Biomedical Engineering: Opening New Doors

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HOW TO SIMULATE THE QUANTUM-MECHANICAL SUPPRESSION OF HIGH-FREQUENCY MODES IN CLASSICAL MOLECULAR DYNAMICS COMPUTATIONS

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The purpose of this talk is to describe a molecular dynamics method which combines two old ideas in a new way. These ideas are the backward-Euler method for the solution of stiff ordinary differential equations and the Langevin-equation approach to the maintenance of thermal equilibrium. The new feature is that the Langevin collision frequency and the backward-Euler dissipation rate are balanced in such a way as to produce a definite cutoff frequency which can be set equal to kT/h to simulate the quantum-mechanical suppression of high-frequency modes. The resulting BACKWARD-EULER/LANGEVIN method has been tested on two physical problems for which both the quantum mechanical and classical results are known: a system of coupled harmonic oscillators and a diatomic molecule. In both cases, the method produces results that correspond much more closely to those of quantum than to those of classical statistical mechanics, despite the classical character of the method. Implementation of the method in the case of large biological molecules will also be discussed.

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REFERENCES:

1. Peskin, C. S. and Schlick, T.: Molecular dynamics by the backward-Euler method. Commun. Pure & Appl. Math. 42: 1001-1039, 1989
2. Schlick, T. and Peskin, C. S.: Can classical equations simulate quantum-mechanical behavior: a molecular dynamics investigation of a diatomic molecule with a Morse potential. Commun. Pure & Appl. Math. 42: 1141-1163, 1989
3. Peskin, C. S.: Analysis of the backward-Euler/Langevin method for molecular dynamics. Commun. Pure & Appl. Math. (in press)

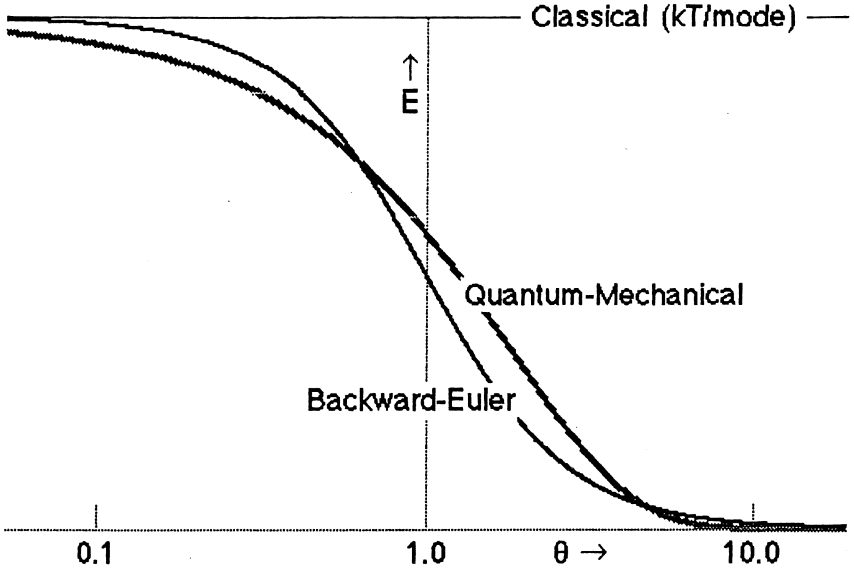

Fig. 1. Partition of mean thermal energy among the vibrational modes of a system of coupled harmonic oscillators ($\theta = h\nu/kT$). Note qualitative agreement between the backward-Euler and the quantum-mechanical results, both of which are in sharp disagreement with the classical equipartition theorem (E independent of θ).