Berry’s conjecture and information theory

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(March 21, 2022)

Abstract

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.
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]. 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[2]. The purpose of this paper is to point out that Berry’s conjecture[3] 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 $\psi_E$ of quantal systems whose classical counterparts are chaotic and ergodic[1]: (1) Such eigenstates appear to be random Gaussian functions $\psi(x)$ on configuration space, (2) with two-point correlations given by

$$\psi^*(x - \frac{s}{2})\psi(x + \frac{s}{2}) = \frac{1}{\Sigma} \int dp e^{i p \cdot s/\hbar} \delta[E - H(x, p)]$$

(1)

Here, $E$ is the energy of the eigenstate, $H(x, p)$ is the classical Hamiltonian describing the system, and $\Sigma \equiv \int dx \int dp \delta[E - H(x, p)]$; if the Hamiltonian is time-reversal-invariant, then $\psi(x)$ is a real random Gaussian function, otherwise $\psi(x)$ is a complex random Gaussian function. Berry’s conjecture thus uniquely specifies, for a given energy $E$, an ensemble $\mathcal{M}_E$ of wavefunctions $\psi(x)$ (i.e. $\mathcal{M}_E$ is the Gaussian ensemble with two-point correlations given

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1 By “chaotic and ergodic”, we mean that all trajectories, except a set of measure zero, chaotically and ergodically explore the surface of constant energy in phase space.
by Eq.1, and states that an eigenstate $\psi_E$ 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 [4] corresponding to the eigenstate $\psi_E$,

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

(2)

where $D$ is the dimensionality of the system. For high-lying states $\psi_E$, this Wigner function, after local smoothing in the $x$ variable, is expected to converge to the microcanonical distribution in phase space [3,5–7]:

$$W_{\text{sm}}^E(x, p) \approx \frac{1}{\Sigma} \delta[E - H(x, p)].$$

(3)

By taking the Fourier transform of both sides of Eq.1, and then smoothing locally in the $x$-variable 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 $\psi_E(x)$ is a Gaussian random function is most easily motivated by viewing $\psi_E(x)$, locally, as a superposition of de Broglie waves with random phases [3]. When the number of these waves becomes infinite, the central limit theorem tells us that $\psi_E(x)$ will look like a Gaussian random function.

We can interpret Berry’s conjecture as making a specific prediction about the eigenstate $\psi_E$: once we compute $\psi_E(x)$ by solving the Schrödinger equation, we can subject it to various tests (see e.g. Ref. [8]), and we will observe that, yes, $\psi_E(x)$ really behaves as a Gaussian random function with two-point correlations given by Eq.1. Alternatively, we can interpret Berry’s conjecture as providing us with the appropriate ensemble of wavefunctions from which to choose a surrogate for the true eigenstate $\psi_E$, if we cannot (or do not care

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2This smoothing is performed on a scale which is large compared with the local correlation length of $\psi(x)$, but small compared with a classically relevant distance scale (see e.g. equations 3.29 and 3.30 of Ref. [5]). This allows us to replace ensemble averaging with local smoothing.
to actually solve for $\psi_E(x)$. In this interpretation, $M_E$ stands to $\psi_E$ 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. I 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 $H(x, p)$ is chaotic and ergodic; and suppose we are told that a high-lying eigenstate of $\hat{H}$ — represented by a wave function $\psi_E(x)$ — exists at energy $E$. Given this limited knowledge, how do we go about making a “best guess” for $\psi_E(x)$? 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 $\psi_E$, 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:

$$ I\{P[\psi]\} = \int P[\psi] \ln P[\psi]. \quad (4) $$

The integral is over all square-integrable functions $\psi(x)$, where $\psi(x)$ 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 [9]: a wavefunction 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,
\[ d\mu = d\psi_1 d\psi_2 \cdots d\psi_N, \text{ where } \psi_i \equiv \psi(x_i). \] 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:

\[ \int P[\psi] = 1. \quad (5) \]

The second constraint is that embodied by Eq. 4:

\[ \int P[\psi] \psi^*(x_1) \psi(x_2) = \frac{1}{\Sigma} \int dp \ e^{ip \cdot s/\hbar} \delta[E - H(x, p)], \quad (6) \]

where \( s \equiv x_2 - x_1 \) and \( x \equiv (x_1 + x_2)/2 \). (Both \( x_1 \) and \( x_2 \) are assumed to be within the classically allowed region; outside this region, the wavefunction is taken to be zero.) As explained briefly above (see also Refs. [3,6,7]), this constraint is motivated by the expectation that the smoothed Wigner function corresponding to \( \psi_E \) will approximate the microcanonical distribution in phase space (Eq. 3). Note that Eq. 4 does not represent a single constraint, but rather a set of constraints, where each member of the set is specified by \( (x_1, x_2) \).

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

\[ A\{P[\psi]\} \equiv I\{P[\psi]\} + \lambda \int P[\psi] + \int \int \Lambda(x_1, x_2) \int P[\psi] \psi^*(x_1) \psi(x_2) \]

\[ = \int P[\psi] \left( \ln P[\psi] + \lambda + \int \int \Lambda(x_1, x_2) \psi^*(x_1) \psi(x_2) \right), \quad (7) \]

where \( \lambda \) is the Lagrange multiplier associated with Eq. 5, \( \Lambda(x_1, x_2) \) is the set of multipliers associated with Eq. 6, and \( \int \int \) is shorthand for \( \int dx_1 \int dx_2 \). For a given distribution \( P[\psi] \), the change in \( A \) induced by a small variation \( \delta P[\psi] \) is, to first order in \( \delta P[\psi] \),

\[ \delta A = \int \delta P \left( \ln P + (\lambda + 1) + \int \int \Lambda(x_1, x_2) \psi^*(x_1) \psi(x_2) \right). \quad (8) \]

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 \( \delta P \). From Eq. 8, it follows that the distribution \( P_E[\psi] \) which accomplishes this minimization has the form:
\[ P_E[\psi] = \mathcal{N} \exp - \int \int \Lambda(x_1, x_2) \psi^*(x_1) \psi(x_2). \quad (9) \]

The constant \( \mathcal{N} \) is determined by normalization (Eq.5), whereas the two-point correlations (Eq.6) uniquely determine \( \Lambda(x_1, x_2) \). (Specifically, the kernel \( \Lambda(x_1, x_2) \) is just the inverse of \( \overline{\psi^*(x_1) \psi(x_2)} \), divided by 2 if \( H \) is time-reversal-invariant [10].)

Once \( \mathcal{N} \) and \( \Lambda(x_1, x_2) \) 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 \( \psi(x) \), with two-point correlations \( \overline{\psi^*(x_1) \psi(x_2)} \) which (by construction) satisfy Eq.1. But is a function sampled from \( P_E \) a Gaussian random function? The answer is yes [8,10]. For a random function \( f(x) \), let \( P_n(f_1, \cdots, f_n) \) denote the joint probability distribution of finding that \( f(x_i) = f_i, \ i = 1, \cdots, n \). Then \( f(x) \) is Gaussian if \( P_n \) is a Gaussian in \( (f_1, \cdots, f_n) \)-space, for any \( (x_1, x_2, \cdots, x_n) \), \( n \geq 1 \) [11]. A function \( \psi(x) \) 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 \( \psi_E(x) \) (by reasonable construction) is a Gaussian random function, with two-point correlations given by Eq.1. This is just another way of stating Berry’s conjecture. (Instead of saying that \( \psi_E \) “looks like” a Gaussian random function, we say that a Gaussian random function is a “best guess” for \( \psi_E \).) 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 \( \psi_E \). When the latter is unobtainable[3] calculations performed with \( \mathcal{M}_E \) may be tractable [12], 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

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3 Note that the computational effort required to solve Schrödinger’s equation grows exponentially with the dimensionality \( N \) of configuration space.
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.

ACKNOWLEDGMENTS

The author wishes to acknowledge useful conversations and correspondence with S.Jain, J.Morehead, and M.Srednicki.
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