Center for Computational Sciences, University of Tsukuba

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Time-dependent Quantum Dynamics

Quantum nuclear fusion

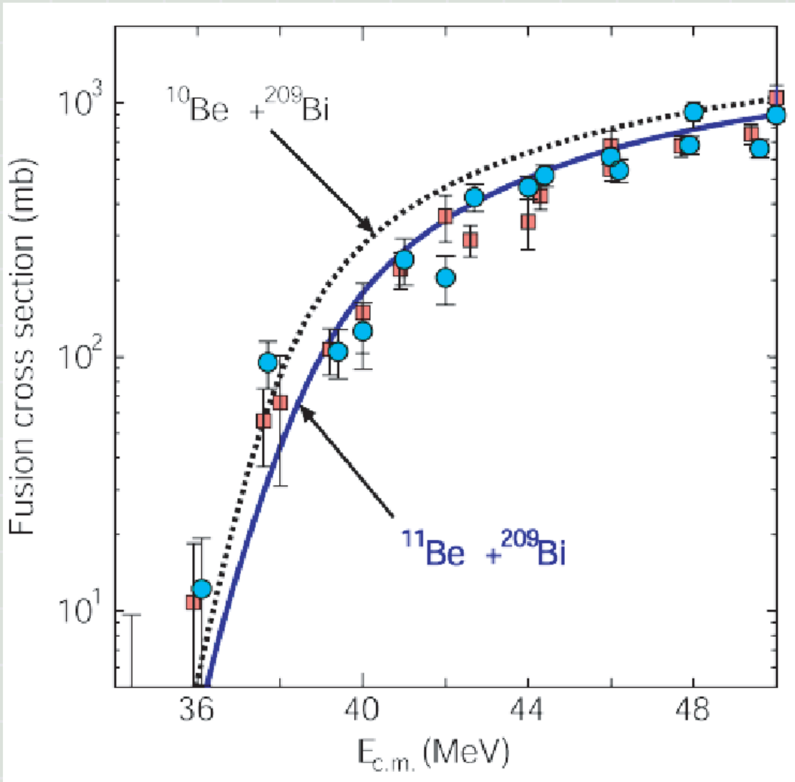
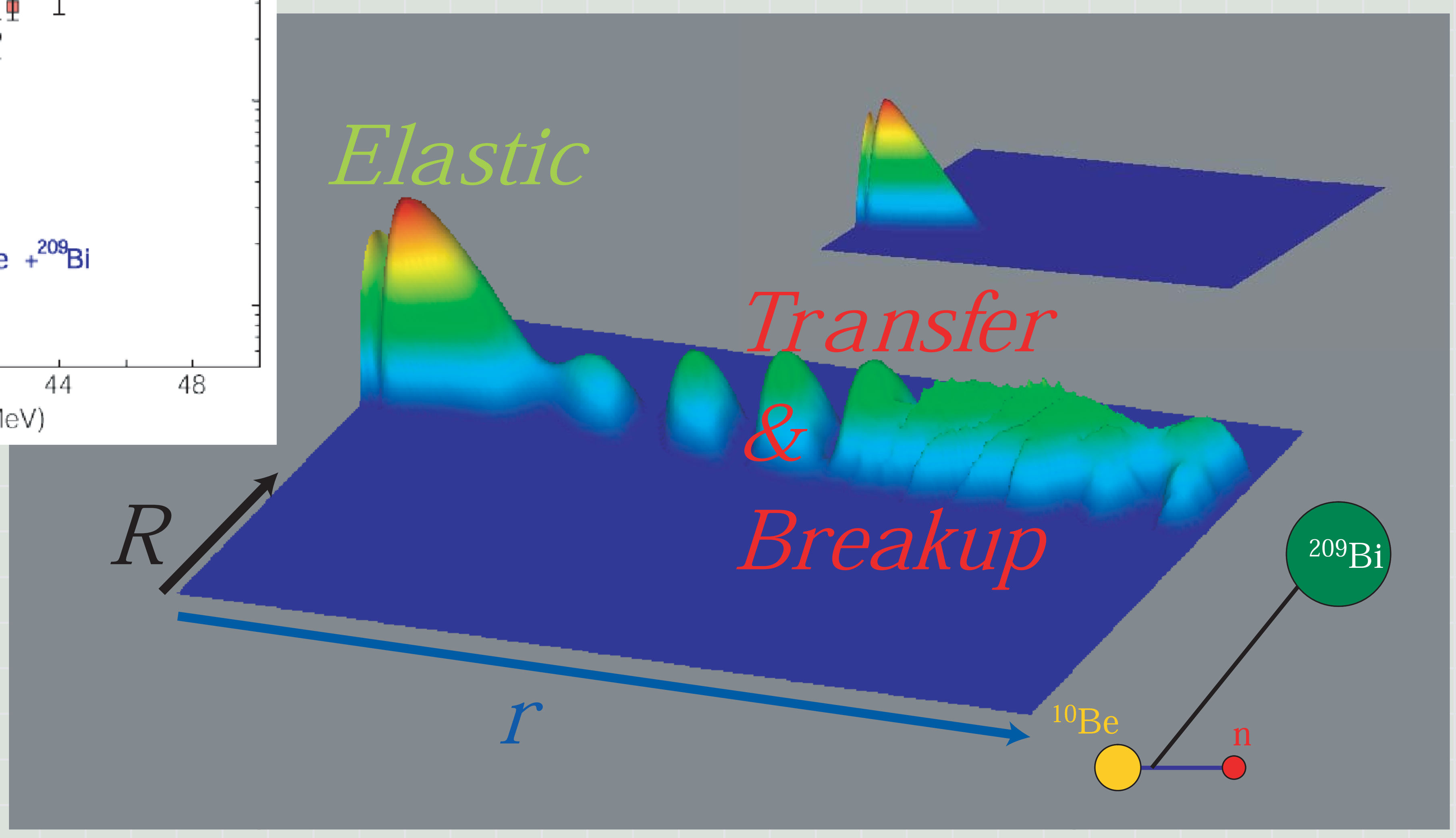


Fig. 2: Fusion cross section (calculation and experiment).

Fig. 1: Calculated time-dependent wave packets for ^{11}Be and ^{209}Bi.



Quantum nuclear fusion is studied with the time-dependent wave-packet (TDWP) method. The time-dependent Schrödinger equation for a three-body system is solved in the discrete variable representation. Figure 1 shows wave packets before and after the collision of ^{11}Be (^{10}Be+n) and ^{209}Bi. Since the last neutron in ^{11}Be is very weakly bound, its wave function, $\Phi(r)$, is spatially extended ("neutron halo"). It has been believed that the extended neutron cloud, playing a role of "glue", would enhance the fusion probability. The large-scale TDWP calculation indicates a significant amount of breakup and transfer of the neutron from ^{11}Be to ^{209}Bi. This leads to a conclusion opposite to the people's belief; suppression of the fusion probability (Fig. 2).

Femto-second electron dynamics

Fig. 3: Density of valence electrons in a naphthalene molecule under a strong laser field.

Femto-second electron dynamics in molecules under an intense laser field is studied with the time-dependent density-functional theory (TDDFT). The ionization mechanism under intense laser field is considered to crucially depend on the laser frequency and molecular size, changing from a quantum tunneling to a nonlinear multi-photon mechanism. Such a behavior is investigated with the TDDFT simulation in the three-dimensional real-space and real-time (Fig.3). The study reveals an importance of the dynamical screening for the external laser field.