Shell Effects in Cluster-Cluster Collisions
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1. Introduction

Collisions between atomic clusters offer a new and interesting field of cluster research. First theoretical studies of cluster-cluster collisions (CCC)$^{1,2,3,4}$ have shown that close analogies to nuclear heavy-ion collisions (HIC) exist. Inspite of the different microscopic forces acting between the constituents, the dynamics of collective (macroscopic) degrees of freedom is similar in both types of systems. The reaction mechanism of HIC and CCC is characterized by dissipation and fluctuation phenomena of a few collective variables coupled to a large, but finite number of intrinsic degrees of freedom (nucleonic and atomic, respectively).$^2$ Therefore, CCC allow to study relaxation phenomena in finite atomic many-body systems.

One of the striking differences between HIC and CCC consists in the role of shell effects. Whereas in HIC nucleonic shell effects are “smoothed” out with increasing excitation energy of the nucleons, they survive almost completely in CCC because the excitation energy is stored mainly in chaotic atomic motion, while the electrons (which mediate the shell effects) remain in their ground state (at sufficiently low bombarding energies). The dominating role of shell effects in CCC shows up in the preferential (almost exclusive) occurrence of “magic” products in the exit channel.$^1$ The decisive influence of shell effects on the energetics$^5$ and dynamics$^6$ of cluster-fission has been demonstrated recently, too (see also the contribution of U. Landman et al., this volume).

Relaxation phenomena should be appropriately treated in terms of transport theories. As a basic entity of any transport theory, the interaction potential as function of the relevant collective degrees of freedom must be known. In the work to be reported here, a microscopic formalism for the calculation of the interaction potential between colliding clusters is presented. It is based on density functional theory in local density and a two-centre
jellium approximation. The potential is calculated as function of the centre-of-mass distance and the size-asymmetry, being important collective degrees of freedom in collisions. First results for the \( \text{Na}_2\text{O} + \text{Na}_2\text{O} \) system are presented. The role of shell effects and their consequences on the collisional dynamics are discussed. Relations to nucleus-nucleus potentials as well as phenomenological potentials\(^4\) will be outlined.

2. The two-centre Kohn-Sham jellium formalism

The potential energy between colliding clusters is defined as the difference between the ground-state total energies of the two-cluster system \( E_{\text{tot}}^{(1+2)} \) and the energies of the two separated clusters

\[
U = E_{\text{tot}}^{(1+2)} - \left( E_{\text{tot}}^{(1)} + E_{\text{tot}}^{(2)} \right)
\]

For the calculation of the energies we adopt the jellium approximation. The electronic ground-state configuration results from the self-consistent solution of the Kohn-Sham equation in local density approximation

\[
\left( -\frac{1}{2} \Delta + V_{\text{eff}}(\vec{r}) \right) \phi_i(\vec{r}) = \varepsilon_i \phi_i(\vec{r})
\]

\[
V_{\text{eff}}(\vec{r}) = V_{\text{eu}}(\vec{r}) + V_{\text{ee}}(\vec{r}) + V_{\text{xc}}(\vec{r})
\]

\[
= V_{\text{eu}}(\vec{r}) + \int \rho(\vec{r}') d^3r' \left| \vec{r} - \vec{r}' \right| + V_{\text{xc}}(\vec{r})
\]

\[
\rho(\vec{r}) = \sum_{i}^{\text{occ.}} \left| \phi_i(\vec{r}) \right|^2
\]

where \( \rho, V_{\text{eu}}, V_{\text{ee}}\) and \( V_{\text{xc}} \) stand for the electronic density, the electron-background potential, the electron-electron and the exchange-correlation potential, respectively. For the exchange-correlation potential and its energy density \( \varepsilon_{\text{xc}} \) we applied the formulae of Gunnarsson and Lundquist [7]. The total energy \( E_{\text{tot}} \) consists of the kinetic energy \( E_{\text{kin}} \), the electrostatic energy \( E_{\text{es}} \) and the exchange-correlation energy \( E_{\text{xc}} \).

The positive charge density \( \rho_+ \) as function of the centre-of-mass distance \( d \) between the interacting clusters is treated in a simple geometrical model\(^5\): For \( d \geq R_1 + R_2 \), two spheres with radii \( R_1 = r_s N_i^{1/3} \) are assumed, where \( r_s \) is the Wigner-Seitz radius \( (r_s = 3.93 \text{ a.u. for Na}) \) and \( N_i \) the number of