ON THE CALCULATION OF RESONANCES BY MEANS OF ANALYTICAL CONTINUATION IN COUPLING CONSTANT

JIŘÍ HORÁČEK[1] and IVANA PAIDAROVÁ[2]

[1]*Institute of Theoretical Physics, Charles University in Prague,*
Faculty of Mathematics and Physics,
V Holešovičkách 2, 180 00 Praha 8, Czech Republic
E-mail: horacek@mbox.troja.mff.cuni.cz
[2]*J. Heyrovský Institute of Physical Chemistry, AS CR, v.v.i.,*
Dolejškova 3, 182 23 Praha 8, Czech Republic
E-mail: ivana.paidarova@jh-inst.cas.cz

Abstract. As is well known resonances play important roles in many processes in plasma physics and plasma chemistry: e.g., in dissociative attachment, associative detachment, vibrational excitation, etc., just to mention a few. For description of the above mentioned resonance processes an accurate knowledge of resonance energies and widths is required. To calculate these is however a complicated problem. There exist very efficient commercial programs for calculation of bound states but not an easy to apply method to calculate resonances. It is therefore natural to ask whether one could obtain some information on the resonance energies and widths using bound state energy calculations only. The answer is affirmative and one method following this idea was proposed already in seventieths in the field of nuclear physics. It works as follows: it is intuitively clear that if we modify our problem in such a way so as to make the interaction between the colliding particle and the molecule more attractive the bound states become more deeply bound; it can be also shown that the resonances decrease their energy as well as their width. If the additional interaction is strong enough the resonances are eventually converted into bound states. One can calculate the bound state energy for various potential strength and then construct an analytic function by means of the so-called analytic continuation. Once the analytical expression is found, the resonance energy and width is determined by simply setting the additional potential strength to zero. Thus from a knowledge of bound state energies for only a slightly modified problem we can determine the resonance parameters. An important restriction of the method is that the bound state energy must be known with a very high accuracy. It is the purpose of this contribution to show that the method is applicable to the treatment of electron-molecule resonances of importance to plasma physics using generally available standard quantum chemistry codes. The method of the analytical continuation combined with the use of the statistical Padé approximation allows us to calculate resonance parameters with an accuracy comparable with other often more elaborate and advanced methods. Here we demonstrate results for the case of $^2\Sigma_u^+$ resonance in the electron – H_2 problem but the method can be easily applied also to large polyatomic molecules.