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Berry's conjecture and information theory

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It is shown that, by applying a principle of information theory, one obtains Berry's conjecture regarding the high-lying quantal energy eigenstates of classically chaotic systems. [S1063-651X(97)03708-2]

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In many problems of physical interest, it is necessary to abandon a search for the exact solution, and to turn instead to a statistical approach. This involves mentally replacing *the* answer which we seek, with an ensemble of possibilities, then adopting the attitude that each member of the ensemble is an equally likely candidate for the true solution. The choice of ensemble then becomes centrally important, and here *information theory* provides a reliable guiding principle. The principle instructs us to choose the least biased ensemble (the one which minimizes information content), subject to some relevant constraints. A well-known illustration arises in classical statistical mechanics: the least biased distribution in phase space, subject to a fixed normalization and average energy, is the canonical ensemble of Gibbs [1]. (The principle of least bias, or maximum entropy, arises in *nonequilibrium* situations as well [2].) Another example appears in random matrix theory: by minimizing the information content of an ensemble of matrices, subject to various simple constraints, one obtains the standard random matrix ensembles [3]. The purpose of this paper is to point out that *Berry's conjecture* [4] regarding the energy eigenstates of chaotic systems, also emerges naturally from this *principle of least bias*.

Berry's conjecture makes two assertions regarding the high-lying energy eigenstates ψ_E of quantal systems whose classical counterparts are chaotic and ergodic: (1) Such eigenstates appear to be random Gaussian functions $\psi(\mathbf{x})$ on configuration space, (2) with two-point correlations given by

$$\overline{\psi^*\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\psi\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)}=\frac{1}{\Sigma}\int d\mathbf{p}e^{i\mathbf{p}\cdot\mathbf{s}/\hbar}\,\delta(E-H(\mathbf{x},\mathbf{p})). \quad (1)$$

Here, E is the energy of the eigenstate, $H(\mathbf{x},\mathbf{p})$ is the classical Hamiltonian describing the system, and $\Sigma\equiv\int d\mathbf{x}\int d\mathbf{p}\,\delta(E-H(\mathbf{x},\mathbf{p}))$; if the Hamiltonian is time-reversal invariant, then $\psi(\mathbf{x})$ is a real random Gaussian function, otherwise $\psi(\mathbf{x})$ is a complex random Gaussian function. Berry's conjecture thus uniquely specifies, for a given energy E, an ensemble $\mathcal{M}_E$ of wave functions $\psi(\mathbf{x})$ [i.e., $\mathcal{M}_E$ is the Gaussian ensemble with two-point correlations given by Eq. (1)], and states that an eigenstate ψ_E at energy E will look as if it were chosen randomly from this ensemble.

The correlations given by Eq. (1) are motivated by considering the Wigner function [5] corresponding to the eigenstate ψ_E,

$$W_E(\mathbf{x},\mathbf{p})\equiv(2\pi\hbar)^{-D}\int d\mathbf{s}\,\psi_E^*\left(\mathbf{x}-\frac{\mathbf{s}}{2}\right)\psi_E\left(\mathbf{x}+\frac{\mathbf{s}}{2}\right)e^{-i\mathbf{p}\cdot\mathbf{s}/\hbar}, \quad (2)$$

where D is the dimensionality of the system. For high-lying states ψ_E, this Wigner function, after local smoothing in the $\mathbf{x}$ variable, is expected to converge to the microcanonical distribution in phase space [4,6–8]:

$$W_E^{\mathrm{sm}}(\mathbf{x},\mathbf{p})\approx\frac{1}{\Sigma}\,\delta(E-H(\mathbf{x},\mathbf{p})). \quad (3)$$

By taking the Fourier transform of both sides of Eq. (1), and then smoothing locally in the $\mathbf{x}$ variable [9] rather than averaging over the ensemble $\mathcal{M}_E$, it is straightforward to show that the correlations given by Eq. (1) produce the desired result, Eq. (3).

The assertion that $\psi_E(\mathbf{x})$ is a Gaussian random function is most easily motivated by viewing $\psi_E(\mathbf{x})$, locally, as a superposition of de Broglie waves with random phases [4]. When the number of these waves becomes infinite, the central limit theorem tells us that $\psi_E(\mathbf{x})$ will look like a Gaussian random function.

It should be noted here that, recently, the spatial correlations of chaotic wave functions have been studied within an alternative, ''supersymmetric'' framework [10]. The results were found to be in agreement with Berry's conjecture, and also with microwave cavity experiments.

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We can interpret Berry's conjecture as making a specific prediction about the eigenstate ψ_E: once we compute $\psi_E(\mathbf{x})$ by solving the Schrödinger equation, we can subject it to various tests (see, e.g., Ref. [11]), and we will observe that, yes, $\psi_E(\mathbf{x})$ really behaves as a Gaussian random function with the two-point correlations given by Eq. (1). Alternatively, we can interpret Berry's conjecture as providing us with the appropriate ensemble of wave functions from which to choose a surrogate for the true eigenstate ψ_E, if we cannot (or do not care to) actually solve for $\psi_E(\mathbf{x})$. In this interpretation, $\mathcal{M}_E$ stands to ψ_E much as, in classical statistical mechanics, the canonical ensemble stands to the instantaneous microscopic state of a system at a given temperature. It is within the context of the second point of view that we will show that Berry's conjecture may be ''derived'' from information theory. Specifically, we will show that, by applying the principle of least bias, and accepting the correlations given by Eq. (1) as a set of relevant constraints, we are led immediately to a statement of Berry's conjecture.

We thus pose the following question. Suppose we have a quantal Hamiltonian $\hat{H}$, whose classical counterpart $H(\mathbf{x},\mathbf{p})$ is chaotic and ergodic; and suppose we are told that a high-lying eigenstate of $\hat{H}$—represented by a wave function $\psi_E(\mathbf{x})$—exists at energy E. Given this limited knowledge, how do we go about making a ''best guess'' for $\psi_E(\mathbf{x})$? By a best guess, we mean not a single wave function, but rather a probability distribution $P_E[\psi]$ in Hilbert space, such that, by sampling randomly from this distribution, we are making a guess which takes into account our limited knowledge regarding ψ_E, but is otherwise unbiased. Information theory provides a general prescription for constructing such a distribution. First, we quantify the information I contained in an arbitrary distribution $P[\psi]$. Next, we identify the constraints on $P[\psi]$ imposed by our limited knowledge. Finally, we minimize $I\{P[\psi]\}$ subject to these constraints. The resulting distribution $P_E[\psi]$ is the least biased one, consistent with our limited knowledge. Let us now implement this procedure.

Given a probability distribution $P[\psi]$ in Hilbert space, the amount of information I contained in this distribution is

$$I\{P[\psi]\}=\int P[\psi]\ln P[\psi]. \tag{4}$$

The integral is over all square-integrable functions $\psi(\mathbf{x})$, where $\psi(\mathbf{x})$ is taken to be real if the Hamiltonian is time-reversal invariant, and complex otherwise. [The integral in Eq. (4) requires a measure $d\mu$ on Hilbert space. We take the usual Euclidean measure of field theories [12]: a wave function is represented by its value at N discrete points in configuration space, and the set of these values is regarded as a (real or complex) Cartesian vector. Hence, $d\mu = d\psi_1 d\psi_2,\ldots,d\psi_N$, where $\psi_i \equiv \psi(\mathbf{x}_i)$. The limit $N\to\infty$ is finally taken.]

Since we will want to minimize $I\{P\}$ subject to relevant constraints on the distribution $P[\psi]$, our next task is to identify those constraints. The first is simply that P ought to be normalized to unity

$$\int P[\psi]=1. \tag{5}$$

The second constraint is that embodied by Eq. (1)

$$\int P[\psi]\psi^*(\mathbf{x}_1)\psi(\mathbf{x}_2)=\frac{1}{\Sigma}\int d\mathbf{p}e^{i\mathbf{p}\cdot\mathbf{s}/\hbar}\delta(E-H(\mathbf{x},\mathbf{p})), \tag{6}$$

where $\mathbf{s}\equiv\mathbf{x}_2-\mathbf{x}_1$ and $\mathbf{x}\equiv(\mathbf{x}_1+\mathbf{x}_2)/2$. (Both $\mathbf{x}_1$ and $\mathbf{x}_2$ are assumed to be within the classically allowed region; outside this region, the wave function is taken to be zero.) As explained briefly above (see also Refs. [4,7,8]), this constraint is motivated by the expectation that the smoothed Wigner function corresponding to ψ_E will approximate the microcanonical distribution in phase space [Eq. (3)]. Note that Eq. (6) does not represent a *single* constraint, but rather a set of constraints, where each member of the set is specified by $(\mathbf{x}_1,\mathbf{x}_2)$.

Finally, we minimize the information $I\{P[\psi]\}$, subject to the constraints in Eqs. (5) and (6). We do this in the usual way, by introducing Lagrange multipliers. That is, we define

$$\begin{aligned} A\{P[\psi]\}\equiv I\{P[\psi]\}+\lambda\int P[\psi] \\ +\int\int\Lambda(\mathbf{x}_1,\mathbf{x}_2)\int P[\psi]\psi^*(\mathbf{x}_1)\psi(\mathbf{x}_2) \\ =\int P[\psi]\Big(\ln P[\psi]+\lambda \\ +\int\int\Lambda(\mathbf{x}_1,\mathbf{x}_2)\psi^*(\mathbf{x}_1)\psi(\mathbf{x}_2)\Big), \end{aligned} \tag{7}$$

where λ is the Lagrange multiplier associated with Eq. (5), $\Lambda(\mathbf{x}_1,\mathbf{x}_2)$ is the set of multipliers associated with Eq. (6), and $\int\int$ is shorthand for $\int d\mathbf{x}_1\int d\mathbf{x}_2$. For a given distribution $P[\psi]$, the change in A induced by a small variation $\delta P[\psi]$ is, to first order in $\delta P[\psi]$,

$$\delta A=\int\delta P\Big(\ln P+(\lambda+1)+\int\int\Lambda(\mathbf{x}_1,\mathbf{x}_2)\psi^*(\mathbf{x}_1)\psi(\mathbf{x}_2)\Big). \tag{8}$$

To minimize A [i.e., to minimize I subject to the constraints imposed by Eqs. (5) and (6)] we insist that $\delta A=0$ for all variations δP. From Eq. (8), it follows that the distribution $P_E[\psi]$ which accomplishes this minimization has the form:

$$P_E[\psi]=\mathcal{N}\exp-\int\int\Lambda(\mathbf{x}_1,\mathbf{x}_2)\psi^*(\mathbf{x}_1)\psi(\mathbf{x}_2). \tag{9}$$

The constant $\mathcal{N}$ is determined by normalization [Eq. (5)], whereas the two-point correlations [Eq. (6)] uniquely determine $\Lambda(\mathbf{x}_1,\mathbf{x}_2)$. (Specifically, the kernel $\Lambda(\mathbf{x}_1,\mathbf{x}_2)$ is just the inverse of $\overline{\psi^*(\mathbf{x}_1)\psi(\mathbf{x}_2)}$, divided by 2 if H is time-reversal invariant [13].)

Once $\mathcal{N}$ and $\Lambda(\mathbf{x}_1,\mathbf{x}_2)$ are determined, Eq. (9) completely specifies a probability distribution P_E on Hilbert space. By randomly sampling from this distribution, we generate a random function $\psi(\mathbf{x})$, with two-point correlations $\overline{\psi^*(\mathbf{x}_1)\psi(\mathbf{x}_2)}$ which (by construction) satisfy Eq. (1). But is a function sampled from P_E a *Gaussian* random function? The answer is yes [11,13]. For a random function $f(\mathbf{x})$, let

$\mathcal{P}_n(f_1, \ldots, f_n)$ denote the joint probability distribution of finding that $f(\mathbf{x}_i) = f_i$, $i = 1, \ldots, n$. Then $f(\mathbf{x})$ is Gaussian if $\mathcal{P}_n$ is a Gaussian in $(f_1, \ldots, f_n)$ space, for any $(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)$, $n \geqslant 1$ [14]. A function $\psi(\mathbf{x})$ obtained by sampling the probability distribution given by Eq. (9) satisfies this condition.

We thus arrive at the following conclusion: given the limited knowledge that an eigenstate of $\hat{H}$ exists at energy E, the least biased guess for $\psi_E(\mathbf{x})$ (by reasonable construction) is a Gaussian random function, with the two-point correlations given by Eq. (1). This is just another way of stating Berry's conjecture. (Instead of saying that ψ_E ''looks like'' a Gaussian random function, we say that a Gaussian random function is a ''best guess'' for ψ_E.) In this sense, Berry's conjecture allows for a statistical description of eigenfunctions, by providing us with the appropriate ensemble $\mathcal{M}_E$ in Hilbert space to use as a stand-in for the true energy eigenstate ψ_E. When the latter is unobtainable [15] calculations performed with $\mathcal{M}_E$ may be tractable [16], just as the canonical ensemble of ordinary statistical mechanics makes possible accurate computations without demanding detailed knowledge of the microscopic state of the system.

The notion that Berry's conjecture is gainfully viewed as a statistical theory—in analogy with classical statistical mechanics, or random matrix theory—has been a guiding theme of this paper. As stressed in the opening paragraph, the first order of business with such theories is to identify the proper ensemble to use in place of an exact description of the object of study (be it the microscopic state of a many-body system, or a complicated Hermitian matrix, or a quantal eigenstate). A common feature of statistical theories is that this ensemble follows in a natural way from the information theoretic principle of least bias. The purpose of this paper has simply been to point out that Berry's conjecture shares this feature.

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[1] D. Chandler, *Introduction to Modern Statistical Mechanics* (Oxford University Press, New York, 1987), Sec. 3.7. Note that minimizing the information content of the ensemble is the same as maximizing its entropy.

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[9] This smoothing is performed on a scale which is large compared with the local correlation length of $\psi(\mathbf{x})$, but small compared with a classically relevant distance scale (see, e.g., Eqs. 3.29 and 3.30 of Ref. [8]). This allows us to replace ensemble averaging with local smoothing.

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[15] Note that the computational effort required to solve Schrödinger's equation grows exponentially with the dimensionality N of the configuration space.

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