



2014年度 物質生命理工学科コロキウム

上智大学 理工学部 物質生命理工学科 主催
理工学部・理工学振興会 共催

Electronically nonadiabatic wave packet propagation using frozen Gaussian scattering.

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場所: 8 - 308



Modern methods to perform wave packet propagation to describe chemical dynamics of many degrees of freedom would be discussed. Significant attention would be paid to approaches which allow incorporation of effects of nonadiabatic transition into such wave packet propagation methods. A novel Frozen Gaussian Scattering (FGS) method to calculate bunches of hopping trajectories to describe various quantum effects would be introduced. It would be demonstrated that since the FGS provides all necessary phase information, it could be used at the first stage of chemical dynamics computations performed with various kinds of modern adiabatic wave packet propagation methods and SC-IVR theories. Thus these techniques could be extended to treat electronically nonadiabatic molecular processes in quite efficient way. As an example implementation of the FGS approach into the Herman-Kluk frozen Gaussian approximation would be presented and efficiency of the result technique would be demonstrated. A ways to extend FGS approach to treat tunneling would be discussed.

学外の方の聴講歓迎・申込不要・参加無料

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