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Fractal Eigenfunctions in (Classically) Nonintegrable Hamiltonian Systems.

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Abstract. – Bound-state eigenfunctions for a (classically) nonintegrable two degrees of freedom Hamiltonian system are studied. Between the de Broglie wavelength and a localization length, the probability density has a statistically fractal structure in some eigenstates. This novel characterization of eigenstates is intrinsically basis-set and coordinate independent and might therefore provide an objective approach to the question of quantum-chaotic behaviour.

A major concern in studying eigenfunctions of systems, which in the classical limit are nonintegrable, is in establishing whether or not a quantum chaos [1] may be associated with some states (*e.g.*, those that form the irregular spectrum [2]). The expectation is that quantum chaotic wave functions have a host of irregular properties and conjectures related variously to the irregularity of nodal patterns [3], Wigner distributions [4], correlation functions of operators [5] and decompositions in Hilbert spaces [6]. The semi-classical limit for regular and irregular wave functions was studied in detail by Berry [7], who pointed out that as $\hbar \to 0$, the morphology is different for the two kinds of wave functions. In particular, chaotic wave functions are expected to have a random pattern of amplitude fluctuations.

In characterizing disordered *materials* (such as the percolation cluster at the percolation threshold [8] or random particle aggregates [9]), it is common to use the notion of a fractal or Hausdorff dimension [10]. Such characterization has also been made for the (electronic) eigenstates of disordered systems like the tight-binding model [11, 12]. The fractal dimension D_f of the probability density in a given eigenstate is defined through

$$A(L) = \int \mathrm{d}\tau \int \mathrm{d}\tau' \, \rho(\boldsymbol{r}) \rho(\boldsymbol{r} + \boldsymbol{r}') \, \theta(L - |r - r'|) \sim L^{D_f}. \tag{1}$$

The notation is $\rho(\boldsymbol{r}) = |\psi(\boldsymbol{r})|^2$, L is a coordinate length, $\mathrm{d}\tau$ is a volume element, θ is the Heaviside step function. Note that all possible choices of origin, r, have been averaged over.

The question we address in this letter is whether such a fractal dimension can be sensibly associated with eigenstates of classically nonintegrable systems. A major motivation for this enquiry is that such characterization is coordinate independent due to the average over

choice of origin, and basis independent, although it is probably not representation independent. A second motivation arises from the suggestive similarity of typical chaotic eigenfunctions (*e.g.*, in the stadium problem [13] to random aggregates [9]). Although we do not, *per se*, equate the notion of possible fractality to possible quantum chaos, the present characterization has some advantages, in that it relates only to scaling properties of probability density. (Coordinate or basis-dependent criteria have been criticized in the past [14].) Similar connections have recently been explored by Singh and Bhattacharjee [12].

Eigenfunctions for a typical nonintegrable Hamiltonian with two degrees of freedom [3, 14, 15] (1),

$$H = -\nabla^2/2 + (ax^2 + by^2)/2 - \lambda x y^2 , \tag{2}$$

with $a = 1.6$, $b = 0.9$, $\lambda = 0.08$ and $\hbar = 1$ are computed. As this problem has a vibrational potential, all quasi-bound eigenstates are localized on large enough length scales, $L_m \sim$ boundary of the potential. (A superior estimate of L_m is provided by the variance of the radius of gyration, $\langle r^2 \varrho(r)\rangle - \langle r\varrho(r)\rangle^2$). Beyond L_m, all eigenfunctions decay exponentially, so for $L > L_m$, states are compact and $D_f \sim 0$. A lower limit is set by the de Broglie wavelength, $\lambda\!\!\!^{-} = \hbar/p$, below which the wave function is smooth, so for $L < \lambda\!\!\!^{-}$, the fractal dimension is merely the embedding Euclidean dimension, which is 2 in this case.

We are, therefore, constrained to work in the range $\lambda\!\!\!^{-} < L < L_m$. In polar coordinates, $x = r\cos\theta$, $y = r\sin\theta$, eq. (1) becomes

$$A(L) = \int_0^{\infty} r\,\mathrm{d}r \int_0^{2\pi} \mathrm{d}\theta\, \varrho(r, \theta) \int_0^{L} r'\,\mathrm{d}r' \int_0^{2\pi} \mathrm{d}\theta'\, \varrho(r + r', \theta') \sim L^{D_f}. \tag{3}$$

As is well known, an infinite hierarchy of such dimensions can be defined [6], and may prove useful in a complete characterization of irregularity in wave functions. Note that the fractal dimension D_f defined in eq. (3) is similar (but not identical) to the correlation dimension D_2 of Hentschel and Procaccia [16].

D_f can be deduced from a graph of $\ln A(L)$ *vs.* $\ln L$. Shown in fig. 1 are such plots for selected individual eigenstates; the system (2) has about 140 bound levels and we include results for illustrative cases (2). The integrals in eq. (3) were evaluated using a Monte Carlo procedure. Uniform sampling of r, θ and θ' is straightforward to implement, but that of r' requires some care to ensure that $A(L)$ is uniformly accurate over the entire range of L (seven «ecades», which is approximately three decades, in this study). The confidence level (3σ) is 98%. We also plot the slope itself *vs.* $\ln L$ in fig. 1 to help identify fractal behaviour. In going from $L < \lambda\!\!\!^{-}$ to $L > L_m$, there are essentially two possibilities: the slope can go continuously from 2 to 0, as in fig. 1*a*), *b*), or with an intermediate plateau, as in fig. 1*c*), *d*). In the latter case, the slope is a constant value (and neither 2 nor 0) over a considerable range of L, indicating fractal behaviour over the relevant intermediate-length scales. This fractal region occupies well over 3/5 of the entire range $\lambda\!\!\!^{-} < L < L_m$ and compares well with the system studied by Soukoulis and Economou [11].

The particular value of D_f is a property of the individual eigenstate; the examples shown here are typical in that several states of the system show similar behaviour—in particular,

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(1) We diagonalize the Hamiltonian (2) in a basis of the lowest 420 states of the unperturbed oscillators. There are slight differences in the eigenvalues above $E = 19$ (cf. ref. [3]). States can be given labels $n_x n_y$ as discussed in [3, 14].

(2) States with low n_x (low n_y) are the most (least) affected by the coupling; see [14].

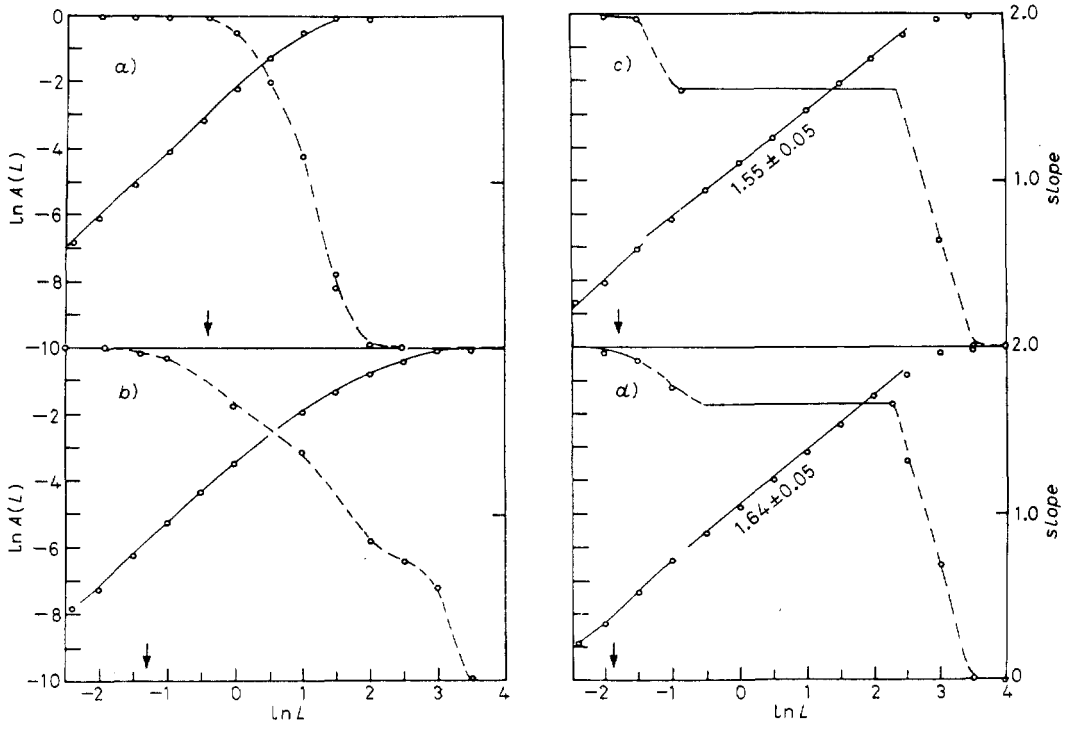

Fig. 1. – Plot of $\ln A(L)$ *vs.* $\ln L$ (solid line) defined in eq. (3), for four eigenstates of Hamiltonian (2). The eigenvalues are also indicated: *a*) state 1, $E = 1.1058$; *b*) state 84, $E = 18.7767$; *c*) state 87, $E = 19.2639$; *d*) state 133, $E = 23.8214$. The slope of $\ln A(L)$ *vs.* $\ln l$ is also plotted (dashed line), to show its variation from 2 below the de Broglie wavelength (marked $\downarrow$) to 0 at large L.

those that are involved in avoided crossings [15]. However, state 87, in fig. 1*c*), can be explicitly semi-classically quantized [17], so that a single fractal dimension less than 2 need not automatically imply a quantum chaos (see also ref. [12]).

This naturally leads to two questions. Firstly, eigenstates of (2) are mixed with respect to the original harmonic basis, so it is of interest to determine how the eigenstates of integrable systems behave under the present analysis. For particular examples, such as rectangle billiards, it is simple to show that the leading behaviour in L yields $D_f = 2$. A more general statement has not been possible here, although we have numerical evidence that pure states typically show a smooth transition from slope 2 to slope 0.

A second question relates to the paradigm of extreme randomness, *viz.* the Gaussian orthogonal ensemble (GOE) matrices [18], which have been seen to share several (eigenvalue related) properties with possibly quantum-chaotic systems [1]. In order to make comparison more direct, we have generated GOE wave functions for this system by diagonalizing GOE matrices and using the same basis as used to diagonalize Hamiltonian (2). To get an ensemble average, $A(L)$ was evaluated for the lowest few such eigenfunctions and averaged over a sampling of GOE matrices; the result is shown in fig. 2. In contrast with the eigenstates of (2), for GOE wave functions, the lower cut-off scale such as λ is not easily defined, although they remain localized for large L. The range over which the slope is constant is smaller than in fig. 1*c*) or 1*d*); however, the value of D_f so obtained is somewhat larger. It is not clear that our present procedure is an unambiguous method for constructing GOE wave functions. A study of billiard systems such as the stadium, wherein such wave functions can be defined more rigorously, will be of value.

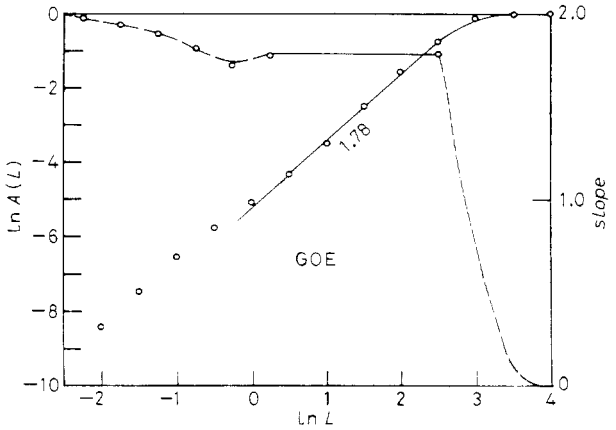

Fig. 2. – As in fig. 1, for the case of ensemble averaged GOE wave functions.

There is some reason to expect such scaling behaviour for sufficiently irregular wave functions. Berry has defined [7] a «locally averaged» (denoted by $\langle\ \rangle$) correlation function, in the semi-classical limit as

$$C(\boldsymbol{r}-\boldsymbol{r}';(\boldsymbol{r}+\boldsymbol{r}')/2)\equiv\langle\psi^*(\boldsymbol{r})\psi(\boldsymbol{r}')\rangle\sim\int \mathrm{d}\boldsymbol{p}\,\exp[i\boldsymbol{p}\cdot(\boldsymbol{r}+\boldsymbol{r}')\hbar/2]\,d(\boldsymbol{r}+\boldsymbol{r}',\boldsymbol{p})\,, \tag{4}$$

where $d(\boldsymbol{r},\boldsymbol{p})$ is the classical phase space density. For the type of system (diagonal kinetic energy + potential) considered here for ergodic motions this has a limiting form [7] in terms of Bessel functions. Using these expressions and replacing $\rho(r)$ in eq. (1) by its local average, allows the estimate

$$A(L)\sim\alpha\lambda L+\beta L^2+\ldots \tag{5}$$

(α and β constants) for $L_m\gg L\gg\lambda$. These estimates are approximate, but if irregular wave functions are similar to Gaussian random functions, as has been conjectured, the above offers some justification for the empirical observation of $D_f<2$.

In summary, here we have shown that over a considerable range, specific eigenfunctions of nonintegrable systems show a fractal character. Such a characterization is state-specific, but coordinate and basis independent. Although we do not equate a single fractal dimension with quantum chaotic character, this may provide a viable approach to a suitable diagnostic for quantum chaos [1, 2], in conjunction with other criteria.

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