It would be necessary, however, to have complete information about the system in the sense that all the values p_0, q_0 are known, or, equivalently, all the values p, q at some other time, in order to determine the motion along a given phase orbit. In practice, this is not normally the case for a macroscopic system where one measures only a few quantities. In thermodynamics, one may not describe a system by more than, say, its pressure and volume or temperature. Suppose the system is composed of $N \cong 10^{23}$ particles. This leaves the very large number $2n = 2 \times 3N$ of data, necessary for the mechanical description, practically unknown and, hence, open to guessing. One is therefore reduced to statistical methods, that is, to a statement of probabilities. In dealing with a mechanical system, it is then necessary, in principle, to consider all possible sets of values p, q that the system may assume at a given time.

Before introducing these statistical methods, however, we prove an important result of pure mechanics, which is known as Liouville's Theorem.

3. Liouville's Theorem(*)

We have seen that the dynamical variables p_i and q_i with $i = 1, 2, \ldots, n$ may be regarded as the coordinates in a $2n$-dimensional space, called the *phase space.* Every set of these variables is thus represented by a point and the quantity

$$d\lambda = \prod_{i=1}^{n} dp_i dq_i \tag{3.1}$$

represents the *volume element* in the phase space. A mechanical system found at the point $P(p_i, q_i)$ at the time t will follow a definite phase orbit so that at a later time t' it will be found at another point $P'(p'_k, q'_k)$ with the set (p'_k, q'_k) obtained from the initial set (p_i, q_i) by forward integration of Hamilton's equations. Since the new values are determined by the initial values in this fashion, we can write

$$\begin{aligned} p'_k &= p'_k(p_i, q_i) \qquad ; k = 1, 2, \ldots, n \\ q'_k &= q'_k(p_i, q_i) \end{aligned} \tag{3.2}$$

These equations can be considered as a transformation of the set of variables (p_i, q_i) to the set (p'_k, q'_k) or, geometrically, as a mapping of the phase space at the time t to that at the time t'. The volume element $d\lambda$ and the corresponding volume element $d\lambda'$, obtained through this transformation (Figure 3.1), are related by the expression

$$d\lambda' = J(t, t')d\lambda \tag{3.3}$$

where $J(t,t')$ is the *jacobian determinant* of the transformation

$$J(t,t') = \left|\frac{\partial(p'_k,q'_k)}{\partial(p_i,q_i)}\right| \equiv \begin{vmatrix} \frac{\partial p'_1}{\partial p_1} & \frac{\partial q'_1}{\partial p_1} & \frac{\partial p'_2}{\partial p_1} & \frac{\partial q'_2}{\partial p_1} & \cdots & \cdots & \frac{\partial p'_n}{\partial p_1} & \frac{\partial q'_n}{\partial p_1} \\ \frac{\partial p'_1}{\partial q_1} & \frac{\partial q'_1}{\partial q_1} & \cdots & & & & & \\ \vdots & & & & & & & \\ \frac{\partial p'_1}{\partial p_n} & \frac{\partial q'_1}{\partial p_n} & \cdots & & & & \frac{\partial p'_n}{\partial p_n} & \frac{\partial q'_n}{\partial p_n} \\ \frac{\partial p'_1}{\partial q_n} & \frac{\partial q'_1}{\partial q_n} & \cdots & & & & \frac{\partial p'_n}{\partial q_n} & \frac{\partial q'_n}{\partial q_n} \end{vmatrix} \tag{3.4}$$

First, let $t' = t$, so that $p'_k = p_k$, $q'_k = q_k$, and therefore

$$\begin{aligned} \frac{\partial p'_k}{\partial p_i} &= \delta_{ik} & \qquad \frac{\partial q'_k}{\partial q_i} &= \delta_{ik} \\ \frac{\partial p'_k}{\partial q_i} &= 0 & \qquad \frac{\partial q'_k}{\partial p_i} &= 0 \end{aligned} \tag{3.5}$$

where δ_{ik} is the Kronecker delta defined by

$$\begin{aligned} \delta_{ik} &= 1 & \qquad for\ i &= k \\ &= 0 & \qquad for\ i &\neq k \end{aligned} \tag{3.6}$$

In this case all terms on the diagonal of J are equal to unity and all others are zero. Therefore

$$J(t,t) = 1 \tag{3.7}$$

Next, let $t' = t + dt$, and keep only first-order terms in dt. One then has from Hamilton's equations

$$\begin{aligned} \dot{p}_k &\equiv \frac{dp_k}{dt} = -\frac{\partial H}{\partial q_k} \\ \dot{q}_k &\equiv \frac{dq_k}{dt} = \frac{\partial H}{\partial p_k} \end{aligned} \tag{3.8}$$

and thus

$$\begin{aligned} p'_k &= p_k - \frac{\partial H}{\partial q_k}dt \\ q'_k &= q_k + \frac{\partial H}{\partial p_k}dt \end{aligned} \tag{3.9}$$

These relations may be differentiated to give

$$\begin{aligned} \frac{\partial p'_k}{\partial p_i} &= \delta_{ik} - \frac{\partial^2 H}{\partial p_i \partial q_k}dt \quad ; \quad & \frac{\partial q'_k}{\partial p_i} &= \frac{\partial^2 H}{\partial p_i \partial p_k}dt \\ \frac{\partial p'_k}{\partial q_i} &= -\frac{\partial^2 H}{\partial q_i \partial q_k}dt \quad ; \quad & \frac{\partial q'_k}{\partial q_i} &= \delta_{ik} + \frac{\partial^2 H}{\partial q_i \partial p_k}dt \end{aligned} \tag{3.10}$$

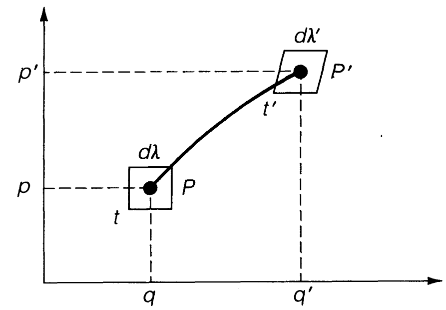

Figure 3.1 The time development of the volume element in phase space as described by Liouville's Theorem (schematic).

In evaluating the determinant in Eq.(3.4), each term containing a non-diagonal element as a factor contains at least another non-diagonal element as a factor. Since all these elements are proportional to dt, these terms are therefore at least of second order in dt and do not contribute to first order. To that order there remains then only the contribution from the diagonal elements

$$\prod_k \left(1 - \frac{\partial^2 H}{\partial p_k \partial q_k} dt\right)\left(1 + \frac{\partial^2 H}{\partial p_k \partial q_k} dt\right)$$

$$\cong 1 + \sum_k \left(\frac{\partial^2 H}{\partial p_k \partial q_k} - \frac{\partial^2 H}{\partial p_k \partial q_k}\right) dt = 1 \tag{3.11}$$

Therefore

$$J(t, t + dt) = J(t, t) + \frac{\partial}{\partial t} J(t'', t)|_{t''=t} dt = 1 \tag{3.12}$$

and since Eq.(3.7) states that $J(t, t) = 1$ we have the result

$$\frac{\partial}{\partial t} J(t'', t)|_{t''=t} = 0 \tag{3.13}$$

On the other hand, besides t and t', consider an arbitrary third time t'' and the corresponding volume element $d\lambda''$ at the time t'' (Figure 3.2) and use Eq.(3.3) with arbitrary t and t'. Then, going from t to t'' we have

$$d\lambda'' = J(t, t'')d\lambda \tag{3.14}$$

and from t'' to t'

$$d\lambda' = J(t'', t')d\lambda'' \tag{3.15}$$

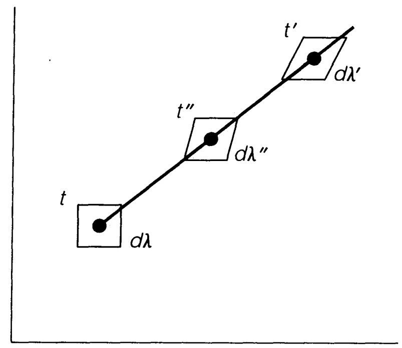

Figure 3.2 Intermediate time t'' and volume element $d\lambda''$ used in proof of Liouville's Theorem.

Therefore

$$d\lambda' = J(t, t'')J(t'', t')d\lambda = J(t, t')d\lambda \tag{3.16}$$

or

$$J(t, t') = J(t, t'')J(t'', t') \tag{3.17}$$

Hence, upon differentiation with respect to the final time t'

$$\frac{\partial J(t, t')}{\partial t'} = J(t, t'')\frac{\partial}{\partial t'}J(t'', t') \tag{3.18}$$

Now on the right side let $t'' = t'$, and this relation becomes

$$\frac{\partial J(t, t')}{\partial t'} = J(t, t')\frac{\partial}{\partial t'}J(t'', t')|_{t''=t'} \tag{3.19}$$

Since Eq.(3.13) holds for any time t, it also holds for t'

$$\frac{\partial}{\partial t'}J(t'', t')|_{t''=t'} = 0 \tag{3.20}$$

Equation (3.19) thus implies

$$\frac{\partial}{\partial t'}J(t, t') = 0 \tag{3.21}$$

This relation now holds for arbitrary t' and provides a first-order differential equation for the jacobian determinant. For $t' = t$ one has the initial condition $J(t,t) = 1$ of Eq.(3.7), and hence

$$J(t,t') = 1 \tag{3.22}$$

for arbitrary t'. It follows from Eq.(3.3) that

$$d\lambda' = d\lambda \tag{3.23}$$

One therefore concludes that *the magnitude of the volume element in phase space does not change in the course of its motion along the phase orbits.*

The same result holds for the volume of any closed finite region R in phase space followed along the phase orbits (Figure 3.3). To every volume element $d\lambda$ within that region at the time t, there corresponds an equal volume element $d\lambda'$ within the region R' at the time t' obtained from R by the equations of motion. Integrating the righthand side of Eq.(3.23) over R corresponds to the integration of the lefthand side over R' so that

$$\int_{R'} d\lambda' = \int_R d\lambda \tag{3.24}$$

or

$$\Omega' = \Omega \tag{3.25}$$

where Ω and Ω' represent the volume contained within R and R' respectively. In abbreviated form, this result is stated by Liouville's Theorem: The phase volume is a constant of the motion.

This theorem can be illustrated for the simplest case of a mass point in free, one-dimensional motion. The hamiltonian is

$$H = \frac{p^2}{2m} \tag{3.26}$$

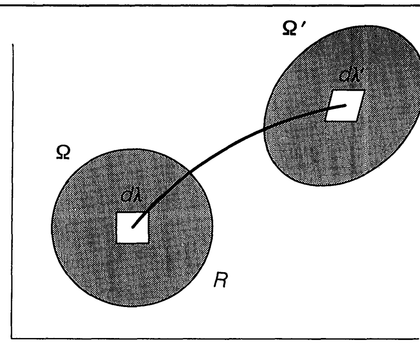

Figure 3.3 Invariance of finite volume elements in phase space followed along the phase orbits (schematic).

and Hamilton's equations give†

$$\begin{aligned} \dot{p} &= -\frac{\partial H}{\partial q} = 0 \\ \dot{q} &= \frac{\partial H}{\partial p} = \frac{p}{m} \end{aligned} \tag{3.27}$$

Integration of these equations yields

$$\begin{aligned} p &= \text{constant} \\ q &= \frac{p}{m}t + \text{constant} \end{aligned} \tag{3.28}$$

which provides a parametric representation of the phase orbit. In the previous notation we have

$$\begin{aligned} p' &= p \\ q' &= q + \frac{p}{m}(t' - t) \end{aligned} \tag{3.29}$$

The jacobian of this transformation can be immediatly evaluated as

$$J(t, t') = \begin{vmatrix} \frac{\partial p'}{\partial p} & \frac{\partial q'}{\partial p} \\ \frac{\partial p'}{\partial q} & \frac{\partial q'}{\partial q} \end{vmatrix} = \begin{vmatrix} 1 & \frac{t'-t}{m} \\ 0 & 1 \end{vmatrix} = 1 \tag{3.30}$$

which illustrates our general result. Consider further the rectangle *abcd* at the time t and the corresponding parallelogram $a'b'c'd'$ at the time t' shown in Figure 3.4. Evidently

$$\begin{aligned} q_{a'} &= q_a + \frac{p_a}{m}(t' - t) \qquad ; \; p_a = p_b \\ q_{b'} &= q_b + \frac{p_b}{m}(t' - t) \qquad ; \; p_c = p_d \\ q_{c'} &= q_c + \frac{p_c}{m}(t' - t) \\ q_{d'} &= q_d + \frac{p_d}{m}(t' - t) \end{aligned} \tag{3.31}$$

Thus

$$\begin{aligned} q_{b'} - q_{a'} &= q_b - q_a \equiv w \\ q_{d'} - q_{c'} &= q_d - q_c \equiv w \end{aligned} \tag{3.32}$$

† We use the customary notation where a dot above a symbol denotes the total time derivative.

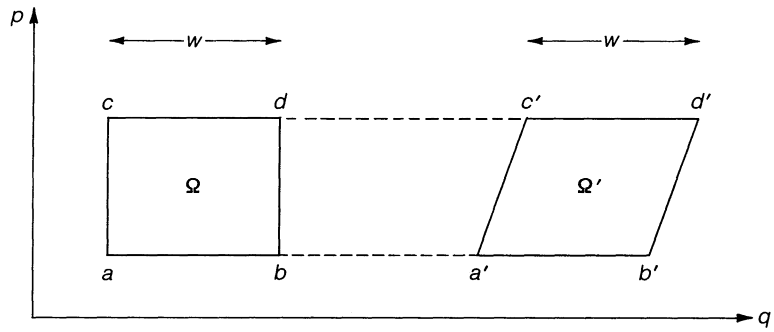

Figure 3.4 Phase volume for free one-dimensional motion of a mass point.

Since $a'b'c'd'$ has the same width w as $abcd$ and the same height $p_c - p_a$, the areas Ω and Ω' are equal, illustrating our general result. The extension to arbitrary regions R and R' (see Figure 3.5) is immediately obtained by dividing the regions into infinitesimally thin horizontal strips and applying the above.

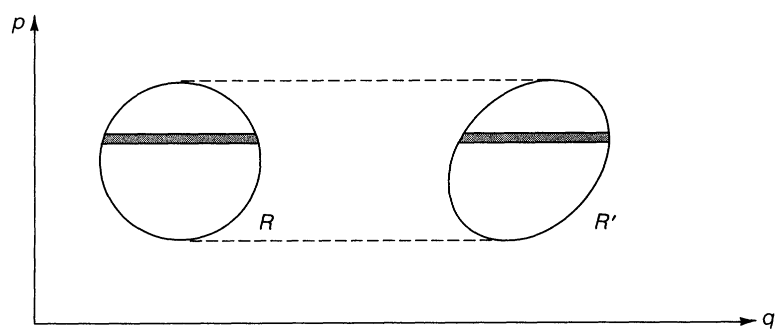

Figure 3.5 Extension of result in Figure 3.4 to a region of arbitrary shape.

Another example is the one-dimensional harmonic oscillator with hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 \tag{3.33}$$

Hamilton's equations give

$$\begin{aligned}\dot{p} &= -\frac{\partial H}{\partial q} = -m\omega^2 q \\ \dot{q} &= \frac{\partial H}{\partial p} = \frac{p}{m}\end{aligned} \tag{3.34}$$

A combination of these relations yields

$$\begin{aligned}\frac{d}{dt}(p + im\omega q) &= \dot{p} + im\omega\dot{q} = -m\omega^2 q + i\omega p \\ &= i\omega(p + im\omega q)\end{aligned} \tag{3.35}$$

and hence, by integration

$$p' + im\omega q' = (p + im\omega q)e^{i\omega(t'-t)} \tag{3.36}$$

The real and imaginary parts of this relation are

$$\begin{aligned}p' &= p \cos\alpha - m\omega q \sin\alpha \\ q' &= \frac{p}{m\omega}\sin\alpha + q\cos\alpha\end{aligned} \tag{3.37}$$

with

$$\alpha \equiv \omega(t' - t) \tag{3.38}$$

the jacobian can be evaluated as

$$J(t,t') = \begin{vmatrix} \frac{\partial p'}{\partial p} & \frac{\partial q'}{\partial p} \\ \frac{\partial p'}{\partial q} & \frac{\partial q'}{\partial q} \end{vmatrix} = \begin{vmatrix} \cos\alpha & \frac{\sin\alpha}{m\omega} \\ -m\omega\sin\alpha & \cos\alpha \end{vmatrix} = \cos^2\alpha + \sin^2\alpha = 1 \tag{3.39}$$

in accord with our previous analysis. Further, upon change of scale

$$\begin{aligned}q &\to m\omega q \\ q' &\to m\omega q'\end{aligned} \tag{3.40}$$

in phase space one has for the area of an arbitrary region in phase space

$$\begin{aligned}\Omega &\to m\omega\Omega \\ \Omega' &\to m\omega\Omega'\end{aligned} \tag{3.41}$$

Now it is evident from Eq.(3.37) that the region R' with area $m\omega\Omega'$, which evolves from the region R with area $m\omega\Omega$, is obtained from R through a rotation around the origin by the angle α (Figure 3.6). Since this does not change the area, one has

$$m\omega\Omega' = m\omega\Omega \tag{3.42}$$

and hence

$$\Omega' = \Omega \tag{3.43}$$

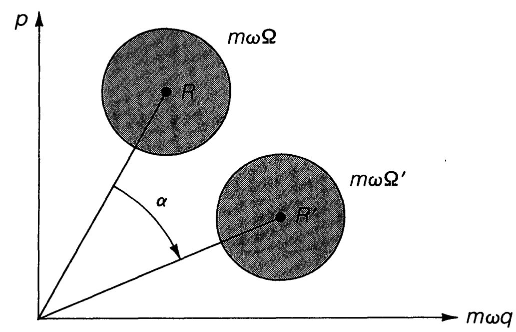

Figure 3.6 Motion of the phase volume along the phase orbits for a one-dimensional harmonic oscillator.