Physikalisches Institut
Fakultät für Mathematik und Physik
Albert-Ludwigs-Universität Freiburg

QE

Quantum Efficiency Seminar und Colloquium

FRANK GROSSMANN

Institut für Theoretische Physik
Technische Universität Dresden

Semiclassical hybrid dynamics and selected applications

The semiclassical initial value formalism to solve the time-dependent Schroedinger equation will be reviewed. Special focus will be laid on the Herman Kluk method [1] and Heller's thawed Gaussians [2]. The semiclassical hybrid formalism that combines both approaches [3] will be introduced.

We then present results for the quenching of quantum interference in Iodine molecules in solution [4] as well as the decoherence dynamics of Iodine in a Krypton matrix, with special emphasis on possible coherence flow into the bath [5].

[1] M. Herman and E. Kluk, Chem. Phys. 91, 27 (1984)
[2] E. J. Heller, J. Chem. Phys. 62, 1544 (1975)
[3] F. Grossmann, J. Chem. Phys. 125, 014111 (2006)
[4] C.-M. Goletz and F. Grossmann, J. Chem. Phys. 130, 244107 (2009)
[5] M. Buchholz et al., J. Phys. Chem. A 116, 11199 (2012)

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