ON THE DESCRIPTION OF ELETRON – MOLECULE COLLISION IN THE SEMICLASSICAL PHASE – SPACE APPROACH

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1. Introduction

Phase-space representations of quantum mechanics play an important role in several branches of physics [1, 2]. Although there exist a large number of phase-space representations discussed in the literature, the Weyl – Wigner representation has come to play the role of a canonical phase-space representation, mainly because of its simplicity. In the present communication, we summarize how one could calculate the elastic differential cross section for the collision between an incident electron and a diatomic molecule. The method makes use of the quantum phase space Wigner function associated to a vibration degree of freedom for the target molecule.

2. Developments

Although the present method could be applied to any kind of reactions, for convenience we are considering a nonreactive collision represented by

$$A + BC\ (n) \rightarrow A + BC(m)$$

where n a m refer to any quantum vibration numbers to be specified.

It is assumed that the molecule vibrational motion can be described by a harmonic oscillator in an " n " state. The corresponding Wigner function is written as

$$W^{(n)} = (-1)^n \frac{1}{\pi\hbar} \exp(\frac{-2E_c}{\hbar\omega}) L_n(\frac{4E_c}{\hbar\omega})$$

where E_c and ω are the classical energy and frequency of the harmonic oscillator and $L_n(x)$ is the Laguerre polynomial. In the present study we are considering the Yukawa type potential to describe the projectile – target interaction.

The quantum full time evolution of the Wigner function is governed by the Weyl-Wigner representation of the quantum von Neumann – Liouville equation. In particular, for harmonic potential interaction, we keep the lowest order term of the corresponding $\hbar$- power series for the Liouville operator,

$$\partial W(p,q,t)/\partial t = -p/m\partial W/\partial q + \partial V/\partial q \partial W/\partial p$$

where $dq/dt = p/m$ and $dp/dt = -\partial V/\partial q$ are the classical Hamilton's equations. In particular, the classical propagation of the Wigner distribution function leads to a exact description of the harmonic oscillator.[3] Each phase-space point of the initial Wigner distribution function (q,p) is propagated along a classical trajectories. Therefore, the resulting Wigner distribution function at time t can be used to determine the final oscillator quantum state. The classical trajectory picture leads to the description of the elastic differential cross section of the reaction.

References

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