Brownian motion in periodic potentials

Friday, April 24, 2009
12:02 PM

Homework 4 to be posted today or tomorrow -- due Monday, May 4 at 5 PM (absolute deadline).

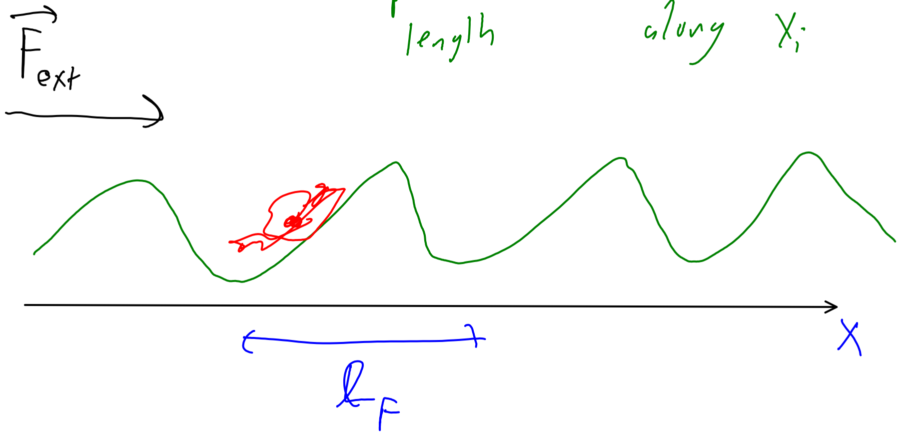
If you have a request for a topic for a special topics lecture after next Tuesday's class, either indicate on the survey to be distributed Tuesday or tell me separately.

Suppose we consider the motion of a particle subjected to a periodic potential, possibly a constant external force, and thermal forces.

$$m\, d\vec{V}(t) = \Big(-\gamma \vec{V} - \underbrace{\vec{F}_{ext}}_{\text{constant applied external force}} - \vec{\nabla}\phi(\vec{X}(t))\Big)\, dt + \sqrt{2\gamma k_B T}\; d\vec{W}(t)$$

$$d\vec{X}(t) = \vec{V}(t)\, dt$$

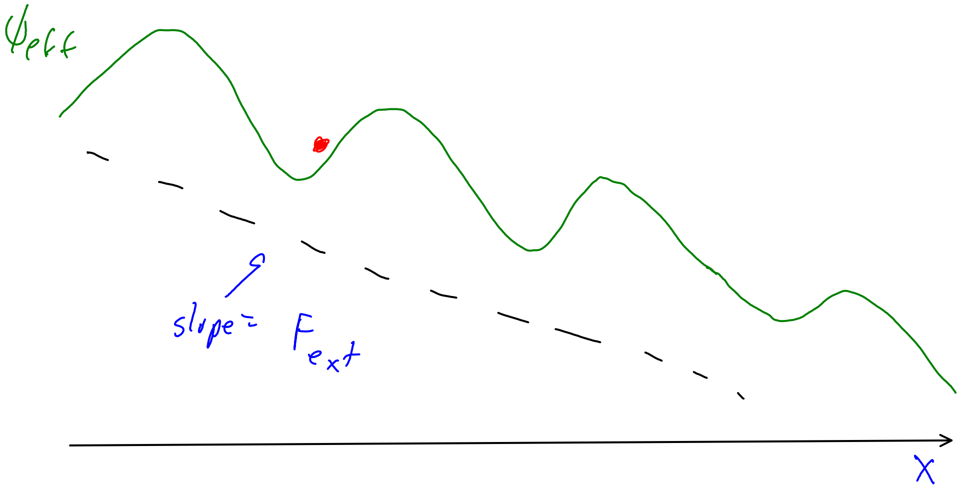
$$\phi(\vec{x}) = \phi(\vec{x} + \underbrace{\ell_F}_{\text{period length}} \underbrace{\hat{e}_i}_{\text{unit coordinate vector along } x_i})$$



One can alternatively visualize the dynamics by simply sketching the total potential from the external force and the periodic variations:

$$\phi_{eff}(\vec{x}) = \phi(\vec{x}) - \vec{F}_{ext} \cdot \vec{x}$$

$$-\vec{\nabla}\phi_{eff} = -\vec{\nabla}\phi + \vec{F}_{ext}$$



Applications (Risken Sec. 11.1):

- stochastically forced pendulum
- motion of ions in an atomic lattice
- superconducting currents
- dipoles in electric field
- phase locked loop for tuning

This also serves as a simple prototype from which to launch a discussion and examination of how Brownian motors work (where the potential fluctuates in time).

How does one approach the analysis of such a system? One fundamental question of interest is...how does the rate of transport of the particle depend on the applied force (and other system properties).

To answer such a question about how an output parameter depends on input parameters, nondimensionalization is a useful tool. For simplicity we'll just look at the overdamped case; underdamped case is more complicated to treat-- see Risken Ch. 11.

$$d\vec{X} = \frac{1}{\gamma}\left(-\vec{\nabla}\phi(\vec{X}) + \vec{F}_{ext}\right)dt + \sqrt{2D}\, d\vec{W}(t)$$

$$D = \frac{k_B T}{\gamma}$$

We will choose as reference units:

reference length scale will be the period length ℓ_F

reference time scale will be $\frac{\gamma \ell_F}{A}$

$$\phi(\vec{x}) = A\,\tilde{\phi}\left(\frac{\vec{x}}{\ell_F}\right)$$

(same as escape problem)

Nondimensionalize as before:

$$d\vec{X} = \left(-\vec{\nabla}_x\tilde{\phi}(\vec{x}) + \vec{f}\right)dt + \sqrt{2\theta}\, d\vec{W}(t)$$

$$\vec{f} = \frac{\vec{F}_{ext}\,\ell_F}{A} \qquad \theta = \frac{k_B T}{A}$$

strength of external force relative to periodic force

strength of thermal energy relative to periodic potential

Notice that by doing this nondimensionalization, we can study how the effective transport rate depends on all the governing parameters by simply studying it as a function of the two nondimensional parameters f, θ

In our escape problem, we considered $\theta \ll 1$

In the case of periodic potentials, we're not so much interested in this limit in general as much as

In the case of periodic potentials, we're not so much interested in this limit in general as much as

$$\theta \lesssim O(1), \qquad |\vec{f}| \lesssim O(1)$$

else some aspect is trivial,

How would we set up a calculation for the transport rate in such a system? One dimension for simplicity but can generalize.

Nondimensionalized Fokker-Planck equation:

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(\left(\frac{d\hat{\varphi}}{dx}(x) - f\right)p\right) + \theta\frac{\partial^2 p}{\partial x^2}$$

$$= -\frac{\partial J}{\partial x}$$

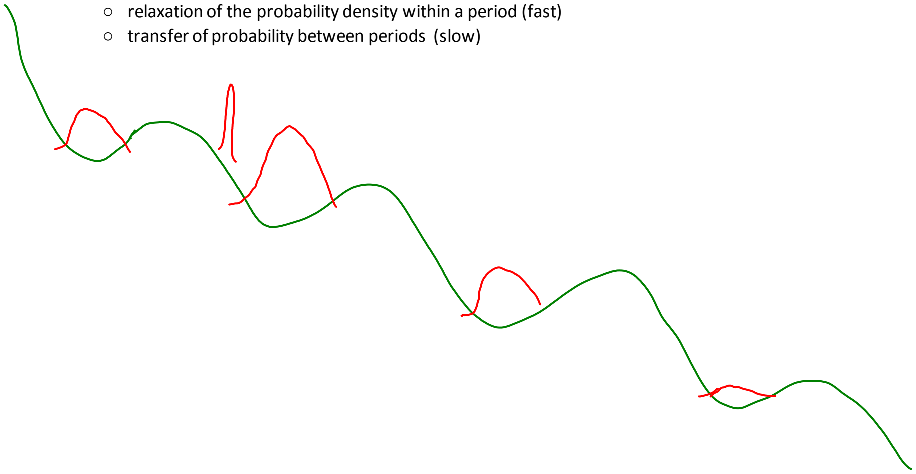
probability flux

$$J(x,t) = \left(-\frac{d\hat{\varphi}}{dx}(x) + f\right)p - \theta\frac{\partial p}{\partial x}$$

How do we analyze this equation? Neither f nor θ are necessarily very small so one doesn't want to set up in general an asymptotic reduction based on these assumptions.

Rather, one observes that the motion itself has two aspects which can be thought of as occuring on different time scales:

- relaxation of the probability density within a period (fast)
- transfer of probability between periods (slow)



Two ways to exploit this observation:

- use reduced densities
- multiscale analysis

We first discuss the method of reduced densities and flux:

Define reduced densities and flux:

$$\hat{p}(x,t) = \sum_{n=-\infty}^{\infty} p(x+n,t)$$

$$\hat{J}(x,t) = \sum_{n=-\infty}^{\infty} J(x+n,t)$$

This gives periodic versions of the probability density and flux which ignores which period the particle is in. Notice in nondimensionalized units, the period is 1.

Apply the summation over integer shifts to the Fokker-Planck equation gives reduced Fokker-Planck equation:

$$\frac{\partial \hat{p}(x,t)}{\partial t} = -\frac{\partial}{\partial x} \hat{J}(x,t)$$

We now compute the effective transport rate for a particle in this arrangement:

$$\left\langle \frac{d\vec{X}}{dt} \right\rangle = \frac{d\langle \vec{X}(t)\rangle}{dt}$$

$$= \frac{d}{dt} \int_{-\infty}^{\infty} x\, p(x,t)\, dx$$

$$= \int_{-\infty}^{\infty} x \frac{\partial p(x,t)}{\partial t}\, dx$$

$$= \int_{-\infty}^{\infty} x \left(-\frac{\partial J}{\partial x}\right) dx$$

↓ integrate by parts

$u = -J \qquad v = x$

$$= -\cancelto{0}{x J(x,t)}\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} 1\,(-J)\, dx$$

$$= \int_{-\infty}^{\infty} J(x,t)\, dx$$

$$= \sum_{n=-\infty}^{\infty} \int_{n}^{n+1} J(x,t)\, dx$$

$x \to n + x'$

$$= \sum_{n=-\infty}^{\infty} \int_{0}^{1} J(x'+n,t)\, dx'$$

$$= \int_{0}^{1} \sum_{n=-\infty}^{\infty} J(x'+n,t)\, dx'$$

$$= \int^{1} 1 \cdot \hat{J}(x',t)\, dx'$$

$$= \int_0^1 \sum_{n=-\infty}^{\infty} J(x'+n,t)\,dx'$$

$$= \int_0^1 1\cdot \hat{J}(x',t)\,dx'$$

int by parts

$u = \hat{J}$ $\quad v = x'$

$$= x'\,\hat{J}(x',t)\Big|_{x'=0}^{x'=1} - \int_0^1 x'\,\frac{\partial \hat{J}}{\partial x'}\,dx'$$

$$= \hat{J}(1,t) - 0 - \int_0^1 x'\left(-\frac{\partial \hat{p}}{\partial t}\right)dx'$$

$$\frac{d\langle \bar{X}(t)\rangle}{dt} = \hat{J}(1,t) + \int_0^1 x'\,\frac{\partial \hat{p}(x',t)}{\partial t}\,dx'$$

This relationship is useful because the reduced probability density and reduced flux should converge relatively quickly to a stationary distribution. This is not true for the original probability density and flux. With this observation, we can simplify the problem by assuming the reduced probability density and flux are time-independent -- this should be the case provided we wait a reasonably small amount of time.

We replace the reduced flux and reduced probability density by their steady values

$$\hat{J}(1,t) = \hat{J}^{(s)}(1)$$

$$\hat{p}(x',t) = \hat{p}^{(s)}(x')$$

where $\cancel{\frac{\partial \hat{p}^{(s)}(x')}{\partial t}} \overset{0}{=} -\frac{\partial \hat{J}^{(s)}(x')}{\partial x'}$ $\quad$ so $\hat{J}^{(s)}$ is a constant

$$\hat{J}^{(s)}(x') = \left(-\frac{d\hat{\varphi}}{dx}(x') + f\right)\hat{p}^{(s)}(x') - \theta\,\frac{d\hat{p}^{(s)}}{dx'}$$

Notice that the equation for the steady probabilty density is just a second order differential equation on the period domain [0,1], which can be solved by integrating factors and using the following two conditions to determine the two integration constants:

- solution must be periodic
- the integral of the reduced probability density must be 1

Now when we solve this equation, notice that

$$\frac{d\langle \vec{X} \rangle}{dt} = \hat{J}^{(s)} \quad (\text{constant})$$

And solving the differential equation would give:

$$\hat{p}^{(s)}(x) = \frac{\int_x^{x+1} e^{(\hat{\varphi}(x') - \hat{\varphi}(x) - fx' + fx)/\theta}\, dx'}{\int_0^1 dx \int_x^{x+1} dx'\, e^{(\hat{\varphi}(x') - \hat{\varphi}(x) - fx' + fx)/\theta}}$$

$$\hat{J}^{(s)} = \frac{\theta\left(1 - e^{-f/\theta}\right)}{\int_0^1 dx \int_x^{x+1} dx'\, e^{(\hat{\varphi}(x') - \hat{\varphi}(x) - fx' + fx)/\theta}}$$

This gives us an explicit formula for how the transport rate depends on the underlying parameters. This can be studied in various simplifying limits…see Risken Sec. 11.3

Such explicit formulas are not generally possible once one looks at more complicated versions of the problem…but the conceptual approach does generalize:

- The relation between the net transport rate and the flux and the reduced probability density
- The notion that the probability density and flux relax more quickly within a period than across periods.

An interesting modern field of research that proceeds from this point is that of Brownian motors, where the periodic potential itself fluctuates in time.

The subject seems to have originated from biological motivation, namely how protein molecules like kinesin and dynein and myosin perform work within the biological cell.