6.C. Ergodic Theory and the Foundations of Statistical Mechanics

Read p.296, Reichl.

Consider a 1-particle system in 1-D space with $H(q, p) = E$. The Hamilton's equations

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} \qquad \frac{dp}{dt} = -\frac{\partial H}{\partial q}$$

can be written as

$$dt = \frac{dq}{\frac{\partial H}{\partial p}} = -\frac{dp}{\frac{\partial H}{\partial q}} \tag{6.33a}$$

Similarly, for an N-particle system in 3-D space with $H(\mathbf{q}^N, \mathbf{p}^N) = E$, we have

$$\frac{dq_{\alpha j}}{dt} = \frac{\partial H}{\partial p_{\alpha j}} \qquad \frac{dp_{\alpha j}}{dt} = -\frac{\partial H}{\partial q_{\alpha j}} \qquad \alpha = x, y, z; \ \ j = 1, \ \ldots, N$$

$$\rightarrow \qquad dt = \frac{dq_{\alpha j}}{\frac{\partial H}{\partial p_{\alpha j}}} = -\frac{dp_{\alpha j}}{\frac{\partial H}{\partial q_{\alpha j}}} \qquad \forall\ \alpha, j \tag{6.33}$$

(6.33) provides $6N$ equations of the form

$$dt = \frac{dX_k}{\frac{\partial H}{\partial X_{k+3N}}} \qquad k = 1, \ \ldots, 3N \tag{6.33b}$$

where

$$\begin{aligned} \mathbf{X}^N &= (\mathbf{q}^N, \mathbf{p}^N) \\ &= (X_1, \ \ldots, X_{3N}, X_{3N+1}, \ \ldots, X_{6N}) \\ &= (q_{x1}, q_{y1}, q_{z1}, \ \ldots, q_{xN}, q_{yN}, q_{zN}, p_{x1}, p_{y1}, p_{z1}, \ \ldots p_{xN}, p_{yN}, p_{zN}) \end{aligned}$$

Integrating(6.33b) gives $6N$ equations

$$t = g_k(\mathbf{X}^N) + c_k \tag{6.33c}$$

where c_k is an integration constant and

$$g_k(\mathbf{X}^N) = \int \frac{dX_k}{\frac{\partial H}{\partial X_{k+3N}}}$$

There are $6N - 1$ equations of time-independent integrals in (6.33c).

For example, eliminating t using the $k = 6N$ equation leaves us with $6N - 1$ equations

$$g_k(\mathbf{X}^N) - g_{6N}(\mathbf{X}^N) = c_{6N} - c_k \qquad k = 1, \ \ldots, 6N - 1$$

or

$$f_k(\mathbf{X}^N) = C_k \qquad \forall\ t \tag{6.34}$$

where

$$f_k(\mathbf{X}^N) = g_k(\mathbf{X}^N) - g_{6N}(\mathbf{X}^N) \qquad = \int dX_k \left(\frac{1}{\frac{\partial H}{\partial X_{k+3N}}} - \frac{1}{\frac{\partial H}{\partial X_{6N+3N}}} \right)$$

$$C_k = c_{6N} - c_k$$

These $f_k(\mathbf{X}^N)$'s are called integrals of the motion. The $6N - 1$ conditions in (6.34) reduces Γ to a 1-D sub-space that is the trajectory of the system, with the C_k's carrying the initial conditions.

More generally, any function of the form (6.34) is called an integral of motion, irregardless of how it is obtained. Note that

$$f(\mathbf{X}^N) = C \qquad \rightarrow \qquad f[\mathbf{X}^N(t)] = C \qquad \forall\ t$$

where $\boldsymbol{X}^N(t)$ describes an arbitrary trajectory of the system.

There are two kinds of integrals of motion: isolating and non-isolating. Each isolating integral reduces the dimension of Γ by 1, while a non-isolating one does not. Thus, isolating integrals control the topology of the possible trajectories of the system and are of great importance.

An example of isolating integral of great importance is

$$H(\boldsymbol{q}^N, \boldsymbol{p}^N) = E \tag{6.34a}$$

For a system of N hard spheres in a box, it is the only one.

Consider a system for which (6.34a) is the only isolating integral. For a given E, trajectories of the system are then restricted to an $(6N-1)$-D surface S_E in Γ.

The flow of the state points is ergodic if, starting from almost anywhere, it passes through arbitrarily close to (but not necessarily through) every point on S_E. Since a line cannot fill a surface of 2 or higher dimensions without intersecting itself, we have inserted the qualifiers "almost" and "arbitrarily close" to exclude those points that must be left out. Fortunately, the excluded points can be reduced to a set of measure zero.

Reminder: the problem of ergodicity is highly technical and requires special mathematical skills.

A criterion for verifying ergodicity is the ergodic theorem.

Let $f(\boldsymbol{X}^N)$ be an integrable function on Γ. If the probability finding the system at any state on the energy surface S_E is the same, then

$$\rho(\boldsymbol{X}^N) = \frac{1}{\Sigma(E)} \delta\left[H^N(\boldsymbol{X}^N) - E\right]$$

where $\Sigma(E)$ is the "area" of S_E, namely,

$$\Sigma(E) = \int_{S_E} d\,S_E = \int_\Gamma d\,\boldsymbol{X}^N\ \delta\left[H^N(\boldsymbol{X}^N) - E\right] \tag{6.36}$$

Hence,

$$\int_\Gamma d\,\boldsymbol{X}^N \rho(\boldsymbol{X}^N) = 1$$

as expected.

The average of $f(\boldsymbol{X}^N)$ on S_E is therefore

$$\langle f \rangle_S = \frac{1}{\Sigma(E)} \int_\Gamma d\,\boldsymbol{X}^N\ \delta\left[H^N(\boldsymbol{X}^N) - E\right] f(\boldsymbol{X}^N) = \frac{1}{\Sigma(E)} \int_{S_E} d\,S_E\ f(\boldsymbol{X}^N) \tag{6.35}$$

We can also define the time average of $f(\boldsymbol{X}^N)$ over a given trajectory $\boldsymbol{X}^N(t)$ by

$$\langle f \rangle_T = \lim_{T\to\infty} \frac{1}{T} \int_{t_0}^{t_0+T} d\,t\ f\left[\boldsymbol{X}^N(t)\right] \tag{6.37}$$

where t_0 is arbitrary.

Birkhoff showed that $\langle f \rangle_T$ exists if $f(\boldsymbol{X}^N)$ is integrable on the trajectory $\boldsymbol{X}^N(t)$.

The ergodic theorem (also due to Birkhoff) then states that :

A system is ergodic if for all $f(\boldsymbol{X}^N)$ on Γ,

(1) $\langle f \rangle_T$ exists for almost all trajectories $\boldsymbol{X}^N(t)$
(except for a set of measure zero).

(2) $\langle f \rangle_T = \langle f \rangle_S$ for all trajectories on which $\langle f \rangle_T$ exists.

Note that in order for $\langle f \rangle_T = \langle f \rangle_S$ for all $f(\boldsymbol{X}^N)$ on a given trajectory, that trajectory must pass through every point on S_E. Thus, a system is ergodic only if almost every trajectory covers the whole S_E.

We now turn to the calculation of S_E for a given $H^N(\boldsymbol{X}^N)$.

To begin, let $\Omega(E)$ be the volume of the region in Γ for which $0 < H^N < E$. By definition, S_E is the area of a constant E shell in Γ. Thus, the volume element between two shells of energies E and $E + dE$ is given by

$$d\,\Omega(E) = \Sigma(E)\, d\,E = \Sigma\left(H^N\right) d\,H^N$$

$$\rightarrow \qquad \Omega(E) = \int_0^E \Sigma\left(H^N\right) d\,H^N \tag{6.39}$$

On the other hand, the volume element of a constant H^N surface element $d\,A_H$ of "height" $d\,n_H$ is given by

$$d\,\boldsymbol{X}^N = d\,A_H\, d\,n_H$$

where $d\,n_H$ is the increment of $\boldsymbol{X}^N$ in the direction normal to $d\,A_H$. Hence,

$$\Omega(E) = \int_{0 < H^N < E} d\,\boldsymbol{X}^N$$

$$= \int_{0 < H^N < E} d\,A_H\, d\,n_H \tag{6.38}$$

Note: although both S_E and A_E represent the same energy surface, the Γ filling families of surfaces they belong to have different spacings ($d\,E$ and $d\,n_H$, respectively). Furthermore, since

$$d\,E = d\,H^N = \left| \nabla_{\boldsymbol{X}} H^N \right| \; d\,n_H \tag{6.38a}$$

the spacing difference varies with $\boldsymbol{X}^N$.

(6.38a) can be used to write (6.38) as

$$\Omega(E) = \int_0^E \int_{S_H} \frac{d\,A_H}{\left| \nabla_{\boldsymbol{X}} H^N \right|}\, d\,H^N$$

$$= \int_0^E \Sigma\left(H^N\right) d\,H^N$$

where S_H is the surface of constant H^N and

$$\Sigma\left(H^N\right) = \int_{S_H} \frac{d\,A_H}{\left| \nabla_{\boldsymbol{X}} H^N \right|} \tag{6.40}$$

Taking the derivative of (6.39) gives

$$\frac{d\,\Omega(E)}{d\,E} = \Sigma(E)$$

$$= \int_{S_E} \frac{d\,A_E}{\left| \nabla_{\boldsymbol{X}} H^N \right|_{H=E}} \tag{6.41}$$

Comparing with (6.36), we have

$$d\,S_E = \frac{d\,A_E}{\left| \nabla_{\boldsymbol{X}} H^N \right|_{H=E}} \tag{6.43}$$

which expresses $d\,S_E$ in terms of the phase space coordinates $\boldsymbol{X}^N$.

$\Sigma(E)$ is also called the structure function. Using (6.43) on (6.35) gives

$$\langle f \rangle_S = \frac{1}{\Sigma(E)} \int_{S_E} \frac{d\,A_E}{\left| \nabla_{\boldsymbol{X}} H^N \right|_{H=E}}\, f(\boldsymbol{X}^N) \tag{6.42a}$$

Now, (6.38) gives

$$\frac{d\,\Omega(E)}{d\,E} = \frac{d}{d\,E}\int_{0<H^N<E} d\,\boldsymbol{X}^N$$
$$= \int_{S_E} \frac{d\,A_E}{\left|\nabla_{\boldsymbol{X}} H^N\right|_{H=E}} \qquad \text{[(6.41) used.]}$$

(6.42a) thus becomes

$$\langle f \rangle_S = \frac{1}{\Sigma(E)}\frac{d}{d\,E}\int_{0<H^N<E} d\,\boldsymbol{X}^N f(\boldsymbol{X}^N) \qquad (6.42)$$

Exercise 6.3.

Compute the structure function for a gas of N non-interacting particles in a box of volume V. Assume that the system has a total energy E.

Answer

$$H^N = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2\,m} \qquad (1)$$

$$\rightarrow \quad \Omega(E) = \int_{V^N} d\,\boldsymbol{q}^N \int_{0<H^N<E} d\,\boldsymbol{p}^N \qquad (2)$$
$$= V^N\,\Omega_p$$

where

$$\Omega_p = \int_{0<H^N<E} d\,\boldsymbol{p}^N$$
$$= \int d\,\boldsymbol{p}^N\,\Theta\!\left(2\,m\,E - \sum_{i=1}^{N} \boldsymbol{p}_i^2\right) \qquad (3)$$

and

$$\Theta(x) = \begin{cases} 1 & x>0 \\ 0 & x<0 \end{cases}$$

Ω_p is therefore the volume of a (3 N)-D sphere of radius $R = \sqrt{2\,m\,E}$. Thus,

$$\Omega_p = A_{3N}\,R^{3N} = A_{3N}\,(2\,m\,E)^{3N/2} \qquad (3a)$$

where A_{3N} is a geometric factor to be determined.

Now, in terms of Cartesian components,

$$\int d\,\boldsymbol{p}^N\,e^{-\sum_{i=1}^{N}\boldsymbol{p}_i^2} = \prod_{i=1}^{N}\int d^3\,p_i\,e^{-\boldsymbol{p}_i^2}$$
$$= \left(\int d^3\,p\,e^{-\boldsymbol{p}^2}\right)^N$$
$$= \left(\int_{-\infty}^{\infty} d\,p_x\,e^{-p_x^2}\int_{-\infty}^{\infty} d\,p_y\,e^{-p_y^2}\int_{-\infty}^{\infty} d\,p_z\,e^{-p_z^2}\right)^N$$
$$= \pi^{3N/2} \qquad (4)$$

Also,

$$\Theta(x-a) = \int_{-\infty}^{x} d\,x'\,\delta(x'-a) = \begin{cases} 0 & x<a \\ 1 & x>a \end{cases}$$

$$\rightarrow \quad \frac{d\,\Theta(x-a)}{d\,x} = \delta(x-a)$$

$$\therefore \qquad \frac{\partial}{\partial R}\Theta\left(R^2-\sum_{i=1}^{N}\boldsymbol{p}_i^2\right)=\frac{dR^2}{dR}\frac{\partial}{\partial R^2}\Theta\left(R^2-\sum_{i=1}^{N}\boldsymbol{p}_i^2\right)$$
$$=2R\,\delta\left(R^2-\sum_{i=1}^{N}\boldsymbol{p}_i^2\right)$$

(3) then gives

$$\frac{\partial\Omega_p}{\partial R}=\int d\boldsymbol{p}^N\frac{\partial}{\partial R}\Theta\left(2mE-\sum_{i=1}^{N}\boldsymbol{p}_i^2\right)$$
$$=\int d\boldsymbol{p}^N\,2R\,\delta\left(R^2-\sum_{i=1}^{N}\boldsymbol{p}_i^2\right)$$

$$\rightarrow \qquad \int_0^\infty dR\frac{\partial\Omega_p}{\partial R}e^{-R^2}=\int d\boldsymbol{p}^N\int_0^\infty dR\,2R\,\delta\left(R^2-\sum_{i=1}^{N}\boldsymbol{p}_i^2\right)e^{-R^2}$$
$$=\int d\boldsymbol{p}^N\int_0^\infty dR^2\,\delta\left(R^2-\sum_{i=1}^{N}\boldsymbol{p}_i^2\right)e^{-R^2}$$
$$=\int d\boldsymbol{p}^N e^{-\sum_{i=1}^{N}\boldsymbol{p}_i^2}$$
$$=\pi^{3N/2} \qquad \text{[(4) used.]} \qquad (5a)$$

On the other hand, (3a) gives

$$\frac{\partial\Omega_p}{\partial R}=3NA_{3N}R^{3N-1}$$

$$\rightarrow \qquad \int_0^\infty dR\frac{\partial\Omega_p}{\partial R}e^{-R^2}=3NA_{3N}\int_0^\infty dR\,R^{3N-1}e^{-R^2}$$
$$=\frac{3}{2}NA_{3N}\int_0^\infty dR^2\,R^{2\left(\frac{3}{2}N-1\right)}e^{-R^2}$$
$$=\frac{3}{2}NA_{3N}\Gamma\left(\frac{3}{2}N\right) \qquad (5)$$

where

$$\Gamma(z)\equiv\int_0^\infty dx\,x^{z-1}e^{-x}$$

is the Gamma function.

Comparing (5) with (5a) gives

$$A_{3N}=\frac{2\pi^{3N/2}}{3N\Gamma\left(\frac{3}{2}N\right)} \qquad (6)$$

so that (2) and (3a) gives

$$\Omega(E)=V^N A_{3N}R^{3N}$$
$$=V^N\frac{2\pi^{3N/2}}{3N\Gamma\left(\frac{3}{2}N\right)}R^{3N}$$
$$=V^N\frac{2\pi^{3N/2}}{3N\Gamma\left(\frac{3}{2}N\right)}(2mE)^{3N/2}$$
$$=\frac{V^N}{\Gamma\left(\frac{3}{2}N+1\right)}(2\pi mE)^{3N/2} \qquad (7)$$

$$\therefore \qquad \Sigma(E) = \frac{d\,\Omega}{d\,E} = \frac{2\,\pi\,m\,V^N}{\Gamma\left(\frac{3}{2}\,N\right)}\,(2\,\pi\,m\,E)^{3\,N/2-1}$$

Microcanonical Ensemble

According to the ergodic theorem, if a system is ergodic, then $\langle f\rangle_T = \langle f\rangle_S$.

To find the time τ_{R_E} the system spends in a region $R_E \subset S_E$, we consider the function

$$\phi_{R_E}(\boldsymbol{X}^N) = \begin{cases} 1 & \boldsymbol{X}^N \in R_E \\ 0 & \boldsymbol{X}^N \notin R_E \end{cases}$$

$$\rightarrow \qquad \langle\, \phi_{R_E}\rangle_S = \frac{1}{\Sigma(E)} \int_\Gamma d\,\boldsymbol{X}^N\ \delta\left(H^N(\boldsymbol{X}^N) - E\right) \phi_{R_E}(\boldsymbol{X}^N)$$

$$= \frac{\Sigma(R_E)}{\Sigma(E)} \qquad (6.44a)$$

where $\Sigma(R_E)$ is the area of R_E.

$$\langle\phi_{R_E}\rangle_T = \lim_{T\to\infty} \frac{1}{T} \int_0^T d\,t\,\phi_{R_E}\left[\boldsymbol{X}^N(t)\right]$$

$$= \lim_{T\to\infty} \frac{\tau_{R_E}}{T} \qquad (6.44b)$$

Equating (6.44a) & (6.44b) gives

$$\lim_{T\to\infty} \frac{\tau_{R_E}}{T} = \frac{\Sigma(R_E)}{\Sigma(E)} \qquad (6.44)$$

Thus, the fraction of time the system spends in R_E is just the fraction of area that R_E occupies in S_E. In other words, the system spends equal times in equal areas on S_E and it has access to every part of S_E. This means there can be no other isolating integrals since their existence will break S_E into separate pieces of lower dimensions so that each trajectory is confined to only one piece.

Next comes the important task of assigning probability to the state points $\boldsymbol{X}^N$. Following (6.44), we set the probability of finding the system in a region $R \subset \Gamma$ to be

$$P(R) = \begin{cases} \dfrac{\Sigma(R)}{\Sigma(E)} & R \subset S_E \\ 0 & R \not\subset S_E \end{cases} \qquad (6.45)$$

This corresponds to a probability density

$$\rho(\boldsymbol{X}^N) = \begin{cases} \dfrac{1}{\Sigma(E)} & \boldsymbol{X}^N \in S_E \\ 0 & \boldsymbol{X}^N \notin S_E \end{cases} \qquad (6.46)$$

which is called the fundamental distribution law by Khintchine, and the microcanonical ensemble by Gibbs.

Finally, we mention that a quantum system is ergodic if and only if its energy spectrum is nondegenerate, which means there can be no observable that commutes with H.

Exercise 6.4.

Consider a dynamical flow on the 2-D unit square defined by

$$0 \le p \le 1 \qquad \text{and} \qquad 0 \le q \le 1$$

and governed by the equations of motion

$$\frac{dp}{dt} = \alpha \text{ and} \qquad \frac{dq}{dt} = 1$$

Assume periodic boundary conditions.

(a) Show that this flow is ergodic.

(b) Given $\rho(q, p, 0)$, compute $\rho(q, p, t)$.

Answer (a)

Integrating the equations of motion gives

$$q(t) = q_0 + t \qquad p(t) = p_0 + \alpha t \qquad (1)$$

where

$$q_0 = q(0) \qquad p_0 = p(0)$$

Incorporating the periodic B.C., we have

$$q(t) = (q_0 + t) \bmod 1 \qquad p(t) = (p_0 + \alpha t) \bmod 1 \qquad (1a)$$

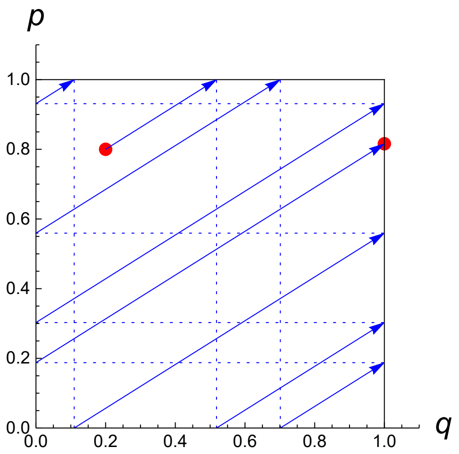
where mod is the modulo operator.

Eliminating t from (1) gives the trajectory

$$p = p_0 + \alpha (q - q_0)$$

which is a straight-line in the q-p plane.

The trajectory of (1a) is much more complicated and consists of a set of line segments of slope α. The following graph shows 8 segments of the trajectory for the case $\alpha = 0.2\pi$, $q_0 = 0.2$, and $p_0 = 0.8$. Red dots mark the start and end points. Trajectory segments within the unit square are shown by arrows. Jumps caused by the periodic B.C. are shown as dotted lines.



Mathematica code for plot is in §Code.

From

$$\boldsymbol{X} = (q, p) \qquad \dot{\boldsymbol{X}} = (1, \alpha)$$

we see that the periods of the motion along the q and p directions, as imposed by the periodic boundary conditions, are

$$\tau_q = 1 \qquad \tau_p = \frac{1}{\alpha}$$

Thus, the entire motion is periodic only if $\frac{\tau_q}{\tau_p} = \alpha$ is a rational number, i.e.,

$$\alpha = \frac{m}{n} \qquad \text{with } m, n \text{ integers}$$

In which case, the period is n.

If α is irrational, the trajectory will cover almost all of the unit square. We shall show that the system is also ergodic.

Since the system is periodic, any well-behaved phase space function can be written as a Fourier series

$$f(q,p) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} A_{mn}\, e^{2\pi i (mq+np)} \qquad (2)$$

$$\rightarrow \qquad \langle f \rangle_T = \lim_{T\to\infty} \frac{1}{T} \int_{t_0}^{t_0+T} dt \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} A_{mn}\, e^{2\pi i [m(q_0+t)+n(p_0+\alpha t)]}$$

$$= \lim_{T\to\infty} \frac{1}{T} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} A_{mn}\, e^{2\pi i (m q_0+n p_0)} \int_{t_0}^{t_0+T} dt\, e^{2\pi i (m+n\alpha)t}$$

The $m = n = 0$ term requires special treatment, giving

$$\lim_{T\to\infty} \frac{1}{T} A_{00} \int_{t_0}^{t_0+T} dt = A_{00}$$

For the other terms,

$$e^{2\pi i (m q_0+n p_0)} \int_{t_0}^{t_0+T} dt\, e^{2\pi i (m+n\alpha)t}$$

$$= e^{2\pi i (m q_0+n p_0)} \frac{e^{2\pi i (m+n\alpha)t_0}\left(e^{2\pi i (m+n\alpha)T} - 1\right)}{2\pi i (m+n\alpha)}$$

$$= e^{2\pi i [m(q_0+t_0)+n(p_0+\alpha t_0)]} \frac{e^{2\pi i (m+n\alpha)T} - 1}{2\pi i (m+n\alpha)}$$

Hence,

$$\langle f \rangle_T = A_{00} + \qquad (3)$$

$$\lim_{T\to\infty} \frac{1}{T} {\sum_{m=-\infty}^{\infty}}' {\sum_{n=-\infty}^{\infty}}' A_{mn}\, e^{2\pi i [m(q_0+t_0)+n(p_0+\alpha t_0)]} \frac{e^{2\pi i (m+n\alpha)T} - 1}{2\pi i (m+n\alpha)}$$

where the prime on the summation denote the exclusion of the 0 term.

For α irrational, $m + n\alpha \neq 0$ so that every term in the sums is finite and hence vanishes as $T \to \infty$. Therefore

$$\langle f \rangle_T = A_{00} \qquad (4)$$

Similarly, since $\Sigma = 1$, we have

$$\langle f \rangle_S = \int_0^1 dq \int_0^1 dp\, f(q,p)$$

$$= \int_0^1 dq \int_0^1 dp \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} A_{mn}\, e^{2\pi i (mq+np)}$$

$$= A_{00} + {\sum_{m=-\infty}^{\infty}}' {\sum_{n=-\infty}^{\infty}}' A_{mn} \frac{e^{2\pi i m} - 1}{2\pi i m} \frac{e^{2\pi i n} - 1}{2\pi i n}$$

$$= A_{00} \qquad (5)$$

which is independent of α.

Hence, the system is ergodic if α is irrational.

Answer (b)

An arbitrary ρ must also be periodic. Hence,

$$\rho(q, p, t) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \rho_{mn}(t)\, e^{2\pi i(mq+np)} \tag{6}$$

Now, (q, p) can be taken as the coordinates of a fixed phase point and $\rho(q, p, t)$ is the value of ρ there at time t. Or, we can take it as the point on the trajectory at which the system is located at time t. This point can be emphasized by writing ρ as $\rho[q(t), p(t), t]$ with $q(t) = q$ and $p(t) = p$. The equations of motion (1) becomes

$$q(t+\Delta t) = q + \Delta t \qquad p(t+\Delta t) = p + \alpha \Delta t \tag{6a}$$

Incorporating the periodic B.C., we have

$$q(t+\Delta t) = (q+\Delta t) \bmod 1 \qquad p(t+\Delta t) = (p+\alpha \Delta t) \bmod 1 \tag{6b}$$

As the system evolves from time t to $t' = t + \Delta t$ according to (6a), the value of ρ at (q, p) is replaced by its value on the trajectory Δt ago, i.e.,

$$\begin{aligned} \rho(q, p, t+\Delta t) &= \rho[q(t-\Delta t), p(t-\Delta t), t] \\ &= \rho\left[(q-\Delta t) \bmod 1,\ (p-\alpha \Delta t) \bmod 1,\ t\right] \end{aligned} \tag{6c}$$

(6) thus gives

$$\rho(q, p, t+\Delta t) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \rho_{mn}(t)\, e^{2\pi i[m(q-\Delta t)+n(p-\alpha\Delta t)]}$$

where the mod operations are no longer necessary since they have no effect on the exponential factors.

Setting $t = 0$ and $\Delta t = t$ then gives

$$\rho(q, p, t) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \rho_{mn}(0)\, e^{2\pi i[m(q-t)+n(p-\alpha t)]} \tag{6d}$$

Comparing with (6) gives

$$\rho_{mn}(t) = \rho_{mn}(0)\, e^{2\pi i(m+n\alpha)t} \tag{6e}$$

Similarly, (6c) gives

$$\rho(q, p, t) = \rho\left[(q-t) \bmod 1,\ (p-\alpha t) \bmod 1,\ 0\right] \tag{7}$$

The form (or shape) of ρ does not change as the system evolves. If it starts at a non-equilibrium state, it will remain so forever. *Mathematica* code for an animation can be found in §Code.

Code

Trajectory Segments

For an initial point X0, XS[X0, α, n] calculates the trajectory points at the square edges for n segments. Output is in the form {X1, X2}, where X1⟦j⟧ and X2⟦j⟧ are the start and end points of the j^{th} segment, respectively.

```
XS[X0_, α_, n_] :=
 Module[{τ, V = {1, α}, X1 = Table[{0, 0}, {j, n}], X2 = Table[{0, 0}, {j, n}]},
      Do[
        If[j == 1, X1[[j]] = X0, X1[[j]] = X2[[j - 1]]];
        Do[ If[Abs[ X1[[j, i]] - 1.] < 10^-6, X1[[j, i]] = 0], {i, 2}];
        τ = Min[ Table[ (1 - X1[[j, i]])/V[[i]] , {i, 2}]];
        X2[[j]] = X1[[j]] + V * τ ,
        {j, 1, n}];
      {X1, X2}
 ]
```

graph[{X1, X2}] plots the trajectory segments for given {X1, X2}.
Red dots mark the start and end points. Trajectory segments within the unit square are shown by arrows. Jumps caused by the periodic B.C.are shown as dotted lines.

```
graph[ {X1_, X2_}] := Module[{n = Dimensions[X1][[1]]},
  G = Graphics[ { Red, PointSize[Large], Point[X1[[1]]], Point[X2[[n]]],
     Black, Line[{{0, 1}, {1, 1}}], Line[{{1, 0}, {1, 1}}],
     Blue, Table[ Arrow[{X1[[j]], X2[[j]]}], {j, n}],
     Dotted, Table[Line[{X1[[j]], X2[[j - 1]]}], {j, 2, n}]}];
  Show[G,
       Axes → True,
       PlotRange → {{0, 1.1}, {0, 1.1}},
       AxesLabel → {"q", "p"}]
 ]
```

```
X0 = {.2, .8}; α = .1 π;
{X1, X2} = XS[X0, α, 5]
```

```
{{{0.2, 0.8}, {0.83662, 0}, {0, 0.0513274}, {0, 0.365487}, {0, 0.679646}},
 {{0.83662, 1.}, {1., 0.0513274}, {1, 0.365487}, {1, 0.679646}, {1, 0.993805}}}
```

```
graph[{X1, X2}]
(* output omitted *)
```

ρ

```
In[6]:= (* This calulates X(t) given X(0)=X0 *)
X[X0_, t_, α_] := { Mod[X0[[1]] + t, 1], Mod[X0[[2]] + α t, 1]}
```

```
In[60]:= (* This calulates ρ(t) given ρ(0)= ρ0.  *)
ρ[ρ0_, t_, α_] := (np = Dimensions[ρ0][[1]];
  Table[ρ0[[Sequence @@ (Mod[Ceiling[X[{i, j} / np, -t, α] * np], np] + 1)]],
   {i, np}, {j, np}])
```

```
(* This plots ρ *)
gr[ρ_] := (np = Dimensions[ρ][[1]];
  Graphics[Table[{If[ρ[[i, j]] == 1, Blue, White], Point[{i, j} / np]}, {i, np}, {j, np}]])
```

The following sets up $\rho 0$ as a disk of radius $r = .1$ and centered at X0 = (.3, .4). The unit square is divided into an np × np grid with np = 50.

In[69]:=
```
α = .2 π;
np = 50; X0 = {.3, .4}; r = .1;
I0 = X0 * np;
ρ0 = Table[If[Sqrt[(I0[[1]] - i)^2 + (I0[[2]] - j)^2] / np ≤ r, 1, 0], {i, np}, {j, np}];

Animate[gr[ρ[ρ0, t, α]], {t, 0, 2, .1}]

(* output omitted *)
```