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 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

$$\frac{d\mathbf{x}_i}{dt}=\frac{\mathbf{p}_i}{m_i},\quad \frac{d\mathbf{p}_i}{dt}=-\frac{\partial\Phi^{(\mathrm{ext})}}{\partial\mathbf{x}_i}-\frac{\partial\Phi^{(\mathrm{int})}}{\partial\mathbf{x}_i}-\alpha\mathbf{p}_i,$$

$$\alpha=-\frac{\sum_i(\mathbf{p}_i/m_i)\cdot(\partial\Phi^{(\mathrm{ext})}/\partial\mathbf{x}_i)}{\sum_i\mathbf{p}_i\cdot\mathbf{p}_i/m_i},\tag{1}$$

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

$$\frac{d\mathbf{x}_i}{dt}=\frac{\mathbf{p}_i}{m_i},\quad \frac{d\mathbf{p}_i}{dt}=-\frac{\partial\Phi}{\partial\mathbf{x}_i}+\gamma\frac{\sum_i(\mathbf{p}_i/m_i)\cdot(\partial\Phi/\partial\mathbf{x}_i)}{\sum_i\mathbf{p}_i\cdot\mathbf{p}_i/m_i}\mathbf{p}_i,\tag{2}$$

which conserve energy $E=\Sigma_i\mathbf{p}_i^2/(2m_i)+(1-\gamma)\Phi$. Here, γ effectively controls the strength of the thermostat from no thermostat ($\gamma=0$), to the GIK thermostat ($\gamma=1$). For any γ 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 $\Phi<0$)

$$\alpha=\frac{\gamma}{2(1-\gamma)}\sum_i\frac{\mathbf{p}_i}{m_i}\cdot\frac{\partial}{\partial\mathbf{x}_i}\ln|\Phi|.\tag{3}$$

Another aspect of a Hamiltonian description of thermostatted systems is that in the physical variables $(\mathbf{x},\mathbf{p})$ there is a phase space volume contraction rate proportional to α, while in the canonical variables $(\mathbf{x},\boldsymbol{\pi})$ phase space volume is conserved. This means that $\boldsymbol{\pi}$ must be greater than $\mathbf{p}$ by a factor equal to $\exp(\int\alpha dt)=|\Phi|^{\gamma/[2(1-\gamma)]}$. Multiplying the zero energy by an arbitrary power of $|\Phi|$ we have

$$H_\beta(\mathbf{x},\boldsymbol{\pi},\lambda)=|\Phi|^{-\gamma/(1-\gamma)+\beta}\sum_i\frac{\boldsymbol{\pi}_i^2}{2m_i}+(1-\gamma)\Phi|\Phi|^{\beta},\tag{4}$$

which, combined with the constraint $H_\beta=0$ and the identifications $dt=|\Phi|^{-\gamma/[2(1-\gamma)]+\beta}d\lambda$ and $\mathbf{p}_i=|\Phi|^{-\gamma/[2(1-\gamma)]}\boldsymbol{\pi}_i$ 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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