Order–chaos transitions in correlation diagrams and quantization of period orbits

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Eigenlevel correlation diagrams has been proved to be a very useful tool to understand eigenstate characteristics of classically chaotic systems.

We illustrate the theory using the vibrational eigenstates of the LiCN molecular system:

$$H = \frac{P_R^2}{2\mu_1} + \frac{P_\theta^2}{2}\left(\frac{1}{\mu_1 R^2} + \frac{1}{\mu_2 r_{eq}^2}\right) + V(R,\theta), \tag{1}$$

where $\mu_1 = m_{Li}(m_C + m_N)/(m_{Li} + m_C + m_N)$ and $\mu_2 = m_C m_N/(m_C + m_N)$ are reduced masses (m_{Li}, m_C, and m_N being the corresponding atomic masses), $r_{eq} = 2.19$ a.u. is the fixed N-C equilibrium length, R is the length between the CN group center of mass and the Li atom, and θ is the angle formed by the corresponding r_{eq} and R directions . Thus, e.g., $\theta = 0$ corresponds to the linear Li-CN configuration, and $\theta = \pi$ rad to the linear CN-Li configuration. Last, P_R and P_θ are the conjugate momenta corresponding to R and θ coordinates, respectively, and $V(R,\theta)$ is the potential energy function describing the interatomic interaction [1]. It presents two minima separated by a saddle at $(R,\theta) = (4.22 a.u., 0.29\pi rad)$ with $V = 3455$ cm^{-1}. These three characteristic points can be connected by the minimum energy path, i.e., the path connecting all characteristic points along which the variation of energy is minimal. Finally, It is worth noting that the well around the absolute minimum (CN-Li isomer) is very anharmonic and, consequently, there is a transition from regular classical motion to chaos in this system [2] that takes place at moderate values of the excitation energy, i.e. around 1700 cm^{-1}.

In particular, we showed in a previous publication [3] how to unveil the formation of the scarring mechanism, a cornerstone in the theory of quantum chaos, using the Planck constant $\hbar$ as the correlation parameter. By increasing $\hbar$ we induced a transition from order to chaos in which scarred functions appeared as interaction of states in broad avoided crossings, at points which formed a well defined line.

In this talk, we demostrate that this frontier can be obtained by semiclassical quantization of the involved scarring periodic orbits. Additionally, in order to calculate the Maslov index of each quantized scarring periodic orbit, we introduce a novel straightforward method based on Lagrangian descriptors.

References

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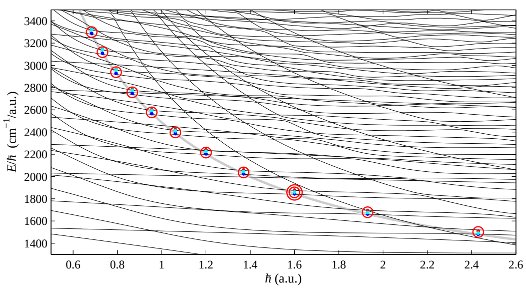

Figure 1: Correlation diagram of eigenenergies versus Planck constant. The semiclassical frontier between order and chaos is depicted in thick gray line.