

Classical systems: moments, continued fractions, long-time approximations and irreversibility

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Let a classical particle, with mass m , position x and momentum p , be subject to a real potential $V = V(x)$, in the presence of a “Heat bath” at equilibrium, at temperature T . The classical Hamiltonian of the particle is: $H = p^2/(2m) + V$. Its probability distribution function is: $W = W(x, p; t) (> 0)$ at time t . The equilibrium distribution is: $W = W_{eq} = \exp[-\beta(p^2/(2m) + V)]$. Let $H_n(q)$ be the standard n -th Hermite polynomial. We introduce the moments $W_n = W_n(x; t)$ ($n = 0, 1, 2, \dots$) of W [1, 2]:

$$W_n = \int dp \frac{H_n(p/q)}{(\pi^{1/2} 2^n n!)^{1/2}} W(x, p; t), \quad q = (2m/\beta)^{1/2} \quad (1)$$

($\beta = (K_B T)^{-1}$, $K_B =$ Boltzmann’s constant). If $W = W_{eq}$, then $W_{eq,0}$ is proportional to $\exp[-\beta V]$ and $W_{eq,n} = 0$, $n = 1, 2, \dots$. Let W_{in} be an initial off-equilibrium distribution, at $t = 0$. The corresponding initial moments, using (1), are $W_{in,n}$. The irreversible Kramers equation (with a friction constant $\sigma > 0$ on the particle due to the “Heat bath”) [1] provides one temporal evolution: $(\partial W/\partial t) + (p/m)(\partial W/\partial x) - (\partial V/\partial x)(\partial W/\partial p) = (1/\sigma)(\partial/\partial p)[p + (m/\beta)(\partial/\partial p)]W$. The latter and (1) yield the infinite irreversible three-term linear hierarchy for W_n ’s ($n = 0, 1, 2, \dots$, $W_{-1} = 0$) [1]:

$$\frac{\partial W_n}{\partial t} = -M'_{n,n+1} W_{n+1} - M'_{n,n-1} W_{n-1} - \frac{n}{\sigma} W_n \quad (2)$$

$M'_{n,n\pm 1}$ being linear operators. From (2), W_n relax the quicker the larger n . W_0 (fulfilling the Smoluchowski equation) dominates the approach towards equilibrium for $t \rightarrow +\infty$.

As a source of insight, we shall treat an idealization (in presence of the “Heat bath” but without friction effects): $(\partial W/\partial t) + (p/m)(\partial W/\partial x) - (\partial V/\partial x)(\partial W/\partial p) = 0$ (the reversible Liouville equation, $\sigma^{-1} = 0$). The infinite reversible three-term linear hierarchy for W_n ’s ($n = 0, 1, 2, \dots$, $W_{-1} = 0$) is the same as in (2), with $\sigma^{-1} = 0$. Let us consider the Laplace transforms $\tilde{W}_n(s) \equiv \int_0^{+\infty} dt W_n \exp(-st)$ and introduce: $g_n = W_{eq,0}^{-1/2} \tilde{W}_n$. This and (2) with $\sigma^{-1} = 0$ yield the symmetric reversible three-term hierarchy for g_n :

$$s g_n = W_{eq,0}^{-1/2} W_{in,n} - M_{n,n+1} g_{n+1} - M_{n,n-1} g_{n-1} \quad (3)$$

$$M_{n,n\pm 1} g_{n\pm 1} \equiv \left[\frac{(n + (1/2)(1 \pm 1)) K_B T}{m} \right]^{1/2} \left[\frac{\partial g_{n\pm 1}}{\partial x} - \frac{(\pm 1) g_{n\pm 1}}{2 K_B T} \frac{dV}{dx} \right] \quad (4)$$

The hierarchy (3) for g_n can be solved formally, in terms of the linear operators:

$$D[n;s] = [s - M_{n,n+1}D[n+1;s]M_{n+1,n}]^{-1} \quad (5)$$

By iteration, $D[n;s]$ becomes an infinite continued fractions of products of linear operators. $D[n;s]$ has been evaluated for $V = 0$ and for a harmonic oscillator [2]. We choose $n_0 (\geq 1)$ and fix $s = \varepsilon \geq 0$ in any $D[n;s]$ (ε suitably small). The $D[n;\varepsilon]$'s are Hermitian, and all their eigenvalues are non-negative (if all eigenvalues of $D[n+1;\varepsilon]$ are ≥ 0 , the same holds for $D[n;\varepsilon]$). The long-time approximation for $n \geq n_0$ reads as follows. One replaces any $D[n';s]$ yielding $\bar{W}_n(s)$, $n' \geq n \geq n_0$, by $D[n';\varepsilon]$: this approximation is not done for $n < n_0$ and is the better, the larger n_0 . We regard $D[n_0;\varepsilon]$ as a fixed (s -independent) operator. For a simpler hierarchy, neglect all $W_{in,n'}$'s for $n' \geq n_0$. Then, for small s : $g_{n_0}(s) \simeq -D[n_0;\varepsilon]M_{n_0,n_0-1}g_{n_0-1}(s)$. The resulting hierarchy for g_n 's ($n = 0, 1, \dots, n_0 - 1$), through inverse Laplace transform, yields a closed approximate irreversible hierarchy for W_n , $n = 0, 1, \dots, n_0 - 1$. The solutions of the last closed hierarchy for W_n relax irreversibly, for large t and reasonable W_{in} , towards $W_{eq,0} \neq 0$ and $W_{eq,n} = 0$, $n = 0, 1, \dots, n_0 - 1$ (thermal equilibrium). As an example, let $n_0 = 1$ and regard the linear operator $D[1;\varepsilon]$ as a real constant (> 0), playing a role similar to $\frac{\sigma}{m}$ (for Kramers equation). One finds the irreversible Smoluchowski equation for the $n = 0$ moment: $\partial W_0 / \partial t = (D[1;\varepsilon] / \beta_{eq})(\partial / \partial x)[(\partial / \partial x) + \beta(\partial V / \partial x)]W_0$, with initial condition $W_{in,0}$.

Finally, we treat a closed large system of many ($N \gg 1$) classical particles, in 3 spatial dimensions. Neither a "Heat bath" nor external friction mechanisms are assumed. The interaction potential is: $V = \sum_{i,j=1,i < j}^N V_{i,j}(|\mathbf{x}_i - \mathbf{x}_j|)$. The classical distribution function is: $W([\mathbf{x}], [\mathbf{p}]; t)$. The initial distribution W_{in} at $t = 0$ describes thermal equilibrium with homogeneous temperature T for large distances and nonequilibrium for intermediate distances (with spatial inhomogeneities). The reversible Liouville equation is:

$$\frac{\partial W}{\partial t} = \sum_{i=1}^N [(\nabla_{\mathbf{x}_i} V)(\nabla_{\mathbf{p}_i} W) - \frac{\mathbf{p}_i}{m}(\nabla_{\mathbf{x}_i} W)]. \quad (6)$$

We introduce moments $W_{[n]}$ of W (using products of Hermite polynomials, by generalizing (1)) and $g_{[n]}$. One gets an infinite reversible three-term linear recurrence for $g_{[n]}$'s, generalizing (3), which is formally solved in terms of continued-fraction operators $D[[n];s]$ for the actual $N (\gg 1)$. One also gets a generalized Hermitian operator $D[[n];\varepsilon]$ with non-negative eigenvalues. All that leads to formulate a similar long-time approximation and to a closed approximate hierarchy, which yields an irreversible evolution towards thermal equilibrium (consistently, approximately, with Fluid Dynamics).

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