The Schwinger Multichannel Method: Basic Aspects of the Theory and Applications

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The Schwinger multichannel method (SMC) [1, 2, 3] is, along with complex-Kohn [4] and R-matrix [5] methods, one of the best suited theoretical approaches for modeling of the scattering problem. During the last two decades, the SMC method has been successfully used in the study of several low-energy electron and positron-molecule collision processes, ranging from elastic scattering to rotational, vibrational and electronic excitations. The effects arising from polarization of the target by the charge of the incident particle, very important at low impact energies, are properly accounted for in the formalism by inclusion of a substantial number of closed electronic channels. The method also allows for an expansion of the total scattering wave function in terms of a square-integrable basis set and, as a consequence, could be applicable to molecules of arbitrary geometry. The evaluation of Green's function matrix elements by numerical quadrature improves the efficiency of the calculations by reducing the size of the basis set, which need only to reflect the dynamical requirements of the scattering wave function. Moreover, it is especially adapted for the use of the so-called norm-conserving pseudopotentials [6]. In this procedure, the core electrons and protons are replaced by a nonlocal but single-particle pseudopotential and only the valence electrons are treated in a many-body framework. This feature has some practical consequences in applications of the SMC method to heavy polyatomic targets, since has allowed for calculations with a significative reduction of the computational effort (processing time and/or memory allocation). In fact, the transferability of the pseudopotential formalism to scattering calculations has established an outstanding progress for the theoretical research in the area of electron-molecule collisions. In this talk we will make an introductory discussion on basic aspects of the SMC theoretical formulation as well as an overview of its more relevant applications and recent developments.

References

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