Semiclassical properties of eigenfunctions and occupation number distribution for a model of two interacting particles

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Abstract

Quantum-classical correspondence for the shape of eigenfunctions, local spectral density of states and occupation number distribution is studied in a chaotic model of two coupled quartic oscillators. In particular, it is shown that both classical quantities and quantum spectra determine global properties of occupation numbers and inverse participation ratio.

Key words: Eigenfunction shape, local density of states, inverse participation ratio, quantum-classical correspondence.

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Recently, the study of the quantum manifestations of classical chaotic systems (quantum chaos) has turned from spectral statistics to properties of eigenfunctions. For the former, statistical aspects of spectral fluctuations are well established: Random matrix predictions follow for chaotic systems and Poisson-like statistics for the integrable ones [1,2]. For eigenfunctions, however, the approach seems not so straightforward. The inherent difficulty here arises essentially from the dependence on the basis. This forces us either to define basis independent quantities, or to specify a basis.

In this letter we shall follow the second possibility, trying to develop a framework as general as possible. We shall concentrate on the quantum-classical

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correspondence of the quantities such as the shape of eigenfunctions (EF), the
total spectral density of states (LDOS) and the single-particle occupation num-
ber distribution \( n_s \). We study a Hamiltonian that displays classical chaos and
has a spreading width in the single particle basis, that is sufficiently large to
allow statistical treatment of the components. We find excellent agreement be-
tween these quantities and their classical analogues in the semiclassical region.
The classical analogues are defined through phase space integrals. Therefore,
they do not depend on dynamical properties such as integrability or chaos of
the full Hamiltonian. We shall also show that this correspondence allows one
to approximately obtain some important characteristics for which quantum
phases of eigenfunctions play no role. In this way, in the semiclassical limit,
one can obtain mean values of single-particle operators without diagonalization
of large matrices. In particular, we present calculations for the inverse
participation ratio which distinguishes localized states from extended ones in
the unperturbed basis. These computations require only the knowledge of the
classical analogue of EF and the spectra of the unperturbed Hamiltonian. We
present our approach for the two-body problem, but essential parts of the
approach can be easily extended to the \( N \)-body problem.

Let us begin with considering a two-body Hamiltonian of the form \( H = H_0 + V \),
and assume that its classical dynamics is fully chaotic. Here, the unperturbed
Hamiltonian is separable and, therefore, integrable in terms of two one-particle
Hamiltonians, i.e. \( H_0 = h_1 + h_2 \). In turn, \( V \) is the potential which couples the
motion of the particles. For our purposes, we shall assume that both \( H \) and
\( H_0 \) remain invariant under the particle interchange (\( h_1 = h_2 = h \)).

For the quantum treatment of such Hamiltonians the unperturbed basis \( H_0 \)
seems a convenient choice for the representation of exact eigenfunctions. The
rate of convergence certainly depends on the strength of the perturbation \( V \).
For instance, if exact eigenfunctions are extended all over the energy range
considered, as it is the case for certain potentials near the dissociation limit [3],
the convergence will be very slow. We, therefore, assume that \( V \) is such that
the perturbed eigenfunctions are extended over a certain energy range as to
allow convergence, but that this range is large enough in terms of the number
of principal components, i.e. that the spreading width is sufficiently large [4].

The unperturbed basis is defined by the eigenfunctions \( |\Phi_k^0\rangle \) of \( H_0 \), reordered
according to increasing eigenvalues, \( E_k^0 < E_l^0 \) for \( k < l \). This basis functions
are written as properly symmetrized linear combinations of products of single-
particle basis states. The single-particle basis is defined by the Schrödinger
equation, \( h|\phi_i\rangle = \epsilon_i|\phi_i\rangle \), and the combination of the basis states is such that
\( E_k^0 = \epsilon_{i_1} + \epsilon_{i_2} \). In this sense, the basis defined by the mean field approximation
coincides with the unperturbed basis when \( V \) is the residual interaction.

Denoting by \( |\Psi_i\rangle \) the eigenstates of the total Hamiltonian and by \( E_i \) the cor-
responding eigenvalues, in terms of the basis states we have

$$|\Psi_i\rangle = \sum_k C^i_k |\Phi^0_k\rangle.$$  \hspace{1cm} (1)

The expansion coefficients $C^i_k$ define some global quantities that we consider here. First, the shape of eigenfunctions (EF), also called the F-function, is defined as the distribution obtained by an average of the squared expansion coefficients as a function of the unperturbed energy \[5\]

$$F^i_k \equiv |C^i_k|^2 = F(E_i, E^0_k).$$  \hspace{1cm} (2)

Here, the average is defined over a small window of perturbed eigenstates around $E_i$. The average has been introduced in order to smooth the fluctuations arising from individual wave functions considered. It has been shown that the F-function defines a kind of thermodynamic partition function for systems of finite number of interacting particles \[5\], if the components meet certain statistical requirements. These will certainly be met, if the classical Hamiltonian leads to chaotic motion and the spreading width is large enough.

The second quantity of our interest, the LDOS gives the distribution of unperturbed eigenstates in terms of the perturbed ones. The LDOS is related to the EF by \[5\]

$$P^i_k \equiv F(E_i, E^0_k) \rho(E_i),$$  \hspace{1cm} (3)

where $\rho(E_i)$ is the level density for exact eigenstates, and the F-function is taken now for a fixed value of the unperturbed energy $E^0_k$. Therefore, the LDOS is a function of the perturbed energy $E_i$.

These quantities have well-defined classical interpretations. For instance, the classical EF is the distribution resulting from the time-dependent unperturbed energy $\mathcal{E}_0(t)$, obtained by substituting the solutions of the equations of motion for the Hamiltonian $H$ into the expression for $H_0$. Since $H$ is assumed to generate fully chaotic and thus ergodic dynamics, we can replace the time integration along one typical orbit by a phase space integral. Therefore, one can write for the classical EF the phase space integral

$$g(\mathcal{E}, \mathcal{E}_0) = A \int \text{d}p \text{d}q \delta(\mathcal{E} - H(p, q)) \delta(\mathcal{E}_0 - H_0(p, q)),$$  \hspace{1cm} (4)

where $q = (q_1, q_2)$, $p = (p_1, p_2)$ are the position and momentum vectors, and $A$ is a normalization constant. For the classical EF in Eq. (4), the independent variable is $\mathcal{E}_0$; the total energy $\mathcal{E}$ is fixed.
The classical LDOS can be obtained in the same terms by integrating the
equations of motion for $H_0$ and substituting the solutions into the expression
for $H$. Since $H_0$ is an integrable Hamiltonian, one is forced to consider an
average over different initial conditions. Then, Eq. (4) serves also to define the
classical LDOS; $\mathcal{E}_0$ is now held fixed and $\mathcal{E}$ is the independent variable. In the
following, we shall use the notation $g(\mathcal{E}_0)$ to indicate the classical EF and $g(\mathcal{E})$
the classical LDOS, when referring to Eq. (4). In this notation, the variable
that is explicitly written is the independent variable.

We notice that the classical and quantum quantities, for instance the EF as
given by Eq. (4) and the F-function Eq. (2), differ in the way they are nor-
malized. The former, being a probability distribution, is normalized according
to $\int g(\mathcal{E}, \mathcal{E}_0) d\mathcal{E}_0 = 1$, which actually defines the value of the constant $A$. For
the latter, the normalization is the unitarity condition for the expansion coef-
ficients, i.e. $\sum_k |C_k^i|^2 = 1$. For a fair comparison of the classical and quantum
results we require the normalizations to be of the same type. This is achieved
including the local density of states, i.e. $\sum_k \int |C_k^i|^2 \delta(E^0 - E_0^k) dE^0 = 1$. Numer-
ically, we shall calculate this expression replacing the local density of states
by a step function, which is different from zero only in a small interval that
includes some levels, where its value is one. Then, we divide the energy range
in a number of bins, and associate to each bin the sum of the intensitie
$|C_k^i|^2$ of the energy levels contained in it.

We shall turn now to the comparison among the quantum EF and LDOS with
their classical counterparts in the following model. We consider two indisti-
guishable coupled quartic oscillators with the Hamiltonian

$$H = \frac{1}{2}(p_1^2 + p_2^2) + \alpha(x_1^4 + x_2^4) + \beta x_1^2 x_2^2 + \gamma(x_1^3 x_2 + x_1 x_2^3). \quad (5)$$

Here, $\alpha > 0$ and we consider $\beta < 0$ in order to have strongly chaotic dynamics
far from the dissociation limit, which is given by $2\alpha + \beta + 2|\gamma| = 0$. For the
results presented below, we have used $\alpha = 10$, $\beta = -5.5$ and $\gamma = 5.6$; the
system is strongly chaotic and the phase space is quite homogeneous [6].

The system defined by the Hamiltonian (5) is obviously integrable for $\beta =
\gamma = 0$; we shall consider this case to define the unperturbed Hamiltonian $H_0$.
We note that in the basis defined by $H_0$ there are diagonal contributions from
the term $\beta x_1^2 x_2^2$. These contributions could be incorporated in the definition
of $H_0$ in order to improve the approximate mean field, but we avoid this
complication.

Since the potential is a homogeneous polynomial, the system scales classically
with the energy. This property can be carried over to the classical expres-
sions for the EF, LDOS and $n_s$. For instance, for the classical EF, one finds
Fig. 1. EF for (a) a typical eigenstate $E_{620} = 664.073$ and, (b) for a localized one $E_{515} = 588.540$. Notice the different vertical scales. Insets: comparison between the classical (continuous curve) and the quantum results (histogram).

Fig. 2. Results for a recentered average involving 21 neighbouring eigenstates: (a) EF around $E_{620}^0$; (b) LDOS around $E_{300}^0 = 469.102$. The unperturbed eigenstate corresponding to the $E_{300}^0$ displays localization properties similar to the state shown in Fig. 1b. The insets show the quantum-classical correspondence for the average.

$$g(E, E_0) = E^{-1}g(1, E_0/E),$$ with obvious extensions to the other quantities.

In the following we present results obtained for fermions of even parity for the Hamiltonian (5); similar results were obtained for other symmetry classes. Figure 1a refers to the EF of a typical eigenstate, which extends over a certain range of unperturbed energies; Fig. 1b shows the EF for the uncommon case of an eigenfunction with a smaller number of principal components, a localized eigenfunction. This can be readily appreciated in the vertical scale (intensity) and on the apparent density of peaks (the eigenfunctions are normalized). The distinction between a localized and an extended eigenstate can be made quantitative, for instance, by considering the number of principal components $l$: In the former case we obtain $l = (\sum_k |C_k|^4)^{-1} = 146.5$, while for the latter we have $l = 18.4$. Similar properties are also found when we consider the LDOS for individual eigenfunctions of $H_0$.  

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Since most eigenstates display similar statistical features, an average considering neighbouring eigenstates will smooth the fluctuations, and we expect a better correspondence. In Figs. 2 we present the results for the EF and the LDOS obtained for a recentered average of eigenstates containing 21 eigenstates. The average was performed by recentering each eigenstate, so the peak associated with the actual energy of the eigenstate is labeled as zero. We notice that this procedure incorporates the fact that neighbouring eigenstates are typically similar.

As shown in the insets of Figs. 1-2, for generic eigenstates there is a clear correspondence between the classical and the quantum results. As it can be appreciated in the plots, in this case, the tails of the distribution are well approximated by the classical calculations, while the central peak is the main concern for the correspondence. The results presented are actually improved as the semiclassical limit is reached. In fact, as we approach the semiclassical limit, the density of states increases and therefore the central classical peak is better resolved. As one would expect, the localized eigenstates display strong deviations from the classical results. Notice though, that after averaging the classical correspondence emerges again, since the main contributions come from the (typical) extended eigenstates. This is appreciated in Fig. 2b, where we present the LDOS obtained for the recentered average taken over 21 eigenstates, where we have chosen the central eigenstate to be localized.

At this point we shall emphasize that no free parameter has been used to fit the data. Namely, the classical energy is taken from the energy of the eigenstate under consideration (and the scaling property is used); for the results involving the average, the energy corresponds to the average energy of the eigenstates within the window. Furthermore, the similarity (under certain reflection) of the LDOS and the EF displayed in Figs. 2 is a consequence of the symmetry of $H$ and $H_0$ in Eq. (4), as given by (3).

The good correspondence found for the EF and the LDOS in the semiclassical limit can be understood by interpreting Eq. (4) as a kind of generalization of the Weyl formula for the intensities of the eigenstates, with respect to a certain basis $H_0$. The fact that this expression is a phase space integral, implies that it contains no information about the integrability or chaos of the classical systems.

While the above quantum-classical correspondence for the LDOS and EF, to a large extent, can be expected from previous studies of other models [7], in what follows we concentrate on the analysis of “single-particle” properties, in particular, the occupation numbers of single-particle states (see also [8] where this quantity was studied for two interacting spins). This may seem of marginal importance for two-particle systems, though it is certainly of great significance as the number of particles increases [9]. Yet, the two-particle system will be an
adequate test ground to study how the semiclassical approach can be applied.

In terms of the expansion coefficients $C_k^i$, the single-particle occupation number distribution $n_s$ is defined as

$$< n_s^i > \equiv \langle \Psi_i | \hat{n}_s | \Psi_i \rangle = \sum_k |C_k^i|^2 n_s^{(k)}, \quad (6)$$

where $\hat{n}_s = a_s^\dagger a_s$ is the occupation number operator, $a_s^\dagger$ and $a_s$ are the creation and annihilation operators, and $n_s^{(k)} = \langle \Phi_0^k | a_s^\dagger a_s | \Phi_0^k \rangle$. Aside from its significance in statistical mechanics, the interest of the occupation number operator is that it allows to calculate mean values of any single-particle operator $< M > = \sum n_s M_{ss}$.

The classical $n_s$ is defined in the same terms of the classical EF or LDOS. Accordingly, it is obtained by computing the time dependent single-particle energy distribution $\epsilon(t)$, using the solutions of the classical equations of motion for $H$. Again, an expression similar to Eq. (4) can be written for the classical occupation number distribution, which is given by

$$g_n(\epsilon, \mathcal{E}) = A' \int d\mathbf{p} d\mathbf{q} \delta(\mathcal{E} - H(\mathbf{p}, \mathbf{q})) \sum_{i=1}^2 \delta(\epsilon - h_i(p_i, q_i)). \quad (7)$$

Here, $\epsilon$ is the independent variable, $\mathcal{E}$ is the energy of the full Hamiltonian, and $h_i$ represents the one-particle Hamiltonian. In the present case we have assumed the particle interchange symmetry, so the sum in Eq. (7) may be absorbed in the normalization constant, which corresponds to the number of particles.
In Fig. 3 we present the results for $n_s$. No free parameter was used to fit the data. A good correspondence of the classical and quantum results is found, although the calculations that involve individual eigenfunctions display very large fluctuations. The correspondence is certainly better if we perform an average over some neighbouring eigenstates, and again is improved as we go deeper into the semiclassical region. It is not clear, however, to what extent the fluctuations observed for individual eigenfunctions are related to quantum localization effects.

The correspondence shown in Figs. 3 is novel and important. First, it has no especial interpretation in the framework of classical mechanics for isolated systems of few interacting particles, although the single-particle occupation number distribution is an important quantity in quantum statistical mechanics, where is linked to the Boltzmann distribution (in the thermodynamic limit). Second, we note that the tail of the $n_s$-distribution, which displays exponential decay, is well reproduced by Eq. (7). This is a non-trivial remark if we recall that we deal with a two-particle system. Clearly, this permits to define an analogous of the Boltzmann parameter for finite systems, although its interpretation as the inverse of the temperature is not generically accepted (see the discussion in [9]).

Once we have shown that good quantum-classical correspondence is found in the semiclassical limit, it is possible to proceed with estimates of other quantities involving the F-function. Our calculations are based on the classical EF as calculated above, and require only the knowledge of the single-particle spectra (that allows to compute the unperturbed spectra) and the perturbed spectra. We shall refer our prescription as “semiquantum approach”. Specifically, we illustrate the method by a calculation of the inverse participation ratio (IPR),

$$P^+(E_i) = \sum_k |C_k^i|^4,$$

which is an important measure of the uniformity of the expansion distribution [4,10]. Other quantities which involve even powers of the expansion coefficients, i.e. where the phase of eigenfunctions does not appear, can be obtained in the same terms.

In order to compute the IPR, we must express our classical (continuous) distribution as an intensity distribution, which is normalized as an eigenfunction. Obviously, our results will depend on how we discretize this distribution, though no free parameter will be involved. The comparison between the semiquantum and the quantum results will thus give insight in the plausibility of the discretization. One possibility for this discretization is the following: We divide the unperturbed energy range into segments, such that every segment contains only one unperturbed eigenvalue, and that they span the whole
interval. We define the limits of each such interval by the middle point of neighboring eigenvalues. Then, we define the classical intensity associated with an unperturbed energy as the value of the area under the classical distribution corresponding to the segment, that contains the unperturbed eigenvalue. This procedure leads to a semiquantum intensity distribution with the required normalization, and can, therefore, be used to obtain quantities like the $n_s$ or a semiquantum version of the IPR. However, the semiquantum intensities obtained in this way will display more zeros than the corresponding quantum ones. This is an obvious consequence of the finite range where the classical density $g(E, E_0)$ is non-zero.

We note that from the classical scaling properties of the EF, $g(E, E_0) \sim E^{-1}$, and the mean level density, $\rho(E) \sim E^{1/2}$, we can obtain a semiquantum estimate for the IPR, which is expected to display a power-law decay of the form $[g(E, E_0)\rho(E)]^2 \sim E^{-1}$. In Figs. 4 we present results for the semiquantum and quantum IPR. The quantum results shown correspond to the direct evaluation of Eq. (8) for individual eigenstates, that is, no average or smoothing prescription has been used. A qualitative agreement is observed between the semiquantum and the quantum data, although quantitative differences arise. The power-law decay predicted from the classical scaling properties of the system (5) is well confirmed. In fact, we have fitted curves of the form $P_i^+ \propto E_i^{-\mu}$ to our results, and obtained that the best fit is provided by $\mu_{sq} = 1.06$ and $\mu_q = 1.07$ for the semiquantum and quantum data, respectively. Analogue results, obtained when considering averages over windows of the eigenstates, show better quantitative agreement. In this case, the features related with large values of the IPR (localized eigenstates) are smeared out.

It is interesting to note that certain semiquantum states display a rather large IPR, which could be associated with some localization properties (scars). In
turn, the quantum results display more of these localized states and the IPR associated is also larger. This enhancement of localization is a well-known quantum effect.

In summary, we have shown that important quantities like the EF, LDOS or \( n_s \) have, in the semiclassical limit, good correspondence to their classical analogues in our model of two interacting non-linear oscillators. The classical quantities are obtained as phase space integrals, assuming that they are applied to the case when the classical dynamics is strongly chaotic. We have used the classical quantities, in particular the classical EF, together with the quantum spectra of the perturbed and unperturbed systems in order to obtain “semiquantum” intensities associated to a given (perturbed) eigenstate. We have compared the quantum results with the semiquantum ones, specifically for the inverse participation ratio, and found good qualitative agreement, although quantitatively they may display differences. In particular, the semiquantum results underestimate the IPR for rather localized (scars) eigenstates, both in their number and magnitude. The energy dependence of the IPR can be understood from the classical scaling properties of our model.

Since quantities like the IPR involve information on the underlying classical mechanics, we believe that semiquantum properties may help to explore quantum localization effects in the semiclassical region. Moreover, expressions like Eq. (4) may help to define a reference from which the study of eigenfunction fluctuations and their relation to the underlying dynamics can be achieved. Our results directly take into account the two-body nature of the inter-particle interaction, and can be easily extended to systems with any number of particles.

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