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Dynamical Switching of a Reaction Coordinate Triggered by Breakdown of a Normally Hyperbolic Invariant Manifold

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In this talk, we present a novel scenario of how a reaction coordinate cease to be a dominant reaction coordinate and what happens after that as the parameters of a system changes in Hamiltonian systems that consists of many degrees of freedom. A hydrogen atom under crossed electric and magnetic field is used for demonstrating the scenario and we found that the reaction coordinate that dominates the reaction dynamics of the system ceases to be a reaction coordinate and it switches into a new reaction coordinate, triggered by the breakdown of the normally hyperbolic invariant manifold, which is the intrinsic phase space structure behind the phenomena

In the system, there is a saddle that connects two different regions, each of which corresponds to the electron bound to the nucleus and that dissociated from the nucleus, respectively (See Fig. 1 (left), Here, (x, y, z) denotes the position of the electron of the hydrogen atom and the origin is set to the saddle.). If the total energy of the system is close to that of the saddle, the instability of the unstable direction of the saddle dominates over that of the other directions and that guarantees the existence of the normally hyperbolic invariant manifold (NHIM) around the saddle [1]. NHIM is invariant under the vector flow that determine the time evolution of the system and its normal stability/instability is more prominent compared with its tangential stability/instability, which is called normal hyperbolicity. At slightly above the saddle energy, the normal direction just corresponds to the unstable direction of the saddle and that serves as the dominant reaction coordinate of the system. However, as the total energy of the system increases, strong chaos starts to develop inside the NHIM and its tangential stability/instability grows due to the chaos and finally that exceeds the normal stability/instability of the NHIM, which ends up with the loss of its normal hyperbolicity [2]. Since the normal hyperbolicity is the very property that guarantees the persistence and smoothness of the NHIM [1], the loss of the normal hyperbolicity generically implies development of its singularities such as cusps and the breakdown of the NHIM.
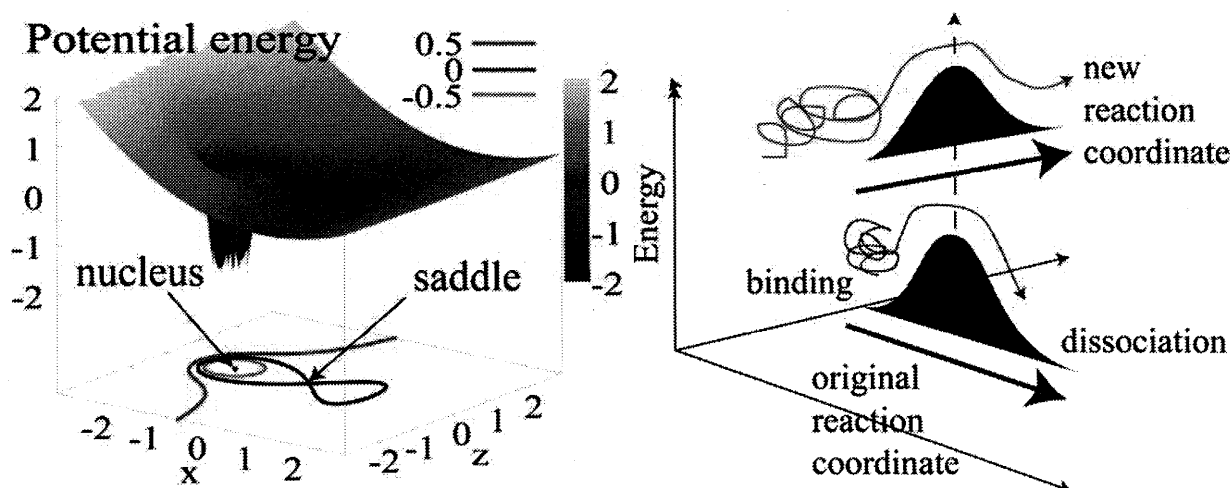

Figure 1: (left) Potential energy surface for the electron is plotted on the section (y=0),

(right) Schematic drawing of the switching mechanism

In order to investigate the mechanism of how the NHIM breaks down and its consequences, first, we constructed the NHIM in the vicinity of the saddle using normal form [5]. However, the normal form is only valid in the vicinity of the saddle and the NHIM cannot be continued up to arbitrary high energy regions

where the NHIM no longer persists using the normal form. Therefore, we do not continue the NHIM itself but continue the unstable periodic orbits in the NHIM, instead. That might sound strange but the unique property of the NHIM that is called isolation property guarantees that if a periodic orbit is in the NHIM in a certain energy region, then, its whole continuous family should also in the NHIM unless it breaks down. The fact makes us possible to follow the NHIM along the branch of each continuous family of the periodic orbits.

By following each branch of the periodic orbits, we found the following facts [3,4];

1. The way of how the NHIM looses its normal hyperbolicity is highly inhomogeneous, that is, strongly depends on each continuous family.

2. Around some periodic orbits that are located on the biggest chaotic sea in the NHIM, switching of the reaction coordinate occurs, that is, the normal direction in the lower energy region ceases to dominate the reaction and another direction starts to work as a new reaction coordinate that connects between different regions of phase space.

3. We created an indicator that provides the necessary condition for the breakdown of NHIM along a homoclinic orbit in the NHIM and, by using the indicator, we found that the NHIM itself actually breaks down along the periodic orbits of 2. on the course of the switching.

Conclusions

The concept of reaction coordinate was thought to be just a static object that solely depends on the topography of the potential energy landscape. The recent theoretical developments [6,7] have revealed that the reaction coordinate is, just as postulated by Wigner [8], a dynamic object that generally depends on the phase space structure and energy in many-dof systems. In this talk, we present a scenario of how the ruin of the reaction coordinate gives birth to a switching to a new reaction coordinate that connects different states.

Acknowledgements

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