Ergodicity of Isothermal Molecular Dynamics Method\(^1\) 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.\(^1\)

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