On the calculation of resonances by means of analytical continuation

J. Horáček
Institute of Theoretical physics
Charles University in Prague
V Holešovičkách 2, 180 00 Praha 8, Czech Republic
jiho@matfyz.cz

As is well known resonances play important roles in many processes in physics and 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 the Hamiltonian in such a way so as to make the interaction between the colliding particles more attractive the bound states become more deeply bound. 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 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. It is the purpose of this contribution to study the numerical performance of the process of analytical continuation on simple analytical models by means of the statistical Padé approximation. It is well known that the process of analytical continuation represents an ill-conditioned problem. It will be shown that the application of the Padé approximation nevertheless allows us to obtain very precise continued data provided the input data were accurate enough.