

BENEMÉRITA UNIVERSIDAD AUTÓNOMA DE PUEBLA

INSTITUTO DE FÍSICA “LUIS RIVERA TERRAZAS”



SEMINARIO “DR. JESUS REYES CORONA”

“SOME USES OF PADÉ APPROXIMANTS IN MOLECULAR PHYSICS”

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Padé approximants constitute a powerful method to make an analytic representation of a function as a ratio of two polynomials. We first consider a class of problems where Padé methods can be used to extract information about resonance energies and the associated wave functions, with an input resulting from a modification of the wave equation, made to ease the numerical treatment. The examples which are treated correspond either to the introduction of a so-called optical potential in the wave equation, with a strong distortion of the results, or to the replacement of the relative coordinate between two entities by a complex coordinate. In the latter case Padé approximants are used to calculate the unnormalizable wave function of a resonance. In the second class of problems, Padé approximants allow the detection of the position of a point in a parameter plane at which there is a failure of the method. This is useful in the context of the theory of exceptional points where there is a coalescence of two complex resonance energies, with a merging of the two wave functions into a unique one. Because this point is a branch point, the Padé approximant breaks down. This failure provides in fact the desired information.

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