Séminaire de Chimie Théorique

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Semiclassical Regge pole analysis: a new tool for understanding reactive cross-sections

In recent years success of state-of-the art experiments (see, for example, [1,2]) and sophisticated numerical modelling [3,4] has made possible detailed investigation of chemical reaction dynamics at low temperatures. At such temperatures quantum mechanical resonances can affect both differential (DSC) and integral (ICS) cross-section. The signatures of resonances may vary, and their identification remains a difficult task after high quality numerical data have been produced by a computer code. A widely used technique is the time-delay analysis [5] of the energy dependence of scattering (S-)matrix.

Here we advocate a different approach which relies on the behaviour of scattering matrix elements in the complex angular moment (CAM) plane. As both the DCS and ICS are obtained by summation over partial waves, one may convert such sums into integrals and identify resonance contributions associated with CAM singularities (Regge poles) of the S-matrix. This allows for a quantitative analysis of the patterns in the cross-sections, often resulting from interference between the direct and resonance mechanisms.

Simple theory based on physical intuition is available for the analysis of state-to-state DCS and ICS. Collision partners may either part after a brief (direct) encounter or form a long-lived complex whose rotation may carry the products into angular regions inaccessible to direct trajectories. Such rotations manifest themselves as exponential 'tails' extending over a wide angular range. Interference between a small number direct and resonance pathways often gives a DCS a complicated shape and produce structure in the corresponding ICS.

Converting the CAM analysis into a practical tool requires software for analytical continuation of the S-matrix element into the CAM plane. A code for this purpose was made available recently [10]. A user-friendly program for semiclassical CAM reconstruction of the scattering amplitude and decomposing a structured DCS into a number of resonance and direct contributions is currently in the making. Similarly, a code for analysing elastic, inelastic and reactive ICS, based on the extension of Mulholland formula [6] is being prepared.

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