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 $W_n = W_n(x;t)$ $(n = 0,1,2,...)$ of W [1, 2]:

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

$(\beta = (K_BT)^{-1}$, $K_B =$ Boltzmann's constant). If $W = W_{eq}$, then $W_{eq,0}$ is proportional to $\exp[-\beta V]$ and $W_{eq,n} = 0$, $n = 1,2,...$. 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 ($n = 0,1,2,...$, $W_{-1} = 0$) [1]:

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

$M'_{n,n\pm1}$ 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 $t \to +\infty$.

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 ($n = 0,1,2,...$, $W_{-1} = 0$) 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:

$$sg_n = W_{eq,0}^{-1/2}W_{in,n} - M_{n,n+1}g_{n+1} - M_{n,n-1}g_{n-1} \tag{3}$$

$$M_{n,n\pm1}g_{n\pm1} \equiv [\frac{(n+(1/2)(1\pm1))K_BT}{m}]^{1/2}[\frac{\partial g_{n\pm1}}{\partial x} - \frac{(\pm1)g_{n\pm1}}{2K_BT}\frac{dV}{dx}] \tag{4}$$

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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 $\tilde{W}_n(s)$, $n' \geq n \geq n_0$, 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 ($n = 0,1,.,n_0-1$), through inverse Laplace transform, yields a closed approximate irreversible hierarchy for W_n, $n = 0,1,.,n_0-1$. 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 $W_{eq,n} = 0$, $n = 0,1,.,n_0-1$ (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: $V = \Sigma_{i,j=1,i<j}^{N} V_{i,j}(\mid \mathbf{x}_i - \mathbf{x}_j \mid)$. 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:

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

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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