Shaking-Induced Transition to a Nonequilibrium State

Rosato *et al.*[1] have simulated a binary system of disks; upon periodic shaking in the presence of gravity, the larger disks rise to the top. This occurs because, as the system relaxes from each shake, the kinetics for the large disk to descend are very slow—requiring an (unlikely) collective motion of many small disks. Here, we present a simpler model, consisting of noninteracting particles and a static potential, which exhibits this evolution away from equilibrium. The particles are periodically excited, allowed to diffuse back into local potential minima, yet particle density "climbs" toward the global potential maximum.

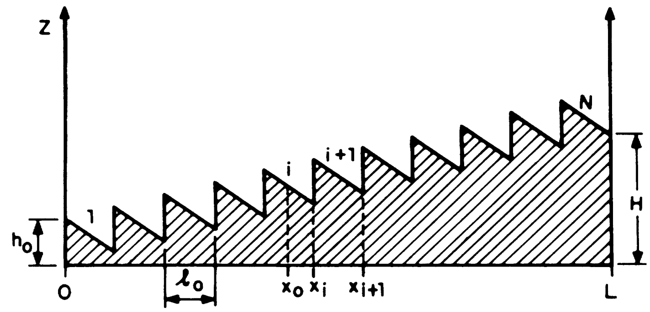

FIG. 1. Model potential is infinite at either end of, and below, ramp. Gravitational field and random force with friction ζ exist above ramp.

Suppose that noninteracting particles of mass m move in a potential $V(z)=mgz$ above a hard, sawtoothed ramp (see Fig. 1). Above the ramp a medium at temperature T provides a constant friction ζ. Periodic "shaking" involves lifting particles to a height $Z>H+h_0$ every τ seconds. Assume that $mgh_0 \gg kT$ and $h_0 \gg Hl_0/L$, so that the rate for activated barrier crossing is small; much smaller than $1/\tau$. If one assumes Smoluchowski dynamics, particles diffuse from (x_0,Z) according to

$$\rho(x,z,t)=(4\pi Dt)^{-1}\exp(-\{(x-x_0)^2+[z-Z+(mg/\zeta)t]^2\}/4Dt), \tag{1}$$

where $D=kT/\zeta$. The distance from Z to the tip of the ith barrier is $\Delta z_i = Z-[(H/L)il_0+h_0]$. In the limit $(2\Delta z_i kT/mg)^{1/2} \ll l_0$, particles diffuse a tiny fraction of the horizontal distance between barriers i and $i\pm 1$ in the time for the center of mass of the distribution ρ to descend the height Δz_i. Defining $E \equiv \frac{1}{2}mgZ$, if $Z(kT/E)^{1/2} \ll l_0$, the diffusion front changes negligibly as the sphere of probability density descends past the ith barrier. If rapid recrossings of the barrier are rare, particles on the left of the barrier are effectively trapped in well i, on the right in well $i+1$, and the uphill rate constant is particularly simple to derive, as follows.

If a particle begins in local thermal equilibrium in well i, after one shake, the fraction of this density which diffuses uphill into well $i+1$ is found to be

$$f_i = \left(\frac{mg\Delta z_i}{kT}\right)^{1/2}\frac{h_0}{l_0}\int_0^\infty \exp\left[-\left(\frac{mg\Delta z_i}{kT}\right)^{1/2}\frac{h_0}{l_0}y\right]\mathrm{erfc}(y)\,dy. \tag{2}$$

If τ is long enough for particles to equilibrate locally, Eq. (2) allows us to write a master equation for p_i, the probability that the particle is in well i in a continuum limit $(t \gg \tau)$:

$$\begin{aligned} dp_i/dt &= k_{i-1}p_{i-1}-k_ip_i, \quad 1<i<N; \\ dp_1/dt &= -k_1p_1; \quad dp_N/dt = k_{N-1}p_{N-1}, \end{aligned} \tag{3}$$

where the uphill rate constant $k_i \equiv f_i/\tau$. Because of barrier asymmetry, downhill motion is (as in Ref. 1) negligible. Equation (3) can be solved via a Laplacian transform. For example, if all particles begin in the ground state, $p_i(0)=\delta_{i1}$, then

$$p_i(t)=[F_1 * F_2 * \cdots * F_i](t)\prod_{j=1}^{i-1}k_j, \tag{4}$$

where $*$ represents convolution and $F_j \equiv \exp(-k_jt)$. The first passage time for a particle to become trapped in the Nth, highest, energy well is just $\mu_1 = \sum_{j=1}^{N-1}k_j^{-1}$.

A simple case is that of $Z \gg (H/L)Nl_0+h_0$ together with $(mgZ/kT)^{1/2}h_0/l_0 \gg 1$, whereupon $k_i \equiv (2\tau)^{-1}$. The uphill progress of the particle density is clear from the solution of Eq. (4) for this case:

$$p_i(t)=(1/2\tau)^{i-1}[t^{i-1}/(i-1)!]\exp(-t/2\tau), \quad i<N. \tag{5}$$

Certainly, if the shaking stops, a Boltzmann distribution of particle density is established; the time scale for this is $(mkT)^{1/2}[1+\exp(-mgHl_0/kTL)]^{-1}\exp[(mg/kT)(h_0-Hl_0/L)]$.

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[1] A. Rosato, K. J. Strandburg, F. Prinz, and R. H. Swendsen, Phys. Rev. Lett. **58**, 1038 (1987).