

QUASICLASSICAL METHOD FOR CALCULATION OF MOLECULAR VIBRATIONAL LEVELS

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The so called quasiclassical method is an approximate Monte-Carlo-type approach to quantum molecular dynamics based on a propagation of a set of independent classical trajectories with their initial conditions given by the preferential sampling of the Wigner distribution of an initial quantum wavepacket Ψ . I will present an improved quasiclassical approximation to the quantum autocorrelation function $\langle \Psi | \exp(-it\hat{H}/\hbar) | \Psi \rangle$ for long-time propagations and the tentative model applications for molecular spectroscopies where excited vibrational levels are measured [1].

[1] P. R. Kapralova-Zdanska, F. Hanak, and J. Lazebnicek, J. Chem. Phys. **128** (2008) 154316.