

Study of the structure of chaotic eigenfunctions in a scar functions basis set

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The central problem studied in this dissertation is the correspondence between classical and quantum mechanics in classically chaotic Hamiltonian systems in the field of 'quantum chaos'. More specifically, we propose a new and efficient method to compute the eigenfunctions of chaotic systems using a set of scar functions. These scar functions play a central role in the study of the quantum manifestations of classical chaos, since they are semiclassical wave functions with a very low dispersion and localized over the invariant manifolds of the periodic orbits that constitute the organizing structure of classical chaos. The method that we have developed has been called "Gram-Schmidt Selective Method" (GSSM), as it constructs the basis set using the conventional Gram-Schmidt Method but taking also into account the dispersion of the scar functions and the length of the periodic orbits along which they are localized. Using the GSSM, we have been able to compute with high accuracy the 2400 lowest-lying eigenfunctions of a highly chaotic quartic oscillator with two coupled degrees of freedom as well as some very excited eigenfunctions of the same system in a small energy window; in both cases, our basis sets were more efficient than those previously reported in the literature. Furthermore, we have applied the GSSM to calculate the eigenfunctions of the isomerizing molecular system LiNC/LiCN, which has a 'mixed' phase space that presents both regular and irregular motion; in this system, we have accurately computed the 66 lowest-lying eigenfunctions.

Finally, we have proposed a perturbative scheme to compute reaction rates in open systems described by anharmonic potentials. With this method, we have obtained the reaction rate of different potentials with one and two degrees of freedom, as well as the isomerizing rate of the molecular system LiNC/LiCN in the presence of (uncorrelated) white noise and embedded in a (correlated) bath of argon atoms. The developed method is independent of the dividing surface and it has enabled us to compute analytical corrections to the famous Kramers formula, allowing at the same time the exact calculation of reaction rates in anharmonic potentials that interact with the environment.