regular region and (4) for an irregular region. In the semiclassical limit all these sequences are independent and the complete spectrum is obtained by their random superposition. The statistical problem of superposing sequences of levels is solved in § 2, and the resulting level spacing distributions are studied in § 3.

The function $P(S)$ describes semiclassical spectra on scales of the order of the mean level spacing $\hbar^f$. On much larger scales, of order $\hbar$, there is long-range oscillatory clustering of the levels; this is not described by $P(S)$ and arises from classical closed orbits, as originally pointed out by Gutzwiller (1967, 1969, 1970, 1971, 1978) and emphasised by Balian and Bloch (1972). On much finer scales the spectrum will be affected by tunnelling between classically separated regions of phase space (Ozorio de Almeida 1984; see also Berry 1984a); even in integrable systems such tunnelling violates our assumption of independence of level sequences from different phase-space regions, but its influence on $P(S)$ is confined to the tiny region $0<S<O(\exp(-\text{constant}/\hbar))$ which is invisible on the scale $\hbar^f$ that we are studying here. On the finest scales of all, spectra are dominated by the effects of degeneracies (which can be made to occur by varying parameters in H), in ways explained by Berry (1984b). A discussion of semiclassical spectra in terms of the features resolved under different magnifications of energy intervals, as measured in comparison with $\hbar$, is given by Berry (1984c). More general reviews of semiclassical mechanics are given by Zaslavsky (1981) and Berry (1983).

2. Superposition of level sequences

Consider N sequences of levels with mean densities ρ_i and spacing distributions $P_i(S)$, so that

$$\overline{S_i}=\int_0^\infty dS\, SP_i(S)=\rho_i^{-1}, \qquad \text{where} \int_0^\infty dS\, P_i(S)=1. \tag{5}$$

The sequences are statistically independent, and we seek the spacing distribution $P(S)$ of the combined sequence obtained by superposing them. This combined sequence has mean level density

$$\rho=\sum_{i=1}^{N}\rho_i, \tag{6}$$

given in terms of the Hamiltonian by equation (1).

We calculate $P(S)$ in terms of the probability that there is no level in the interval E to $E+S$, given that there is a level at E. This probability is $\int_S^\infty P(x)\,\mathrm{d}x$ and is given as the sum of N independent contributions, the ith of which corresponds to E being a level of the ith sequence. Thus

$$\int_S^\infty \mathrm{d}x\,P(x)=\sum_{i=1}^{N}\left(\frac{\rho_i}{\rho}\int_S^\infty \mathrm{d}y\,P_i(y)\prod_{\substack{j=1\\ j\neq i}}^{N}Q_j(S)\right) \tag{7}$$

where in each term the factor ρ_i/ρ is the probability that E belongs to the ith sequence, $\int_S^\infty \mathrm{d}y\,P_i(y)$ is the probability that no further level of this sequence lies in the interval, and $Q_j(S)$ is the probability that no level of the jth sequence lies in the interval.

To find $Q_j(S)$, we note that in

$$\{\mathrm{d}\sigma\,P_j(\sigma)\sigma\rho_j\}\{(1-S/\sigma)\theta(\sigma-S)\} \tag{8}$$

the first factor is the probability that E, which is uncorrelated with the jth sequence, lies in a gap of length σ to $\sigma+\mathrm{d}\sigma$ of that sequence; and the second factor is the probability of having no level of this sequence in an interval of length S inside this gap (θ denotes the unit step function). Integration over σ then gives $Q_j(S)$ as

$$Q_j(S)=\rho_j\int_S^\infty \mathrm{d}\sigma\,P_j(\sigma)(\sigma-S). \tag{9}$$

Thus (7) becomes

$$\int_S^\infty \mathrm{d}x\,P(x)=\frac{1}{\rho}\left(\prod_{k=1}^{N}\rho_k\right)\sum_{i=1}^{N}\left(\left(\int_S^\infty \mathrm{d}y\,P_i(y)\right)\prod_{\substack{j=1\\ j\neq i}}^{N}\int_S^\infty \mathrm{d}\sigma\,P_j(\sigma)(\sigma-S)\right). \tag{10}$$

This result takes a much simpler form if we define

$$Z_i(S)\equiv\int_S^\infty \mathrm{d}\sigma\int_\sigma^\infty \mathrm{d}x\,P_i(x)=\int_S^\infty \mathrm{d}\sigma\,P_i(\sigma)(\sigma-S) \tag{11}$$

and integrate (10) over S, to give a factorised expression which embodies the statistical independence of the N sequences, namely

$$Z(S)\equiv\int_S^\infty \mathrm{d}\sigma\int_\sigma^\infty \mathrm{d}x\,P(x)=\frac{1}{\rho}\prod_{i=1}^{N}\rho_i Z_i(S), \tag{12}$$

whose correctness is easily verified by differentiating the product with respect to S. In terms of this, the level spacing distribution of the full spectrum is

$$P(S)=\mathrm{d}^2Z(S)/\mathrm{d}S^2. \tag{13}$$

To show that this function is normalised to unity and gives the mean level spacing as ρ^{-1}, we need only realise that (5) and (11) imply

$$Z_i(0)=\rho_i^{-1}, \qquad dZ_i(0)/dS=-1 \tag{14}$$

and observe that the product (12) implies corresponding relations for $Z(0)$ and $dZ(0)/dS$, provided ρ satisfies (6).

For later reference we note that from (11)–(13) it follows that $P(0)$, whose value is a simple index of fine-scale level clustering, is

$$P(0)=\rho+\frac{1}{\rho}\sum_{i=1}^{N}\rho_i(P_i(0)-\rho_i), \tag{15}$$

and that higher moments of the spacing distribution are given by

$$\overline{S^n}\equiv\int_0^\infty dS\, S^nP(S)=n(n-1)\int_0^\infty dS\, S^{n-2}Z(S) \qquad (n\geq 2). \tag{16}$$

The integrals converge for all n because of the exponential decay of all the factors Z_i contributing to Z.

Gurevich and Pevsner (1956) determined the statistics of the superposition of two independent level sequences, and introduced the functions $Z_i(S)$. Lane (1957) also considered this problem, in unpublished work cited by Rosenzweig and Porter (1960). The latter authors studied the superposition of N sequences all of whose separate $P_i(S)$ have the same form but whose weightings ρ_i are different. Our formulae (11)–(13) constitute a slight generalisation of these results, and will now be applied in a semiclassical context.

3. Spacing distributions

According to the programme outlined in § 1, the sequences to be superposed have spacing distributions $P_i(S)$ of the form (3) for those phase-space regions which support regular motion, and (4) for those supporting chaotic motion, with ρ_i proportional to the Liouville measures of the regions.

It is obvious physically that superposition of all the Poisson-type level sequences corresponding to regular motion will produce a sequence which is itself a Poisson process, $P(S)$ being of the form (3) with ρ given by the sum of the level densities of the separate regular regions. And this result follows from (12) because the factors ρ_iZ_i corresponding to regular regions have, from (11) and (3), the form $\rho_iZ_i=\exp(-\rho_iS)$. From now on we shall denote by ρ_1 the level density of all the regular sequences taken together; the corresponding contribution to (12) is

$$Z_1(S)=\exp(-\rho_1S)/\rho_1. \tag{17}$$

The remaining phase-space regions $i=2,\ldots,N$ are chaotic, and (11) and the approximation (4) give

$$Z_i(S)=\operatorname{erfc}(\tfrac{1}{2}\sqrt{\pi}\rho_iS)/\rho_i \qquad (i\geq 2) \tag{18}$$

where

$$\operatorname{erfc} x\equiv(2/\sqrt{\pi})\int_x^\infty dt\, e^{-t^2}. \tag{19}$$

The level spacing distribution is now obtained from (12) and (13) as

$$P(S)=\frac{1}{\rho}\frac{\mathrm{d}^2}{\mathrm{d}S^2}\left[\mathrm{e}^{-\rho_1 S}\prod_{i=2}^{N}\operatorname{erfc}\left(\frac{\sqrt{\pi}}{2}\rho_i S\right)\right]. \tag{20}$$

This is our central result. When $S=0$

$$P(0)=\rho-\frac{1}{\rho}\sum_{i=2}^{N}\rho_i^2. \tag{21}$$

For systems with three or more freedoms, Arnold diffusion will ensure that there is just one chaotic region forming a connected web; this phenomenon has its origin in the fact that f-dimensional tori do not stratify the $(2f-1)$-dimensional energy surface if $f\geqslant 3$ (see Lichtenberg and Lieberman 1983). Of course there are, generically, infinitely many regular regions (tubes filled with tori), but we have seen that these can be amalgamated into a single level sequence with density ρ_1. Thus for $f\geqslant 3$ we can take $N=2$, with ρ_2 proportional to the measure of the whole chaotic region. The particularly simple form of $P(S)$ in this case will be written explicitly later.

When $f=2$ there are, generically, infinitely many chaotic regions, which manifest themselves as separate stochastic components on a Poincaré surface of section (Lichtenberg and Lieberman 1983). In such cases we expect that in practice (20) will be applied for finite N, with $N-1$ being the number of chaotic regions considered to have significant measure. But it is important to have a way of choosing N, and to confirm that the infinitely many chaotic regions thus neglected have negligible influence on $P(S)$; this we now do.

Let $\nu(\rho')\,\mathrm{d}\rho'$ be the number of classical chaotic regions giving sequences with level densities between ρ' and $\rho'+\mathrm{d}\rho'$. This function must satisfy the normalisation

$$\rho-\rho_1=\int_0^{\rho-\rho_1}\mathrm{d}\rho'\,\rho'\nu(\rho'), \tag{22}$$

where as before ρ is the total mean level density. The interesting case is that for which the total number of chaotic regions, $\int_0^{\rho-\rho_1}\mathrm{d}\rho'\,\nu(\rho')$, diverges, whereas (22) is finite. This implies that

$$\text{if } \nu(\rho')\to\text{constant}/(\rho')^{\alpha} \text{ as } \rho'\to 0 \qquad \text{then } 1\leqslant\alpha\leqslant 2. \tag{23}$$

To gauge the effect of the divergence of $\nu(\rho')$ we write the infinite product for $Z(S)$ in the form of N factors corresponding to the regular region plus the predominant chaotic regions, multiplied by a continuous 'tail' from the chaotic regions of small measure. Equations (12), (17) and (18) now give

$$Z(S)=\frac{1}{\rho}\mathrm{e}^{-\rho_1 S}\prod_{i=2}^{N}\operatorname{erfc}\left(\frac{\sqrt{\pi}}{2}\rho_i S\right)\exp\left\{\int_0^{\rho_{\min}}\mathrm{d}\rho'\,\nu(\rho')\ln\left[\operatorname{erfc}\left(\frac{\sqrt{\pi}}{2}\rho' S\right)\right]\right\} \tag{24}$$

where $\rho_{\min}$ is the density of the level sequence corresponding to the largest of the small chaotic regions, given by

$$\int_0^{\rho_{\min}}\mathrm{d}\rho'\,\rho'\nu(\rho')=\rho-\rho_1-\sum_{i=2}^{N}\rho_i. \tag{25}$$

Obviously $\rho_{\min}\ll\rho$. If in addition we consider only S satisfying

$$\rho_{\min}S\ll 1, \tag{26}$$

use of (19) with x small enables the logarithm in (24) to be written as

$$\ln[\operatorname{erfc}(\tfrac{1}{2}\sqrt{\pi}\rho' S)] \approx -\rho' S. \qquad (27)$$

Equations (25) and (24) now show that the combined effect of all the small chaotic regions can be considered as a small modification to the regular density ρ_1. The condition (26) has a simple physical interpretation, which also provides a criterion for choosing N: 'small' chaotic regions are those giving rise to level sequences so sparse that there is a negligible chance of finding such a level in an energy interval S. Evidently N must be taken larger if $P(S)$ is required for larger S.

The foregoing argument confirms that even if $f=2$ the level spacing distribution (20) can be well approximated by considering a finite number $N-1$ of chaotic regions.

The most important case of (20) occurs when $N=2$; this applies, as we have seen, when $f \geqslant 3$, and also when $f=2$ if one chaotic region predominates. We normalise the energy scale to ensure that the mean density ρ, and thus the mean level spacing, are unity, and denote the spacing distribution by $P_2(S, \rho_1)$; ρ_1 is now simply the fraction of the energy surface for which motion is regular. Then $Z(S) = \exp(-\rho_1 S)\operatorname{erfc}(\tfrac{1}{2}\sqrt{\pi}\bar{\rho}S)$

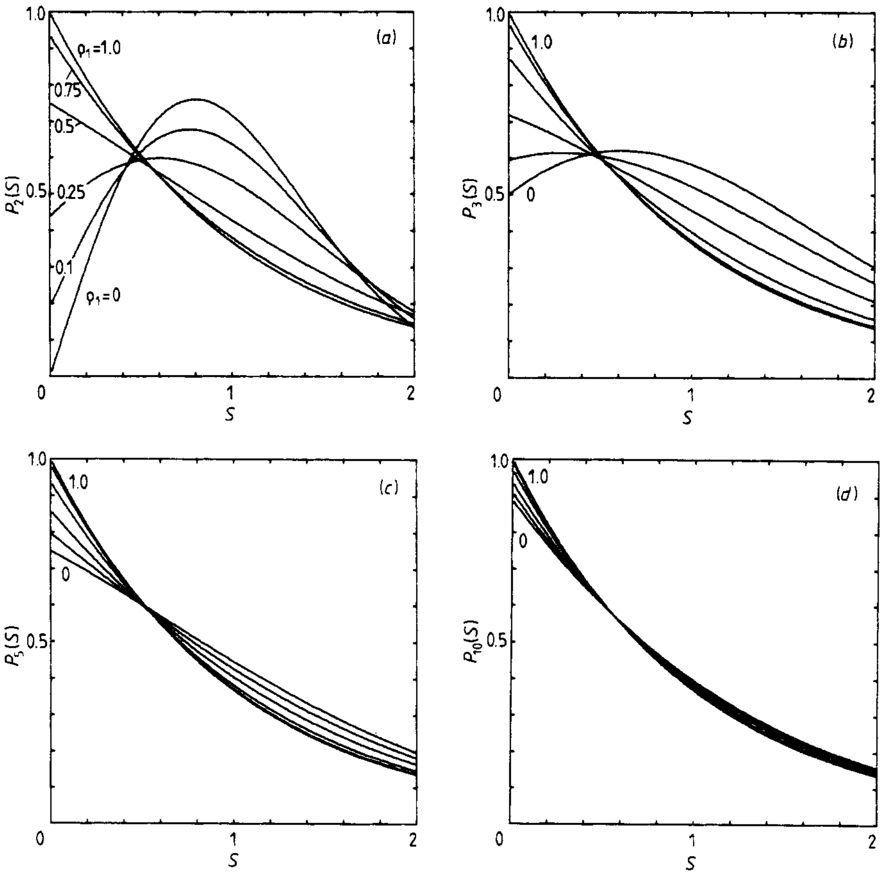

Figure 1. Level spacing distributions $P_N(S, \rho_1)$ computed from (28) and (33) for $\rho_1 = 0, 0.1, 0.25, 0.5, 0.75$ and 1.0: (*a*) $N=2$; (*b*) $N=3$; (*c*) $N=5$; (*d*) $N=10$. ρ_1 is the fraction of the classical energy surface for which the orbits lie on tori; the remainder of the energy surface is assumed to be divided into $N-1$ separate chaotic regions of equal measure.

and (20) give the simple expression

$$P_2(S, \rho_1) = \rho_1^2 \,\mathrm{e}^{-\rho_1 S} \operatorname{erfc}(\tfrac{1}{2}\sqrt{\pi}\bar{\rho}S) + (2\rho_1\bar{\rho} + \tfrac{1}{2}\pi\bar{\rho}^3 S) \exp(-\rho_1 S - \tfrac{1}{4}\pi\bar{\rho}^2 S^2) \qquad (\bar{\rho} \equiv 1 - \rho_1). \tag{28}$$

Figure 1(*a*) shows the form of P_2 for several ρ_1 values interpolating between $\rho_1 = 0$ (Wigner distribution) and $\rho_1 = 1$ (Poisson distribution). Evidently a sensitive indicator of the regular fraction ρ_1 is (cf (21))

$$P_2(0, \rho_1) = 1 - \bar{\rho}^2 = \rho_1(2 - \rho_1). \tag{29}$$

A less sensitive indicator is (from (16)) the mean square spacing

$$\overline{S^2} = (2/\rho_1)[1 - \exp(\rho_1^2/\pi\bar{\rho}^2) \operatorname{erfc}(\rho_1/\sqrt{\pi}\bar{\rho})], \tag{30}$$

which increases from $4/\pi$ ($\rho_1 = 0$) to 2 ($\rho_1 = 1$). Higher moments are given by

$$\overline{S^{n+2}} = \tfrac{1}{2}(n+1)(n+2)(-1)^n \,\mathrm{d}^n\overline{S^2}/\mathrm{d}\rho_1^n. \tag{31}$$

To illustrate the effect of more than one chaotic region, we consider the case where they all have the same measure $\bar{\rho}$, so that (again choosing $\rho = 1$)

$$\bar{\rho} = (1 - \rho_1)/(N - 1). \tag{32}$$

Equation (20) gives, for the spacing distributions which we now denote by $P_N(S, \rho_1)$,

$$P_N(S, \rho_1) = \mathrm{e}^{-\rho_1 S}[\operatorname{erfc}(\tfrac{1}{2}\sqrt{\pi}\bar{\rho}S)]^{N-3}\{\rho_1^2[\operatorname{erfc}(\tfrac{1}{2}\sqrt{\pi}\bar{\rho}S)]^2 + (N-1)\operatorname{erfc}(\tfrac{1}{2}\sqrt{\pi}\bar{\rho}S) \times \exp(-\tfrac{1}{4}\pi\bar{\rho}^2 S^2)(2\rho_1\bar{\rho} + \tfrac{1}{2}\pi\bar{\rho}^3 S) + (N-1)(N-2)\bar{\rho}^2 \exp(-\tfrac{1}{4}\pi\bar{\rho}^2 S^2)\}. \tag{33}$$

Figures 1(*b*–*d*) show the forms of P_3, P_5 and P_{10} for a sequence of ρ_1 values. It is clear that even when the regular density ρ_1 is negligible the superposition of $N-1$ independent Wigner distributions of equal strength tends rapidly to a Poisson distribution as N increases, and indeed this follows from a trivial asymptotic analysis of (33).

4. Discussion

The central result of this paper is the family of level spacing distributions (20), whose calculation requires only a knowledge of the purely classical quantities ρ_i. Is it feasible to attempt numerical tests of these predicted forms for $P(S)$, by comparing them with quantum mechanically computed level spacing distributions? For the most commonly studied quantal systems displaying both regular and chaotic classical motion, namely particles moving in the fields of nonlinearly perturbed multidimensional harmonic oscillators, we think such a comparison is probably not feasible at present. The reason is that for these systems the relative measures of regular and chaotic regions change with energy, and in order to calculate $P(S)$ corresponding to a given energy E, as described in § 1, the energy interval ΔE must be small. To get enough levels in this interval to enable $P(S)$ to be computed to sufficient accuracy would require an $\hbar$ so small as to demand the diagonalisation of prohibitively large matrices. (The histograms of level spacing distributions for coupled Morse oscillators, recently published by Matsushita and Terasaka (1984), incorporate levels over a wide energy range and so should not be compared with the curves in figure 1.)

This difficulty could be avoided by choosing systems whose Hamiltonians have scaling properties which imply that the classical phase-space structure is the same at all energies. Then the restriction to levels within ΔE is unnecessary, and any sequence may be employed to compute $P(S)$, provided the energies are scaled to have uniform mean density. For example, non-relativistic particles moving in potentials scaling as

$$V(\alpha q_1 \ldots \alpha q_f) = \alpha^s V(q_1 \ldots q_f) \quad (34)$$

would allow $P(S)$ to be calculated not from the levels E_m but by using the scaled sequence

$$\varepsilon_m = E_m^{f+f/s-1}. \quad (35)$$

A particularly suitable class of systems of this type is planar quantum billiards, for which $f=2$ and $s \to \infty$. Among billiards with analytic boundaries, and inside which the classical motion exhibits both regularity and chaos, are the ovals studied by Berry (1981b) and the heart shapes studied by Robnik (1983, 1984).

Finally, J H Hannay has remarked to us that our procedure for obtaining the semiclassical $P(S)$ can be considered as associating with each classical invariant manifold a Wigner-distributed level sequence, whose level density is proportional to the Liouville measure of the manifold, and then superposing all the sequences. An irregular region is a single indecomposable manifold with finite measure and contributes a Wigner distribution with finite density as explained in § 3. A regular region decomposes into infinitely many tori; each of them contributes a Wigner distribution of infinitestimal strength, whose superposition gives the Poisson distribution for the whole regular region (usually this is considered (Berry and Tabor 1977) to arise from the superposition of the sequences of equally spaced levels obtained by varying one quantum number at a time).

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Note added in proof. A series of curves qualitatively similar to figure 1(a) have been computed by Seligman *et al* (1984) for the levels of a family of two-dimensional non-integral potentials exhibiting different degrees of stochasticity.

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