2004 Vol.41 No.3 pp.357-361 DOI:

Studies of Rigid Rotor-Rigid Surface Scattering in Dynamical Lie Algebraic Method

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(Received: 2003-6-16; Revised:)

Abstract: The dynamical Lie algebraic method is used for the description of statistical mechanics of rotationally inelastic molecule-surface scattering. It can give the time-evolution operators about the low power of $a^\dagger$ and a by solving a set of coupled nonlinear differential equations. For considering the contribution of the high power of $a^{\dagger}$ and a, we use the Magnus formula. Thus, with the time-evolution operators we can get the statistical average values of the measurable quantities in terms of the density operator formalism in statistical mechanics. The method is applied to the scattering of $N_{2 }$ (rigid rotor) by a flat, rigid surface to illustrate its general procedure. The results demonstrate that the method is useful for describing the statistical dynamics of gas-surface scattering.

PACS: 03.65.Fd,

Key words: Lie algebraic method, scattering, rigid rotor

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