

REPLACEMENT OF VAN DER WAALS PAIRS AT COLLISIONS IN THE THREE-BODY PROBLEM

Kim S.E., Popov E.N.

ITMO University, Russia, 197101, St. Petersburg, Kronverksky Pr., 49, bldg. A;
codeilece@gmail.ru, +7 952 922 32 13; enp-tion@yandex.ru, +7 981 941 42 06

As known, van der Waals pairs form in triple collisions in hot gas when one of atoms transfers excess energy, cooling the other two atoms trapped in a potential field of van der Waals forces [1]. In this work, we numerically simulate the dynamics of van der Waals pair destruction based on the three-body problem [2]. Of interest is the dynamics of van der Waals pair destruction, in which one of the atoms in the bonded pair is dislodged by a third atom, thus taking the place of the dislodged atom. We call this phenomenon "replacement" and evaluate the conditions and frequency of its occurrence.

A sample of van der Waals pairs with the mutual location of atoms and their relative velocities was obtained ahead of time. Then, we described and modeled the act of collision of an atomic pair with a third atom. Modeling of the process is associated with the difficulty of finding an analytical formula for calculating the atomic pair by initial conditions on account of the interaction potential, with degrees -6 and -12. Simulating many times different collisions in the conditions of van der Waals interaction revealed that "replacement" is not a rare phenomenon for atoms with masses of the same order. We assume that this is related to the peculiarity of the introduced potential. Therefore, at sufficient proximity, the atoms repel each other, as in an absolutely elastic collision, which allows us to interpret the phenomenon of "replacement" as Newton's cradle, where the colliding objects swap momentum.

The results obtained can be used to investigate the spin-exchange interaction between atoms, which occurs when atoms approach each other for a time longer than the double collision time [3, 4].

References.

1. *Lu T., Chen Q.*, van der Waals potential: an important complement to molecular electrostatic potential in studying intermolecular interactions //Journal of Molecular Modeling. – 2020. – T. 26. – №. 11. – C. 315.
2. *Nielsen E. et al.* The three-body problem with short-range interactions //Physics Reports. – 2001. – T. 347. – №. 5. – C. 373-459.
3. *Walker T. G., Larsen M. S.*, Spin-exchange-pumped NMR gyros //Advances in atomic, molecular, and optical physics. – Academic Press, 2016. – T. 65. – C. 373-401.
4. *Kelley M., Branca R. T.*, Theoretical models of spin-exchange optical pumping: Revisited and reconciled //Journal of Applied Physics. – 2021. – T. 129. – №. 15.