Quantum classical correspondence for the statistical moments of eigenfunctions in closed systems with chaotic dynamics

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Abstract. Quantum classical correspondence, QCC, is a wide subject of interest from the historical approaches to current studies in simple and complex systems, including time dependent Hamiltonians. Quantum eigenfunctions, or wave-functions, are part of the quantities analysed in recent years, including the implementation due to M V Berry and A Voros in 1977 of a suitable quantity to be considered as the classical eigenfunction counterpart. Here we present the calculation of the statistical moments of eigenfunctions in energy representation for anharmonic oscillators. The classical counterpart of the system is fully chaotic. The comparison of the quantum version in order to test for quantum classical correspondence is analysed using a slightly modified formula of the proposed by Berry and Voros. The agreement is good with the corresponding classical counterpart being at the bottom of the quantum version for all the energy range considered.

1. Introduction
The correspondence between quantum and classical phenomena is a wide and old area of research. How the quantum behaviour became part of the classical world was the concern of N Bohr in what is named the Principle of Correspondence [1,2,3]. Quantum behaviour is related with observables, operators which eigenvalues and eigenvector are measurable. Usually the physical quantum behaviour is associated with quantities with units of action, energy times time, that are directly related with Planck constant, \( \hbar \), but not restricted to them. Among others quantities, the energy spectrum is a traditional test for the quantum classical correspondence. An example is the Weyl formula for the spectra of closed systems in the Thomas-Fermi approximation. Such a formula, for the density of states, is:

\[
\rho(\mathcal{E}) = \frac{1}{(2\pi\hbar)^{2N}} \int dp \, dq \, \delta(H - \mathcal{E})
\]

Where the integral considers the sum on all the phase space coordinates which coincide with the energy shell of radius \( \mathcal{E} \), for a system described for the Hamiltonian. The unit of phase space for a quantum is \( 2\pi\hbar \) or \( \hbar \), for \( N_p \) particles. The \( \delta(\cdot) \) stand for the Dirac delta function. As a remainder, the quantumness of a quantity, or how close to have quantum behaviour, must be related in terms of how close of \( \hbar \) we are, but notice that it means that it is related to quantities with the units of \( \hbar \), or action units. Such a units are energy times time. In this sense the fulfilment of the quantum area in phase space is \( dpdq \sim 2\pi \hbar \).

Inspired by formulation in (1) in 1977 M V Berry [4] and A Voros [5] proposed that the semiclassical analogue for the eigenfunctions, EFs, in a different basis from the proper one. The explanation of this idea and the realisation of it presented in [6,7] in the energy representation is matter of the next section. Some details added in [8] are explained as well. But the results we present in the current paper are related to the statistical properties of the eigenfunctions or wavefunctions of quantum closed systems, focusing in those with a chaotic classical dynamics. Since the squared eigenfunction times a proper representation is a Probability Density Function, PDF, considering the raw moments of such a distribution is an interesting matter. We have interest in these properties mainly because they can be calculated for all the eigenfunctions given a numerical precision and reliability.
That is not a single state test for quantum classical correspondence but an overall test. As in the case of the Weyl formula, where the reliability of the numerical calculation of spectra for quantum systems is contrasted with a proper estimation of density of states, as in equation (1). To the later topic is devoted the section 3, conclusion appear at section 4.

2. Quantum classical correspondence for eigenfunctions or wavefunctions

Eigenfunctions of quantum operators have a simple description only in its own basis, as they are members of a vectorial space, the Hilbert space. However, analysis of their properties or properties related to them require of a projection in other basis. This is important from both theoretical and experimental point of view.

In undergraduate programs the selected basis for describe the EFs is the basis of coordinates x, with vector $|x\rangle$, that stands for a column vector with real index, x. Here, and in the rest of the paper we shall use the Dirac notation for simplicity, emphasizing that it is a notation not a quantum signature. See [9] for an explanation for undergraduates.

Hence the eigenfunction, $|\Psi_i\rangle$, of a given Hamiltonian is the solution of the stationary Schrödinger equation:

$$H |\Psi_i\rangle = E_i |\Psi_i\rangle$$

For eigenvalue or eigenenergy $E_i$, labelled with $i$, in the integers in this case. Hence, the wavefunctions is usually written in a coordinate basis as:

$$\Psi(x) = \langle x |\Psi_i\rangle$$

But the expansion could be in a different basis, for instance in the eigenvectors, $|\varphi_k\rangle$, of a new Hamiltonian, named $H_0$ with the expression:

$$|\Psi_i\rangle = \sum_k \langle \varphi_k |\Psi_i\rangle |\varphi_k\rangle$$

Where is not needed to have $H = H_0 + \lambda V$, for a perturbative parameter $\lambda$. Here, we label the energies of $H_0$ as $E_k^0$. Since the basis vectors correspond to the energy we consider equation (4) as an expansion in unperturbed energies. Meanwhile;

$$|\varphi_k\rangle = \sum_i \langle \Psi_i |\varphi_k\rangle |\Psi_i\rangle$$

stands for the so called Local Density of States, or a function of perturbed states. This expression is of relevance in experimental physics. The quantum energies will denoted as normal E’s with sub or superscripts, meanwhile the classical, or semiclassical, energies will be denoted with calligraphic E’s, that is $E$ and $E^0$.

2.1. The classical analogue of wavefunctions in energy representation

It is usual to discuss two examples, the harmonic oscillator and the hydrogen atom. Both with several symmetries and fully integrable, the later implies the existence of a sufficient number of constants of motion and hence the sufficient number of good quantum numbers. In such a system it is possible to build a Complete Set of Commuting Observables or CSCO. In such a system the theoretical quantum classical correspondence could be fulfilled straightforward in the coordinate representation for the EF using WKB approach, for instance [2,3,10]. But such a system is the exception not the rule. That is one of the reasons that a more general approach was needed. Even more how the quantum classical correspondence is achieved is a matter of discussion, for simple, integrable systems to open time-dependent ones, from purely theoretical models to experimental ones [3].

A semiclassical version for eigenfunctions in energy representation was proposed by M V Berry [4] and A Voros [5] as intersection of the two energy shells, one for the system and one for the basis. A further development is appeared in a set of papers [11] where the quantity:

$$g(\epsilon, E^0) = \frac{1}{(2\pi\hbar)^3} \int dp dq \delta(\epsilon - H(p, q)) \delta(\epsilon^0 - H_0(p, q))$$

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is assumed as the classical analogue of the eigenfunction. This quantity considers the intersection between two energy shells, one from the Hamiltonian, $H$, and the other from the unperturbed one or test Hamiltonian, $H_0$. Notice that the sum is performed for those values in coordinates and momenta consistent with both conditions, for $\mathcal{E}$ and $\mathcal{E}_0$. As noticed in [8,12] a detail is needed to fulfil the quantum classical correspondence, the density of states in energy. It is named as:

$$N(\mathcal{E}) = \int d\mathcal{E}_0 \, \tilde{g}(\mathcal{E}, \mathcal{E}_0) \, \rho_0(\mathcal{E}_0)$$  \hspace{1cm} (8)

for the wavefunction and

$$N(\mathcal{E}_0) = \int \tilde{g}(\mathcal{E}, \mathcal{E}_0) \, \rho(\mathcal{E}) \, d\mathcal{E}$$  \hspace{1cm} (9)

for the Local Density of States, LDoS. Such a correction is relevant as the densities of energy are far from uniformity. Such a condition is noticeable mainly for large values of energy.

An easy way to interpret the classical eigenfunction is to see, for instance, the phase space of a harmonic oscillator of angular frequency, $\omega$, and fixed energy $E$. The time evolution corresponds to periodic orbits in time. Now, consider a new harmonic oscillator, at a different frequency and energy. For some of the values of $p$ and $q$ in the full Hamiltonian will coincide with the energy of the new Hamiltonian.

The quantum classical correspondence for eigenfunctions has been corroborated for a series of systems, as well as their Gaussian fluctuations around the average [8,11]. A less visible feature is its overall behaviour. Here we discuss a very particular aspect: the moments of eigenfunctions in the energy representation or the much more usual for measures, the Local Density of States or LDoS. As in many cases, the large numbers law is expected, but it is not the case, as we shall see later, eigenfunctions in the energy representation are not described by a Gaussian in general. Even when the studied system has a chaotic classical dynamic such a shape does not appear.

2.2. The systems

In order to test the quantum classical correspondence we considered an one dimensional anharmonic oscillator with four particles. In order to have generic properties we search for values of the parameters that allow that the classical dynamics gets fully chaotic. The Hamiltonian is:

$$H = T + V$$  \hspace{1cm} (10)

with the potential operator written as:

$$V = \alpha \sum_{i=1}^{N_p} q_i^2 + \beta \sum_{1 \leq i < j \leq N_p} q_i^2 q_j^2 + \gamma \sum_{1 \leq i < j \leq N_p} q_i^2 q_j^3$$  \hspace{1cm} (11)

for $N_p = 4$ particles. We consider as the unperturbed Hamiltonian:

$$H^0 = \sum_{i=1}^{N_p} h^0(\hat{p}_i \hat{q}_i)$$  \hspace{1cm} (12)

being:

$$h^0(\hat{p}_i \hat{q}_i) = \frac{1}{2} p_i^2 + \alpha q_i^2$$  \hspace{1cm} (13)

The single particle Hamiltonian. The number of particles considered in this work is four, since it is well known that the three chaotic particles case is full of symmetries.

The parameters for the current work have been tested for positive Lyapunov exponents [8] and their values are:

$$\alpha = 10, \beta = -2.1, \gamma = -2.2$$
Figure 1. Quantum (solid line) and classical (dashed line) statistical raw moments, from the first to the fourth, for the eigenfunctions of an anharmonic oscillator with four particles given by equation (10). Notice that the classical case, given by equation (16) is almost below all the quantum values, equation (15). See text for details.

The values were obtained by trial and error. The units where choose in order to get $m = 1$, $\hbar = 1$ and we do not consider electrical charge. The quantum states are obtained by direct diagonalisation of the Hamiltonian in a finite harmonic oscillator basis. The matrix considered has dimensions of 10000 times 10000 and was diagonalised using the algorithm of Bunge et al. [13] in a Fortran code. The classical wavefunctions were obtained by Monte Carlo integration in phase space for the proper and scale version of (7).

3. The quantum classical correspondence in moments
Quantum classical correspondence could be tested in several ways and, one of them is to look for the statistical raw moments of the eigenfunctions in energy representation. Such a comparison could be interesting since it is considered for all the states. Formally the m-th raw moment is calculated as:

$$\mu_m = \int x^m P(x) dx$$

(14)

for a probability density $P(x)$.

For the quantum wavefunctions such a quantity is

$$\mu_m^q(E') = \sum_k (E_k^p)^m \langle \varphi_k | \Psi_t > |^2$$

(15)

for the perturbed state $| \Psi_t >$ on the $| \varphi_k >$ basis. The superscript $q$ stands for quantum. For a practical purpose, the quantum PDF can be obtained from the diagonalisation of the full Hamiltonian in the basis of the test Hamiltonian.

For the classical case, the formulation is similar,

$$\mu_m^c(E) = \int (E^q)^m \tilde{\varrho} (\langle E^q, E^0 \rangle \rho_0 \langle E^0 \rangle ) dE^0$$

(16)
An explicit for $\mu_3$ can be obtained for scalable systems as the anharmonic oscillator presented here. For $N_p$ degrees of freedom we have, by direct calculation using Hamiltonian (10-13), that:

$$\mu_3 = \frac{c}{\rho(E)} \int dq \left( E - (V(q) - V^0(q)) \right)^3 \left[ 2(E - V(q)) \right]^{\frac{N_p-2}{2}} \Theta(E - V(q))$$  \hspace{1cm} (17)

$$c = \frac{2\pi^{\frac{N_p}{2}}}{\Gamma(\frac{N_p}{2})}$$  \hspace{1cm} (18)

Noticing that the expression (6) for $g$ can be simplified as:

$$g(E, E^0) = \frac{2\pi^{\frac{N_p}{2}}}{\Gamma(\frac{N_p}{2})} \int dq \left( E - V(q) - (E^0 - V^0(q)) \right) \left( E - V(q) + E^0 - V^0(q) \right)^{\frac{N_p-2}{2}} \Theta(E - V(q)) E^0 - V^0(q))$$  \hspace{1cm} (19)

We can obtain the explicit form for the moments given by:

$$\mu_m = \frac{c}{\rho(E)} I_{N_p, m} E^{\frac{3N_p-1}{4}}$$  \hspace{1cm} (20)

here:

$$I_{N_p, m} = \int d\tilde{q} (1 - V(q))^{m} \left[ 2(1 - V(q)) \right]^{\frac{N_p-2}{2}} \Theta(1 - V(q))$$  \hspace{1cm} (21)

and the variables with a hat are the scaled ones. The integrals can be calculated using Monte Carlo procedure and do not depend on $E$. The result for the first four moments using equation (17) and their comparison with the quantum case of equation (15) is shown in figure 1. There the scale is log-log. In all cases, the classical analogue is near the lower edge of the quantum result and being their envelope. The first moment is consistent with a linear growth as a function of the unperturbed energy. Mutatis mutandis, we obtain the same results for the LDoS where the integral is:

$$I_{N_p, m} = \int d\tilde{q} (1 - V(q))^{m} \left[ 2(1 - V(q)) \right]^{\frac{N_p-2}{2}} \Theta(1 - V(q))$$  \hspace{1cm} (22)

For the central moments, we have a binomial–like structure as usual which can be calculated as well. An interesting point would be to see under which conditions the fourth central moment depends only on the second and first raw moments, that is, under which conditions we would have a Gaussian shape.

4. Conclusions

Quantum classical correspondence is an important subject of research, for a wide range of systems, being simple, complex, closed or open [3]. Here we contribute to the discussion with the comparison of the statistical raw moments for the quantum wavefunctions in energy representation and their classical analogue. Looking for general properties we performed the calculations using a Hamiltonian of anharmonic oscillators in one dimension. The classical dynamics is fully chaotic and additionally, the system is scalable. As a consequence, the classical analogue is explicitly calculated in energy representation. For the moments of EFs components, the vast majority of them have larger values than the classical analogue. It could be interesting that comparison is on all the states under the numerical reliability and not restricted to a particular form of the eigenfunction. In the current case no Gaussian shape was found in the quantum case.

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