From Newton's second law to Liouville's equation and back in an intuitive way

Let us start by looking at a classical particle and its Newtonian dynamics. Furthermore, let us assume that the force that acts on the particle, of mass m, is conservative. In one dimension, to simplify the analysis, we have

$$F = -\frac{\partial}{\partial z} V(z),$$

where F is the force along the z-axis and $V(z)$ is the potential energy whose spatial derivative gives the force. Newton's second law gives

$$\frac{dp}{dt} = -\frac{\partial}{\partial z} V(z). \tag{1}$$

In the phase space we can choose a region $\mathscr{R}$ given a, say, compact set of initial conditions, that is, at $t = 0$. If we let each one of the points in $\mathscr{R}$ evolve during a time $t > 0$, we are going to have the same volume of phase space as we had in $\mathscr{R}$, according to Liouville's theorem. In this case of a single spacial dimension, we actually mean area of phase space, instead of volume, but the word volume is the standard for all dimensions, even if we have more than three spatial dimensions (for more than one particle comprising the system).

Now, after a time interval $t > 0$ has elapsed, let us choose a particular phase-space volume $dzdp$ about the point (z, p) and let $\rho_{cl}(z, p, t)\, dzdp$ be the probability of finding the particle inside the volume element $dzdp$. If, instead, we think of $\rho_{cl}(z, p, t)$ as the density of N non-interacting particles at the point (z, p) at time t, we see that they left, at time $t = 0$, the region $\mathscr{R}$ from the neighborhood of the point $(z_{cl}(0), p_{cl}(0))$, where z_{cl} and p_{cl} are the functions of time describing the trajectory described by Eq. (1) that, at time t, ends up at the phase-space point (z, p). By Liouville's theorem, if we have $dzdp\rho_{cl}(z, p, t)$ particles in the region of volume $dzdp$ about the point (z, p) at time $t > 0$, these are the particles that came from the region of phase-space volume value also given by $dzdp$, but centered about the point $(z_{cl}(0), p_{cl}(0))$ at $t = 0$. Therefore, the number of particles about the two different points of phase space is the same, that is,

$$\frac{d}{dt}\left[dzdp\rho_{cl}(z_{cl}(t), p_{cl}(t), t)\right] = 0$$

and, since $dzdp$ is the same along the whole trajectory of all the N particles, we can write:

$$\frac{d}{dt}\rho_{cl}(z_{cl}(t), p_{cl}(t), t) = 0,$$

or, equivalently,

$$\frac{dz_{cl}}{dt}\frac{\partial}{\partial z_{cl}}\rho_{cl}(z_{cl}, p_{cl}, t) + \frac{dp_{cl}}{dt}\frac{\partial}{\partial p_{cl}}\rho_{cl}(z_{cl}, p_{cl}, t) + \frac{\partial}{\partial t}\rho_{cl}(z_{cl}, p_{cl}, t) = 0.$$

Since

$$p_{cl} = m\frac{dz_{cl}}{dt}, \tag{2}$$

using Eq. (1) we obtain

$$\frac{\partial}{\partial t}\rho_{cl}(z_{cl}, p_{cl}, t) + \frac{p_{cl}}{m}\frac{\partial}{\partial z_{cl}}\rho_{cl}(z_{cl}, p_{cl}, t) - \frac{\partial V(z_{cl})}{\partial z_{cl}}\frac{\partial}{\partial p_{cl}}\rho_{cl}(z_{cl}, p_{cl}, t) = 0.$$

Therefore, for any point (z,p) of phase space at time t, the dynamics of the probability distribution function is written as

$$\frac{\partial}{\partial t}\rho_{cl}\left(z,p,t\right)+\frac{p}{m}\frac{\partial}{\partial z}\rho_{cl}\left(z,p,t\right) \;=\; \frac{\partial V\left(z\right)}{\partial z}\frac{\partial}{\partial p}\rho_{cl}\left(z,p,t\right), \tag{3}$$

which is the classical Liouville equation.

Now we want to show how to obtain the force out of the distribution function and its equation of motion. The same procedure will be used when we deal with the force acting on the atom that we want to decelerate, for example. Let us consider an initially very localized distribution centered at point (z_0, p_0) of phase space. Because the basic volume element associated with non-negligible values of the distribution function is going to be conserved, since the dynamics is Hamiltonian, then the distribution will propagate through phase space as time passes, but will remain localized as at $t = 0$. Because of this and supposing the time evolution is finite, the function $\rho_{cl}\left(z,p,t\right)$ is going to tend to zero as the magnitude of z or p tends to infinity. Hence, we intuitively see that

$$\begin{aligned}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dzdp\,z\rho_{cl}\left(z,p,t\right) &\approx z_{cl}\left(t\right)\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dzdp\,\rho_{cl}\left(z,p,t\right)\\ &\approx z_{cl}\left(t\right),\end{aligned} \tag{4}$$

if we normalize the distribution function so that

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dzdp\,\rho_{cl}\left(z,p,t\right) \;=\; 1. \tag{5}$$

We also have:

$$\begin{aligned}\int_{-\infty}^{+\infty}dp\int_{-\infty}^{+\infty}dz\,z\left[p\frac{\partial}{\partial z}\rho_{cl}\left(z,p,t\right)\right] &= \int_{-\infty}^{+\infty}dp\,p\int_{-\infty}^{+\infty}dz\,\frac{\partial}{\partial z}\left[z\rho_{cl}\left(z,p,t\right)\right]\\ &\quad-\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dzdp\,p\rho_{cl}\left(z,p,t\right)\\ &\approx -p_{cl}\left(t\right),\end{aligned} \tag{6}$$

where we used

$$\int_{-\infty}^{+\infty}dz\,\frac{\partial}{\partial z}\left[z\rho_{cl}\left(z,p,t\right)\right] \;=\; \left[z\rho_{cl}\left(z,p,t\right)\right]_{z=\infty}-\left[z\rho_{cl}\left(z,p,t\right)\right]_{z=-\infty}=0, \tag{7}$$

because the probability density goes to zero at infinite points of phase space, and

$$\int_{-\infty}^{+\infty}dz\int_{-\infty}^{+\infty}dp\,p\rho_{cl}\left(z,p,t\right) \;\approx\; p_{cl}\left(t\right), \tag{8}$$

since the distribution function (or probability density) is localized in phase space for all time. In an analogous fashion, we calculate:

$$\begin{aligned}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dzdp\,z\frac{\partial}{\partial p}\rho_{cl}\left(z,p,t\right) &= \int_{-\infty}^{+\infty}dz\,z\int_{-\infty}^{+\infty}dp\frac{\partial}{\partial p}\rho_{cl}\left(z,p,t\right)\\ &= \int_{-\infty}^{+\infty}dz\,z\left\{\left[\rho_{cl}\left(z,p,t\right)\right]_{p=\infty}-\left[\rho_{cl}\left(z,p,t\right)\right]_{p=-\infty}\right\}=0.\end{aligned} \tag{9}$$

Thus, multiplication of Eq. (3) by z and integrating over the whole phase space gives, according with Eqs. (4-9),

$$\frac{dz_{cl}}{dt}-\frac{p_{cl}}{m} = 0,$$

which is just Eq. (2).

We now proceed by multiplying Eq. (3) by p and integrating over phase space. Then,

$$\begin{aligned}\frac{d}{dt}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dzdp\,p\rho_{cl}\left(z,p,t\right)+\frac{1}{m}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dzdp\,p^{2}\frac{\partial}{\partial z}\rho_{cl}\left(z,p,t\right) &=\\ \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dzdp\,p\frac{\partial V\left(z\right)}{\partial z}\frac{\partial}{\partial p}\rho_{cl}\left(z,p,t\right),&\end{aligned}$$

giving

$$\frac{dp_{cl}}{dt}+\frac{1}{m}\int_{-\infty}^{+\infty}dp\,p^{2}\int_{-\infty}^{+\infty}dz\frac{\partial}{\partial z}\rho_{cl}\left(z,p,t\right) = \int_{-\infty}^{+\infty}dz\frac{\partial V\left(z\right)}{\partial z}\int_{-\infty}^{+\infty}dp\,p\frac{\partial}{\partial p}\rho_{cl}\left(z,p,t\right). \tag{10}$$

But,

$$\int_{-\infty}^{+\infty}dz\frac{\partial}{\partial z}\rho_{cl}\left(z,p,t\right) = \left[\rho_{cl}\left(z,p,t\right)\right]_{z=\infty}-\left[\rho_{cl}\left(z,p,t\right)\right]_{z=-\infty}=0 \tag{11}$$

and

$$\begin{aligned}\int_{-\infty}^{+\infty}dp\,p\frac{\partial}{\partial p}\rho_{cl}\left(z,p,t\right) &= \int_{-\infty}^{+\infty}dp\,\frac{\partial}{\partial p}\left[p\rho_{cl}\left(z,p,t\right)\right]-\int_{-\infty}^{+\infty}dp\,\rho_{cl}\left(z,p,t\right)\\ &= \left[p\rho_{cl}\left(z,p,t\right)\right]_{p=\infty}-\left[p\rho_{cl}\left(z,p,t\right)\right]_{p=-\infty}-\int_{-\infty}^{+\infty}dp\,\rho_{cl}\left(z,p,t\right)\\ &=-\int_{-\infty}^{+\infty}dp\,\rho_{cl}\left(z,p,t\right).\end{aligned} \tag{12}$$

Hence, using Eqs. (11) and (12) in Eq. (10), we get

$$\frac{dp_{cl}}{dt} = -\int_{-\infty}^{+\infty}dz\frac{\partial V\left(z\right)}{\partial z}\int_{-\infty}^{+\infty}dp\,\rho_{cl}\left(z,p,t\right)=-\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dzdp\,\frac{\partial V\left(z\right)}{\partial z}\rho_{cl}\left(z,p,t\right)$$

and, using the fact that $\rho_{cl}\left(z,p,t\right)$ is localized about $\left(z_{cl}\left(t\right),p_{cl}\left(t\right)\right)$, this equation is found to be

$$\frac{dp_{cl}}{dt} \approx -\frac{\partial V\left(z_{cl}\right)}{\partial z_{cl}}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}dzdp\,\rho_{cl}\left(z,p,t\right)=-\frac{\partial V\left(z_{cl}\right)}{\partial z_{cl}},$$

where we have used Eq. (5). We see that this last result is just Eq. (1), as expected. The procedure we have been depicting here is exactly analogous to the one we will employ when calculating the force acting on the atom, for example.

A crash introduction to the Wigner function and, then, to the Wigner operator

Let us consider a quantum particle of mass m subject to the potential operator $V\left(Z\right)$, where Z is the position operator. Before talking about operators here, let us look at the more basic formulation in terms of wave functions. Suppose that at

$t = 0$ the state of the particle is described by the wave function $\psi(z, 0)$. Schrödinger's equation gives the time evolution of the wave function:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\psi(z,t) + V(z)\psi(z,t) = i\hbar\frac{\partial}{\partial t}\psi(z,t), \tag{13}$$

where z, of course, is the point in one-dimensional space where we are calculating the probability amplitude $\psi(z,t)$ of finding the particle. As usual, the probability of finding the particle within the region of size dz about the point z is given, according to the Born principle, by $|\psi(z,t)|^2 dz$. Similarly, the probability of finding the particle within the region of size dp about the momentum p, in momentum space, is given by $\left|\tilde{\psi}(p,t)\right|^2 dp$, where $\tilde{\psi}(p,t)$ is the Fourier transform of $\psi(z,t)$, namely,

$$\tilde{\psi}(p,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} dz\,\psi(z,t)\exp\left(-i\frac{pz}{\hbar}\right). \tag{14}$$

We could say that the Fourier transform of the position wave function changes the position description of the particle to one in terms of its momentum.

Using the formalism of wave functions we can define the density-matrix elements in position space as

$$\rho(z,z',t) \equiv \psi(z,t)\psi^*(z',t), \tag{15}$$

where $\psi^*(z,t)$ stands for the complex conjugate of $\psi(z,t)$. Notice that Eq. (15) is the density-matrix element, taken between the position eigenvalues z and z', for a pure quantum state represented by the wave function $\psi(z,t)$. For $z = z'$, the density-matrix element $\rho(z,z,t)$ is just the probability density for finding the particle at position z at instant t. For $z \neq z'$, however, the element $\rho(z,z',t)$ is what is called the coherence, let us say, between positions z and z'. Incidentally, it might be illustrative to remember that

$$\begin{aligned}|\psi(t)\rangle &= \int_{-\infty}^{+\infty} dz\ |z\rangle\langle z|\psi(t)\rangle \\ &= \int_{-\infty}^{+\infty} dz\ |z\rangle\,\psi(z,t).\end{aligned}$$

Therefore, if we focus attention at a central position z and look at the coherence between two other points separated by a distance $|s|$, but symmetrically located in relation to this particular central position z, we have

$$\rho(z+s/2, z-s/2, t) = \psi(z+s/2,t)\psi^*(z-s/2,t). \tag{16}$$

Equivalently, we can also say that, given a reference position z, Eq. (16) describes, relative to it, the coherences between the points a distance $|s|/2$ apart from z. Now, classically, if a particle passes through two different points in space, then we conclude that the particle has momentum (and, of course, it passes through each point at a different time). Could our coherences, somehow, be related with the momentum description of the quantum state? [I am being very imprecise here, but my intention is to make the definition of the Wigner function more intuitive.] We then can take the Fourier transform of Eq. (16) with respect to s and keep z intact to get:

$$\begin{aligned}w(z,p,t) &\equiv \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} ds\,\rho(z+s/2,z-s/2,t)\exp\left(-i\frac{ps}{\hbar}\right) \\ &= \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} ds\,\psi(z+s/2,t)\psi^*(z-s/2,t)\exp\left(-i\frac{ps}{\hbar}\right),\end{aligned} \tag{17}$$

where $w(z,p,t)$ is called the Wigner function. It is now seen that

$$\begin{aligned}
\int_{-\infty}^{+\infty} dp\, w(z,p,t) &= \int_{-\infty}^{+\infty} ds\, \psi(z+s/2,t)\, \psi^*(z-s/2,t) \left[\frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dp\, \exp\left(-i\frac{ps}{\hbar}\right) \right] \\
&= \int_{-\infty}^{+\infty} ds\, \psi(z+s/2,t)\, \psi^*(z-s/2,t)\, \delta(s) = |\psi(z,t)|^2
\end{aligned}$$

and, using the inverse of Eq. (14), namely,

$$\psi(z,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} dp\, \tilde{\psi}(p,t) \exp\left(i\frac{pz}{\hbar}\right),$$

we also obtain

$$\begin{aligned}
\int_{-\infty}^{+\infty} dz\, w(z,p,t) &= \int_{-\infty}^{+\infty} ds\, \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dz\, \psi(z+s/2,t)\, \psi^*(z-s/2,t) \exp\left(-i\frac{ps}{\hbar}\right) \\
&= \int_{-\infty}^{+\infty} ds\, \frac{1}{(2\pi\hbar)^2} \int_{-\infty}^{+\infty} dz \int_{-\infty}^{+\infty} dp_1\, \tilde{\psi}(p_1,t) \exp\left[i\frac{p_1}{\hbar}(z+s/2)\right] \\
&\quad \times \int_{-\infty}^{+\infty} dp_2\, \tilde{\psi}^*(p_2,t) \exp\left[-i\frac{p_2}{\hbar}(z-s/2)\right] \exp\left(-i\frac{ps}{\hbar}\right),
\end{aligned}$$

that is,

$$\begin{aligned}
\int_{-\infty}^{+\infty} dz\, w(z,p,t) &= \int_{-\infty}^{+\infty} dp_1 \int_{-\infty}^{+\infty} dp_2\, \tilde{\psi}(p_1,t)\, \tilde{\psi}^*(p_2,t) \left\{ \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dz\, \exp\left[i\frac{z}{\hbar}(p_1-p_2)\right] \right\} \\
&\quad \times \left\{ \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} ds\, \exp\left[-i\frac{s}{\hbar}\left(p - \frac{p_1+p_2}{2}\right)\right] \right\} \\
&= \int_{-\infty}^{+\infty} dp_1 \int_{-\infty}^{+\infty} dp_2\, \tilde{\psi}(p_1,t)\, \tilde{\psi}^*(p_2,t)\, \delta(p_1-p_2)\, \delta\left(p - \frac{p_1+p_2}{2}\right) = \left|\tilde{\psi}(p,t)\right|^2.
\end{aligned}$$

Thus we see that the Wigner function gives a distribution in phase space analogous to the distribution $\rho_{cl}(z,p,t)$ of the previous section. If integrated over p, it gives the probability density to find the particle about the point z, irrespective of its momentum, and, if integrated over z, it gives the probability density to find the particle about momentum p, irrespective of its position. However, the Wigner function is not, in general, positive for all points in phase space; it is not a probability distribution.