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F. J. Lin* (fjlin@usc.edu), University of Southern California, Department of Mathematics, KAP 108, 3620 S. Vermont Avenue, Los Angeles, CA 90089-2532. Quantum and classical geometric phases in N-body molecular dynamics each describe the motion of a moving frame corresponding to internal angular momentum. Preliminary report.

In differential geometric terms, a geometric phase is the holonomy of a connection. In N-body molecular dynamics, for example, a geometric phase arises in the solution of differential equations: (1) the time-dependent Schrodinger equation for a wavefunction in quantum mechanics and (2) Hamilton's equations for a trajectory in phase space in classical mechanics. In quantum dynamics, a geometric phase in the wavefunction is a phase shift corresponding to the expected value of the internal/vibrational angular momentum of the N-body system within its moving frame. In classical dynamics, a geometric phase of a moving frame is its net rotation corresponding to the internal/vibrational momentum of the N-body system within its moving frame. The geometric phase is also called a Berry phase and arises in further situations in both quantum and classical mechanics. (Received June 22, 2010)