Time-dependent quantum wave packet dynamics to study charge transfer in heavy particle collisions

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Synopsis The method of time-dependent quantum wave packet dynamics has been successfully extended to study charge transfer/exchange process in low energy two-body heavy particle collisions. The collision process is described by coupled-channel equations with diabatic potentials and (radial and rotational) couplings. The time-dependent coupled equations are propagated with multiconfiguration time-dependent Hartree method and the modulo squares of *S*-matrix is extracted from the wave packet by the flux operator with complex absorbing potential method (FCAP). The calculations of charge transfer process $1^2\Sigma^+\ \mathrm{H}^-(1s^2)+\mathrm{Li}(1s^2 2s) \rightarrow 2^2\Sigma^+/3^2\Sigma^+/1^2\Pi\ \ \mathrm{H}(1s)+\mathrm{Li}^-(1s^2 2s2l)\ (l=s,p)$ at the incident energy of about [0.3, 1.3] eV are illustrated as an example. It shows the calculated reaction probabilities by the present FCAP reproduce that of quantum-mechanical molecular-orbital close-coupling (QMOCC) very well, including the peak structures contributed by the resonances. Since time-dependent external interactions can be directly included in the present FCAP calculations, the successful implementation of FCAP provides us a powerful potential tool to study the quantum control of heavy particle collisions by lasers in the near future.

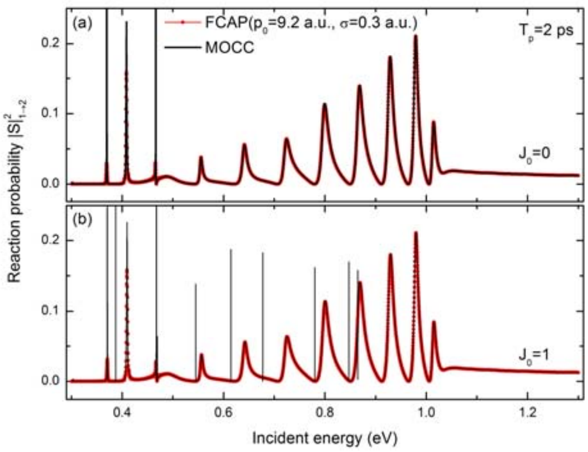

FIG. 1. $1^2\Sigma^+ \rightarrow 2^2\Sigma^+$ reaction probability $|S|^2_{1\rightarrow 2}$ for J_0=0 and 1 as a function of incident energy. The thin line shows the results from QMOCC calculations, the dot line shows the present FCAP calculations (p_0=9.2 a.u., σ=0.3 a.u., T_p=2 ps).

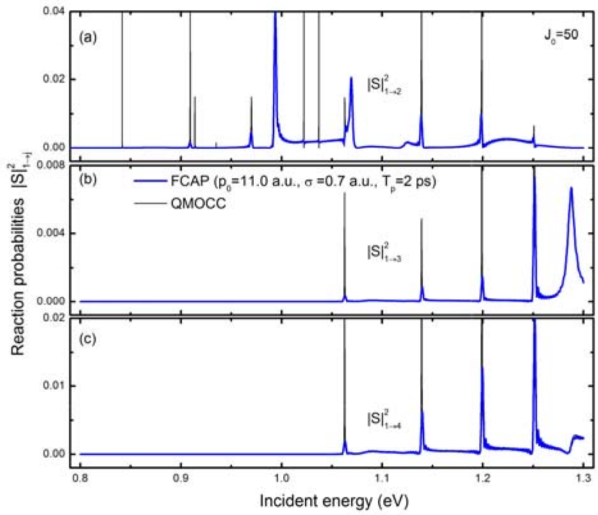

Fig. 2. Reaction probabilities $|S|^2_{1\rightarrow 2}$, $|S|^2_{1\rightarrow 3}$ and $|S|^2_{1\rightarrow 4}$ for J_0=50. The thin line and bold line show the results from QMOCC and FCAP (p_0=11.0 a.u., σ=0.7 a.u., T_p=2 ps), respectively.

References

[1] S. B. Zhang, Y. Wu, and J. G. Wang, J. Chem. Phys. **145**, 224306 (2016)

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