

Construction and Test of Thermostats and Twirlers for Molecular Rotations

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Z. Naturforsch. **58a**, 377 – 391 (2003); received May 28, 2003

The equations of motion are coupled with a dynamical variable, referred to as twirler, which randomizes the angular momentum. The equations are time-reversal invariant, just as those for the standard Gaussian, Nosé-Hoover and configurational thermostats. The derivation of the basic equations is outlined. Test calculations are performed for the two-dimensional isotropic harmonic oscillator and for a nonlinear elastic dumbbell, used as a simple model to study properties of polymer molecules. Graphs of characteristic quantities and orbits, some of which are rather intriguing, are displayed. As applications, the rotational diffusion and the influence of a shear flow on the angular velocity and the deformation of the model polymer are analyzed.

Key words: Molecular Rotations; Dumbbell; Thermostats; Diffusion; Shear Flow.