

Abstract Submitted  
for the MAR08 Meeting of  
The American Physical Society

**Ergodicity of Isothermal Molecular Dynamics Method<sup>1</sup>** HIROSHI WATANABE, Nagoya University — A condition for equations of motion for isothermal dynamics is derived, and the Nosé–Hoover method is generalized on the basis of this condition. The ergodicity of the one-variable thermostats are studied, and it is shown that the one-variable thermostat coupled with the one-dimensional harmonic oscillator loses its ergodicity with large enough relaxation time. A stochastic process of the Nosé–Hoover method is also discussed based on the Markovian approximation.

<sup>1</sup>This research was partially supported by the Ministry of Education, Science, Sports and Culture, Grant-in-Aid for Young Scientists (B), 19740235, 2007.

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Date submitted: 29 Oct 2007

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