Hamiltonian for a restricted isoenergetic thermostat

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Nonequilibrium molecular dynamics simulations often use mechanisms called thermostats to regulate the temperature. A Hamiltonian is presented for the case of the isoenergetic (constant internal energy) thermostat corresponding to a tunable isokinetic (constant kinetic energy) thermostat, for which a Hamiltonian has recently been given. [S1063-651X(99)01612-8]

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Thermostats are modifications to the equations of motion of a classical system to simulate thermal interaction of a system with the environment. The Nosé-Hoover thermostat is used to simulate fluctuations in energy of an equilibrium system corresponding to the canonical ensemble of statistical mechanics, and the Nosé-Hoover and Gaussian thermostats, among others, are used to remove heat from a system driven by external forces into a nonequilibrium stationary state [1]. There has been recent interest in thermostatted equations of motion, focused on the symplectic structure of the equations of motion, and the related pairing of the Lyapunov exponents. Both a Hamiltonian and pairing of the Lyapunov exponents are known for Nosé-Hoover and Gaussian isokinetic (GIK: constant kinetic energy) thermostats [1–3]. Numerical evidence against pairing (and hence the existence of a Hamiltonian) are discussed in [4] for the GIK thermostat applied to shearing systems and in [5] for the Gaussian isoenergetic (GIE: constant internal energy) thermostat. The latter paper does, however show that in a special case of the GIE thermostat, involving one rather than two arbitrary potentials, the Lyapunov exponents are paired. The purpose of this Brief Report is to present a Hamiltonian for this case.

The GIE thermostat has equations of motion of the form

\[ \frac{dx_i}{dt} = \frac{p_i}{m_i}, \quad \frac{dp_i}{dt} = -\frac{\partial\Phi^{(\text{ext})}}{\partial x_i} - \frac{\partial\Phi^{(\text{int})}}{\partial x_i} - \alpha p_i, \]

\[ \alpha = -\frac{\sum_i (p_i/m_i) \cdot (\partial\Phi^{(\text{ext})}/\partial x_i)}{\sum_i p_i \cdot p_i/m_i}. \]

(1)

where \( \Phi^{(\text{ext})} \) is the external driving potential, \( \Phi^{(\text{int})} \) the interparticle potentials, and \( \alpha \) is the thermostat term which ensures that the equations conserve internal energy \( E = \sum_i p_i^2/(2m_i) + \Phi^{(\text{int})} \). The equations reduce to no thermostat when \( \Phi^{(\text{ext})} = 0 \) and to GIK when \( \Phi^{(\text{int})} = 0 \). A more general example of a limit involving only one arbitrary potential is the case \( \Phi^{(\text{ext})} = \gamma \Phi, \Phi^{(\text{int})} = (1 - \gamma)\Phi \), leading to the equations

\[ \frac{dx_i}{dt} = \frac{p_i}{m_i}, \quad \frac{dp_i}{dt} = -\frac{\partial\Phi/\partial x_i}{\partial x_i} + \gamma \sum_i \frac{(p_i/m_i) \cdot (\partial\Phi/\partial x_i)}{\sum_i p_i \cdot p_i/m_i} p_i, \]

(2)

which conserve energy \( E = \sum_i p_i^2/(2m_i) + (1 - \gamma)\Phi \). Here, \( \gamma \) effectively controls the strength of the thermostat from no thermostat (\( \gamma = 0 \)), to the GIK thermostat (\( \gamma = 1 \)). For any \( \gamma \) the Lyapunov exponents are paired [5], suggesting the existence of a Hamiltonian.

Following the GIK case [3], the conservation law is enforced by setting the numerical value of the Hamiltonian equal to the conserved energy, assigned the value zero by a shift in the potential energy. This allows the kinetic energy term in the denominator of Eq. (1) to be replaced by minus the potential energy (note \( \Phi < 0 \))

\[ \alpha = \frac{\gamma}{2(1 - \gamma)} \sum_i \frac{p_i}{m_i} \frac{\partial}{\partial x_i} \ln|\Phi|. \]

(3)

Another aspect of a Hamiltonian description of thermostatted systems is that in the physical variables \((x, p)\) there is a phase space volume contraction rate proportional to \( \alpha \), while in the canonical variables \((x, \pi)\) phase space volume is conserved. This means that \( \pi \) must be greater than \( p \) by a factor equal to \( \exp(\int dt) = |\Phi|^{\gamma(1 - \gamma)} \). Multiplying the zero energy by an arbitrary power of \(|\Phi|\) we have

\[ H_\beta(x, \pi, \lambda) = |\Phi|^{-\gamma(1 - \gamma) + \beta} \sum_i \frac{\pi_i^2}{2m_i} + (1 - \gamma)\Phi|\Phi|^{\beta}, \]

(4)

which, combined with the constraint \( H_\beta = 0 \) and the identifications \( dt = |\Phi|^{-\gamma(1 - \gamma) + \beta} d\lambda \) and \( p_i = |\Phi|^{-\gamma(1 - \gamma)} \pi_i \) leads to the equations of motion (2). Interesting cases are \( \beta = \gamma(2(1 - \gamma)) \) for which there is no time scaling, \( \beta = 0 \) has a certain simplicity, \( \beta = -\gamma(1 - \gamma) \) yields the familiar form of kinetic plus potential energy, and \( \beta = -1 \) for which the Hamiltonian is that of a geodesic in a conformally flat space, see Ref. [3].

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