known, $q_j = q_j(t)$, the problem is completely solved. The generalized velocities can be calculated from

$$\dot{q}_j(t) = \frac{d}{dt} q_j(t)$$

and the generalized momenta are

$$p_j = \frac{\partial}{\partial \dot{q}_j} L(q_j, \dot{q}_j, t)$$

The essential point is that, whereas the q_j and the $\dot{q}_j$ are related by a simple time derivative *independent of the manner in which the system behaves,* the connection between the q_j and the p_j are the *equations of motion themselves.* Finding the relations that connect the q_j and the p_j (and thereby eliminating the assumed independence of these quantities) is therefore tantamount to solving the problem.

7.12 Phase Space and Liouville's Theorem (Optional)

We pointed out previously that the generalized coordinates q_j can be used to define an s-dimensional *configuration space* with every point representing a certain state of the system. Similarly, the *generalized momenta* p_j define an s-dimensional *momentum space* with every point representing a certain condition of motion of the system. A given point in configuration space specifies only the position of each of the particles in the system; nothing can be inferred regarding the motion of the particles. The reverse is true for momentum space. In Chapter 3, we found it profitable to represent geometrically the dynamics of simple oscillatory systems by phase diagrams. If we use this concept with more complicated dynamical systems, then a $2s$-dimensional space consisting of the q_j and the p_j allows us to represent both the positions *and* the momenta of all particles. This generalization is called **Hamiltonian phase space** or, simply, **phase space.***

EXAMPLE 7.13

Construct the phase diagram for the particle in Example 7.11.

Solution. The particle has two degrees of freedom (θ, z), so the phase space for this example is actually four dimensional: θ, p_θ, z, p_z. But p_θ is constant and therefore may be suppressed. In the z direction, the motion is simple harmonic, and so the projection onto the z-p_z plane of the phase path for any total energy H is just an ellipse. Because $\dot{\theta}$ = constant, the phase path must represent motion increasing uniformly with θ. Thus, the phase path on any surface H = constant is a **uniform elliptic spiral** (Figure 7-11).

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*We previously plotted in the phase diagrams the position versus a quantity proportional to the velocity. In Hamiltonian phase space, this latter quantity becomes the generalized momentum.

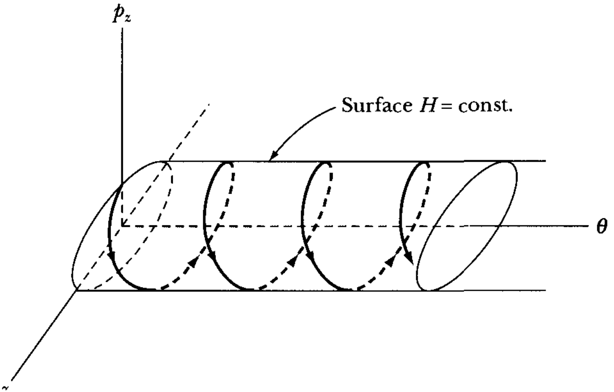

FIGURE 7-11 Example 7.13. The phase path for the particle in Example 7.11.

If, at a given time, the position and momenta of all the particles in a system are known, then with these quantities as initial conditions, the subsequent motion of the system is completely determined; that is, starting from a point $q_j(0), p_j(0)$ in phase space, the representative point describing the system moves along a unique phase path. In principle, this procedure can always be followed and a solution obtained. But if the number of degrees of freedom of the system is large, the set of equations of motion may be too complicated to solve in a reasonable time. Moreover, for complex systems, such as a quantity of gas, it is a practical impossibility to determine the initial conditions for each constituent molecule. Because we cannot identify any particular point in phase space as representing the actual conditions at any given time, we must devise some alternative approach to study the dynamics of such systems. We therefore arrive at the point of departure of statistical mechanics. The Hamiltonian formulation of dynamics is ideal for the statistical study of complex systems. We demonstrate this in part by now proving a theorem that is fundamental for such investigations.

For a large collection of particles—say, gas molecules—we are unable to identify the particular point in phase space correctly representing the system. But we may fill the phase space with a collection of points, each representing a *possible* condition of the system; that is, we imagine a large number of systems (each consistent with the known constraints), any of which could conceivably be the actual system. Because we are unable to discuss the details of the particles' motion in the actual system, we substitute a discussion of an *ensemble* of equivalent systems. Each representative point in phase space corresponds to a single system of the ensemble, and the motion of a particular point represents the independent motion of that system. Thus, no two of the phase paths may ever intersect.

We may consider the representative points to be sufficiently numerous that we can define a *density in phase space* ρ. The volume elements of the phase space defining the density must be sufficiently large to contain a large number of representative points, but they must also be sufficiently small so that the density

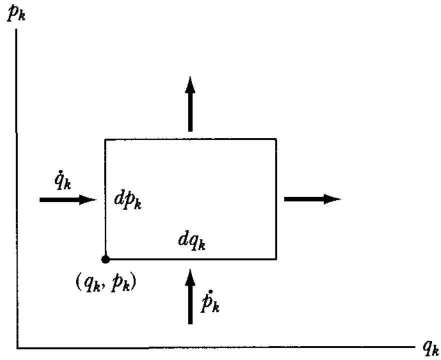

FIGURE 7-12 An element of area $dA = dq_k\, dp_k$ in the q_k–p_k plane in phase space.

varies continuously. The number N of systems whose representative points lie within a volume dv of phase space is

$$N = \rho\, dv \tag{7.190}$$

where

$$dv = dq_1\, dq_2 \cdots dq_s\, dp_1\, dp_2 \cdots dp_s \tag{7.191}$$

As before, s is the number of degrees of freedom of each system in the ensemble.

Consider an element of area in the q_k–p_k plane in phase space (Figure 7-12). The number of representative points moving across the left-hand edge into the area per unit time is

$$\rho \frac{dq_k}{dt}\, dp_k = \rho \dot{q}_k\, dp_k$$

and the number moving across the lower edge into the area per unit time is

$$\rho \frac{dp_k}{dt}\, dq_k = \rho \dot{p}_k\, dq_k$$

so that the total number of representative points moving *into* the area $dq_k\, dp_k$ per unit time is

$$\rho(\dot{q}_k\, dp_k + \dot{p}_k\, dq_k) \tag{7.192}$$

By a Taylor series expansion, the number of representative points moving *out* of the area per unit time is (approximately)

$$\left[\rho \dot{q}_k + \frac{\partial}{\partial q_k}(\rho \dot{q}_k)\, dq_k\right] dp_k + \left[\rho \dot{p}_k + \frac{\partial}{\partial p_k}(\rho \dot{p}_k)\, dp_k\right] dq_k \tag{7.193}$$

Thus, the total increase in density in $dq_k\, dp_k$ per unit time is the difference between Equations 7.192 and 7.193:

$$\frac{\partial \rho}{\partial t}\, dq_k\, dp_k = -\left[\frac{\partial}{\partial q_k}(\rho \dot{q}_k) + \frac{\partial}{\partial p_k}(\rho \dot{p}_k)\right] dq_k\, dp_k \tag{7.194}$$

After dividing by $dq_k\, dp_k$ and summing this expression over all possible values of k, we find

$$\frac{\partial \rho}{\partial t} + \sum_{k=1}^{s} \left(\frac{\partial \rho}{\partial q_k} \dot{q}_k + \rho \frac{\partial \dot{q}_k}{\partial q_k} + \frac{\partial \rho}{\partial p_k} \dot{p}_k + \rho \frac{\partial \dot{p}_k}{\partial p_k} \right) = 0 \tag{7.195}$$

From Hamilton's equations (Equations 7.160 and 7.161), we have (if the second partial derivatives of H are continuous)

$$\frac{\partial \dot{q}_k}{\partial q_k} + \frac{\partial \dot{p}_k}{\partial p_k} = 0 \tag{7.196}$$

so Equation 7.195 becomes

$$\frac{\partial \rho}{\partial t} + \sum_{k} \left(\frac{\partial \rho}{\partial q_k} \frac{dq_k}{dt} + \frac{\partial \rho}{\partial p_k} \frac{dp_k}{dt} \right) = 0 \tag{7.197}$$

But this is just the total time derivative of ρ, so we conclude that

$$\boxed{\frac{d\rho}{dt} = 0} \tag{7.198}$$

This important result, known as **Liouville's theorem,*** states that the density of representative points in phase space corresponding to the motion of a system of particles remains constant during the motion. It must be emphasized that we have been able to establish the invariance of the density ρ only because the problem was formulated in *phase space*; an equivalent theorem for configuration space does not exist. Thus, we must use Hamiltonian dynamics (rather than Lagrangian dynamics) to discuss ensembles in statistical mechanics.

Liouville's theorem is important not only for aggregates of microscopic particles, as in the statistical mechanics of gaseous systems and the focusing properties of charged-particle accelerators, but also in certain macroscopic systems. For example, in stellar dynamics, the problem is inverted and by studying the distribution function ρ of stars in the galaxy, the potential U of the galactic gravitational field may be inferred.

7.13 Virial Theorem (Optional)

Another important result of a statistical nature is worthy of mention. Consider a collection of particles whose position vectors $\mathbf{r}_\alpha$ and momenta $\mathbf{p}_\alpha$ are both bounded (i.e., remain finite for all values of the time). Define a quantity

$$S \equiv \sum_{\alpha} \mathbf{p}_\alpha \cdot \mathbf{r}_\alpha \tag{7.199}$$

*Published in 1838 by Joseph Liouville (1809–1882).