Probabilistic Classical Mechanics

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Abstract

The framework of classical mechanics is founded on deterministic information: if we specify with perfect precision the initial conditions of any mechanical system, the state of that system at any desired moment t is strictly fixed. This quite clearly means that the perfect precision in the estimation of quantities and initial conditions is practically impossible because we usually measure the initial conditions with a specific error. In other words, our data are probabilistic.

In this paper, we first consider a general mechanical system and examine how the system's state at time t is represented as a probability distribution if the initial conditions are given as a probability distribution. Later on, we reduce this consideration to one-dimensional single-particle systems, and we will analyze them.

1 Hamiltonian Field: A Fluid Perspective in Phase Space

Since the state of an N-particle mechanical system at any instant is entirely defined by the momenta and positions of its particles. We can now imagine a $6N$-dimensional space, where each point denotes the set of position and momentum coordinates of the N particles, and the state of the system corresponds to a point in the $6N$-D space.

If the Hamiltonian function of the system is known, the evolution of any point in the phase space can be determined. Since the equations of motion are first-order differential equations, placing the system at a specific point in phase space will immediately result in motion with a certain velocity. This concept implies that for a given Hamiltonian, there exists a velocity field in the phase space, analogous to a fluid flow. Thus, placing the system at any point causes it to move along the streamlines of this velocity field.

2 Incompressible Fluid

For an ideal incompressible fluid, the equations of motion can be written as follows:

- Newton's second law:
$$\rho \frac{D\mathbf{v}}{Dt} = \rho \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\, \mathbf{v} \right) = -\nabla\phi - \nabla p$$
- Mass conservation:
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$
- Incompressibility:
$$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \nabla \rho = 0$$

The first equation represents the equation of motion, which will be derived in later sections for our specific problem. The last two equations are constraint equations that characterize the fluid. The mass conservation equation can be rewritten as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \rho \cdot \mathbf{v} + \rho \nabla \cdot \mathbf{v} = 0$$

By substituting the first term, $\partial\rho/\partial t$, from the incompressibility equation, this equation becomes:

$$-\nabla \rho \cdot \mathbf{v} + \nabla \rho \cdot \mathbf{v} + \rho \nabla \cdot \mathbf{v} = \rho \nabla \cdot \mathbf{v} = 0$$

Thus, mass conservation and fluid incompressibility imply that the fluid's velocity field has no divergence:

$$\nabla \cdot \mathbf{v} = 0$$

3 Incompressibiliy of Phase Space Fluid

Now we examine the mentioned fluid in phase space. First, we define the position vector and the velocity field in this space:

$$\mathbf{r} \equiv \sum_{i=1}^{3N} q_i \hat{q}_i + p_i \hat{p}_i$$

$$\mathbf{v}(\mathbf{r}) \equiv \sum_{i=1}^{3N} \dot{q}_i(\mathbf{r}) \hat{q}_i + \dot{p}_i(\mathbf{r}) \hat{p}_i$$

The unit vectors are chosen according to the defined phase space. The quantities $\dot{q}_i$ and $\dot{p}_i$ are related to the system placed at that point, making this defined velocity a vector field on $\mathbf{r}$.

From Hamilton's equations, we have:

$$\dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i}$$

$$\dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i}$$

$$\mathbf{v} = \sum_{i=1}^{3N} \frac{\partial \mathcal{H}}{\partial p_i} \hat{q}_i - \frac{\partial \mathcal{H}}{\partial q_i} \hat{p}_i$$

The Nabla operator in this space is defined as:

$$\nabla \equiv \sum_{i=1}^{3N} \frac{\partial}{\partial p_i}\hat{p}_i + \frac{\partial}{\partial q_i}\hat{q}_i$$

Thus, the divergence of the velocity field of this fluid is:

$$\nabla \cdot \mathbf{v} = \sum_{i=1}^{3N} \frac{\partial^2 \mathcal{H}}{\partial p_i \partial q_i} - \frac{\partial^2 \mathcal{H}}{\partial q_i \partial p_i} = 0$$

It appears that the Hamiltonian fluid and phase space form an incompressible fluid. For a precise proof, we use the conservation of the number of systems, which is analogous to mass conservation in an ideal fluid. The quantity ρ is defined as the number of systems per unit volume (volume in the $6N$-dimensional phase space). Its conservation is expressed as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = \frac{\partial \rho}{\partial t} + \nabla \rho \cdot \mathbf{v} + \rho \nabla \cdot \mathbf{v} = 0$$

Given that we have shown $\nabla \cdot \mathbf{v} = 0$, the convective derivative of the system density is zero:

$$\frac{\partial \rho}{\partial t} + (\mathbf{v} \cdot \nabla)\, \rho = \frac{D\rho}{Dt} = 0$$

This indicates the incompressibility of the fluid. Consequently, if a number of systems are released in a specific volume in phase space to evolve, the volume occupied by this collection of systems remains constant over time. This fact is crucial for our subsequent derivation and analysis, as it underpins the behavior of the system in phase space and forms the foundation for the results presented in this work.

4 Evolution of Probability Distribution Density

Notation: Here, whenever q, p are mentioned without an index, they refer to the set of all q_i, p_i's:

$$q \equiv \{q_1, q_2, \cdots\} \quad , \quad p \equiv \{p_1, p_2, \cdots\}$$

Definition of Probability Distribution: If, at time t, the probability distribution of the system in phase space is $f(q, p, t)$, this means that the probability of finding the system in the volume element dv in phase space is:

$$f(q, p, t)\, dv$$

The volume element in phase space is:

$$dv = \prod_{i=1}^{3N} dp_i\, dq_i$$

This function is also normalized because the total probability must equal one. Therefore, we have:

$$\int_V f(q,p,t)\,dv = 1$$

Here, we represent the probability distribution in phase space as follows, noting that we will change its notation slightly later:

$$f\left(q,p,t \mid f_0(q_0,p_0,t_0)\right)$$

This function represents the phase space probability distribution at time t, given that the probability distribution at time t_0 is $f_0(q_0,p_0,t_0)$. Considering that only $s \equiv t - t_0$ matters, the probability distribution can also be expressed as:

$$f(q,p,s \mid f_0(q_0,p_0))$$

Now, to derive the evolution equation of the probability distribution, we proceed as follows: in a short time interval τ, the "increase in the probability of the system being in the volume element dv" equals the "decrease in the probability of the system leaving this volume to elsewhere" plus the "increase in the probability of the system entering this volume from elsewhere." This reasoning is mathematically expressed as:

$$\begin{aligned}\frac{\partial f}{\partial s}\tau dv = &-\int_{v'} f(q,p,s|f_0(q_0,p_0))\ dv\ f(q',p',\tau|f_0(q,p))\ dv' \\ &+\int_{v'} f(q',p',s|f_0(q_0,p_0))\ dv\ f(q,p,\tau|f_0(q',p'))\ dv'\end{aligned}$$

The left side of the equality is actually $\tau\, dv\, \frac{\partial}{\partial s} f(q,p,s \mid f_0(q_0,p_0))$.

In the first integral, terms that are not functions of the primed variables are taken out of the integral:

$$-f(q,p,s \mid f_0(q_0,p_0))\,dv \int_{v'} f(q',p',\tau \mid f_0(q,p))\,dv'$$

Due to the normalization of the probability distribution function, the integral equals one:

$$-f(q,p,s \mid f_0(q_0,p_0))\,dv$$

Thus, the evolution equation of the probability distribution is:

$$\begin{aligned}\frac{\partial f}{\partial s}\tau = &\int_{v'} f(q',p',s|f_0(q_0,p_0))\ f(q,p,\tau|f_0(q',p'))\ dv' \\ &- f(q,p,s|f_0(q_0,p_0))\end{aligned}$$

The equations written so far are constraint equations that we expect the distribution function to follow, but they do not incorporate any laws of physics. In fact, the physics of the problem is embedded in the second term of the integral; specifically, the laws of physics determine the probability of entering from other points in phase space to the desired volume.

To derive this term, we use the theorem proved in Section 3. Given that the phase space fluid is incompressible, systems that are in a volume dv at one moment must have been in another region of the same volume dv a short time τ before this moment.

Using the mentioned point, we see that the system can move from the volume element located at

$$\mathbf{r}' = (q_1', q_2', \cdots, p_1', p_2', \cdots)$$

to the volume element located at

$$\mathbf{r} = (q_1, q_2, \cdots, p_1, p_2, \cdots)$$

only if:

$$q_i = q_i' + \frac{\partial \mathcal{H}}{\partial p_i}\tau$$
$$p_i = p_i' - \frac{\partial \mathcal{H}}{\partial q_i}\tau$$

We express this for a probability distribution as:

$$f(q, p, \tau \mid f_0(q', p'))\, dv = \prod_{i=1}^{3N} \delta\left(q_i - q_i' - \frac{\partial \mathcal{H}}{\partial p_i}\tau\right) \delta\left(p_i - p_i' + \frac{\partial \mathcal{H}}{\partial q_i}\tau\right)\, dv$$

This expression utilizes the fact that there is the same volume element on both sides. By substituting this expression into the evolution equation of the probability distribution, we have:

$$\frac{\partial f}{\partial s}\tau = -f(q, p, s|f_0(q_0, p_0)) + f\left(q - \frac{\partial \mathcal{H}}{\partial p_i}\tau, p + \frac{\partial \mathcal{H}}{\partial q_i}\tau|f_0(q_0, p_0)\right)$$

Given the time interval τ is infinitesimal, this equation becomes:

$$\boxed{\frac{\partial f}{\partial t} = \sum_{i=1}^{3N} -\frac{\partial f}{\partial q_i}\frac{\partial \mathcal{H}}{\partial p_i} + \frac{\partial f}{\partial p_i}\frac{\partial \mathcal{H}}{\partial q_i}}$$

This equation specifies the evolution of the probability distribution function over the phase space. It can also be expressed using the Poisson bracket notation:

$$\frac{\partial f}{\partial t} = \{\mathcal{H}, f\}$$

5 Stationary Distributions

A case that might seem interesting is determining the probability distribution in phase space at the initial moment such that this probability distribution does not change over time. For this purpose, we require that the term $\partial f/\partial t$ be equal to zero:

$$\sum_{i=1}^{3N} -\frac{\partial f}{\partial q_i}\frac{\partial \mathcal{H}}{\partial p_i} + \frac{\partial f}{\partial p_i}\frac{\partial \mathcal{H}}{\partial q_i} = 0$$

6 One-Dimensional Single-Particle Systems

To further develop this topic, we consider simpler systems. Here, we focus on one-dimensional single-particle systems.

To have a more intuitive understanding, we denote position by x and momentum by y. In this two-dimensional phase space, the evolution equation of the distribution function is:

$$\frac{\partial f}{\partial t} = -\frac{\partial f}{\partial x}\frac{\partial \mathcal{H}}{\partial y} + \frac{\partial f}{\partial y}\frac{\partial \mathcal{H}}{\partial x}$$

For a single-particle system, we have:

$$\mathcal{H}(x,p) = \frac{p^2}{2m} + U(x)$$

$$\frac{\partial \mathcal{H}}{\partial p} = \frac{p}{m} \quad , \quad \frac{\partial \mathcal{H}}{\partial x} = \frac{dU}{dx} = U'(x)$$

Thus, the evolution equation becomes:

$$\frac{\partial f}{\partial t} = -\frac{y}{m}\frac{\partial f}{\partial x} + U'(x)\frac{\partial f}{\partial y}$$

In terms of the force field $F(x)$, we have:

$$\boxed{-\frac{\partial f}{\partial t} = \frac{y}{m}\frac{\partial f}{\partial x} + F(x)\frac{\partial f}{\partial y}}$$

And for the stationary state case:

$$\boxed{\frac{y}{m}\frac{\partial f}{\partial x} + F(x)\frac{\partial f}{\partial y} = 0}$$

We can use separation of variables to find some stationary state distributions:

$$f(x,y) = X(x)Y(y)$$

$$-\frac{1}{F(x)X(x)}\frac{dX}{dx} = \frac{m}{yY(y)}\frac{dY}{dy}$$

Given that the left side is only a function of x and the right side is only a function of y, each must equal a constant, which we denote by $-c$:

$$\frac{m}{yY(y)}\frac{dY}{dy} = -c \Rightarrow Y(y) = a_y \exp\left[-c\frac{y^2}{2m}\right]$$

$$\frac{1}{F(x)X(x)}\frac{dX}{dx} = c \Rightarrow X(x) = a_x \exp\left[-cU(x)\right]$$

$$f(x,y) = A\exp\left[-c\left(\frac{y^2}{2m} + U(x)\right)\right]$$

This result shows that in separable stationary states (separable as $X(x)Y(y)$), the probability distribution at each point is exponentially related to the Hamiltonian at that point:

$$f(x,y) = Ae^{-c\mathcal{H}(x,y)}$$

For illustrative purposes, we can define a temperature for the separable stationary probability distribution:

$$T \equiv \frac{1}{k_B c}$$

Thus, the separable stationary probability distributions can be written as:

$$f(x, y) = A \exp\left[-\frac{\mathcal{H}}{k_B T}\right]$$

We obtain the constant A from the normalization of the function f:

$$\boxed{f(x, y) = \frac{1}{Z} \exp\left[-\frac{\mathcal{H}(x, y)}{k_B T}\right] \quad , \quad Z \equiv \iint \exp\left[-\frac{\mathcal{H}(x, y)}{k_B T}\right] \, dx \, dy}$$

As can be seen, separable stationary state distribution functions are closely related to the Boltzmann distribution and the partition function.

6.1 Probability Distribution of Position and Momentum

The probability distribution function $f(x, y, t)$ that we have introduced so far is the probability distribution over phase space. From this probability distribution, we can calculate the separate probability distributions of position and momentum:

- Position probability distribution:

$$f_x(x, t) = \int_{-\infty}^{\infty} f(x, y, t) \, dy$$

- Momentum probability distribution:

$$f_y(y, t) = \int_{-\infty}^{\infty} f(x, y, t) \, dx$$

These probability distributions indicate the likelihood of finding a particle with the specified position or momentum.

6.2 Free Particle

To investigate a free particle, we set $F(x)$ to zero, yielding:

$$-\frac{\partial f}{\partial t} = \frac{y}{m} \frac{\partial f}{\partial x}$$

As expected, for a free particle, the momentum distribution remains unchanged over time:

$$\frac{\partial f_y}{\partial t} = -\frac{y}{m} \int_{-\infty}^{\infty} \frac{\partial f}{\partial x} \, dx = 0$$

However, the position distribution changes as follows:

$$\frac{\partial f_x}{\partial t} = -\frac{1}{m} \frac{\partial}{\partial x} \int_{-\infty}^{\infty} y f(x, y, t) \, dy$$

6.3 Harmonic Oscillator

For a harmonic oscillator setting the unit system such that $k = 1$ and $m = 1$, the evolution equation becomes:

$$-\frac{\partial f}{\partial t} = y\frac{\partial f}{\partial x} - x\frac{\partial f}{\partial y}$$

For the stationary state, we have:

$$y\frac{\partial f}{\partial x} = x\frac{\partial f}{\partial y}$$

Dividing both sides by xy and using separation of variables, we obtain:

$$f(x, y) = X(x)Y(y)$$

$$\frac{1}{Xx}\frac{dX}{dx} = \frac{1}{Yy}\frac{dY}{dy} = c$$

Solving these differential equations, we get:

$$X(x) = a_x e^{cx^2} \quad , \quad Y(y) = a_y e^{cy^2}$$

Thus, the distribution function is:

$$f(x, y) = Ae^{-c(x^2+y^2)}$$

where c is a constant, and A is determined from the normalization condition (for the function to be normalizable, c must be positive):

$$\iint_{-\infty}^{\infty} f(x, y)\, dx\, dy = 1$$

$$\frac{A}{c}\pi = 1 \Rightarrow A = \frac{1}{\pi c}$$

$$\boxed{f(x, y) = \frac{1}{\pi c} e^{-c(x^2+y^2)}}$$

The graph of this function is shown in Figure 1.

This solution represents a separable stationary state; however, we see that the general equation also holds for the harmonic oscillator stationary state in the following form:

$$f(x, y) = g(x^2 + y^2)$$

The obtained separable solution is of this type. Therefore, if the distribution function has cylindrical symmetry in the xy plane at the initial moment, this distribution will not change over time.

This result is expected given the nature of the problem, as the motion of a harmonic oscillator in the given Hamiltonian describes a circular path in the phase plane. Thus, if we have a distribution with cylindrical symmetry, each component of it moves on a circular trajectory, and this symmetry ensures that the motion does not alter the distribution. This demonstrates one of the key successes of the derived theory and evolution equation.

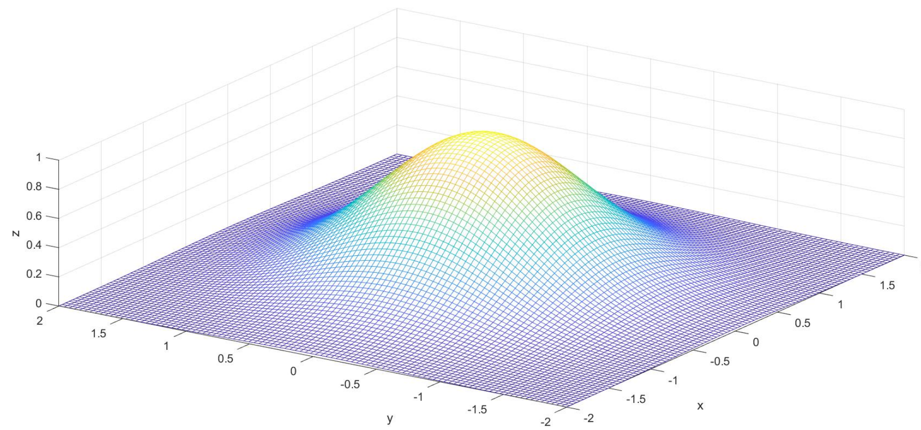

Figure 1: Stationary distribution of the harmonic oscillator

6.4 Keplerian Motion

In Keplerian motion, the effective potential energy is given by:

$$U_{\text{eff}}(r) = \frac{L^2}{2mr^2} - \frac{GmM}{r}$$

The force field corresponding to this potential is:

$$-F(r) = \frac{\partial U_{\text{eff}}}{\partial r} = \frac{L^2}{mr^3} - \frac{GmM}{r^2}$$

By substituting this force field into the stationary probability distribution equation, we obtain the following equation:

$$\frac{y}{m}\frac{\partial f}{\partial x} = \left(\frac{L^2}{mx^3} - \frac{GmM}{x^2}\right)\frac{\partial f}{\partial y}$$

$$\frac{m}{y}\frac{\partial f}{\partial y} = \frac{mx^3}{L^2 - Gm^2Mx}\frac{\partial f}{\partial x}$$

Again, we use separation of variables:

$$f(x, y) = X(x)Y(y)$$

The separated equations become:

$$\frac{m}{Yy}\frac{dY}{dy} = c$$

$$\frac{mx^3}{L^2 - Gm^2Mx}\frac{1}{X}\frac{dX}{dx} = c$$

The solutions to these equations are:

$$Y(y) = a_y e^{-cy^2/2m}$$

$$X(x) = a_x \exp\left[c\left(\frac{GmM}{x} - \frac{L^2}{2mx^2}\right)\right]$$

Thus, the final solution is:

$$f(x,y) = A\exp\left[-c\left(\frac{y^2}{2m} + \frac{L^2}{2mx^2} - \frac{GmM}{x}\right)\right]$$

The general form of the graph of this function is shown in Figure 2.

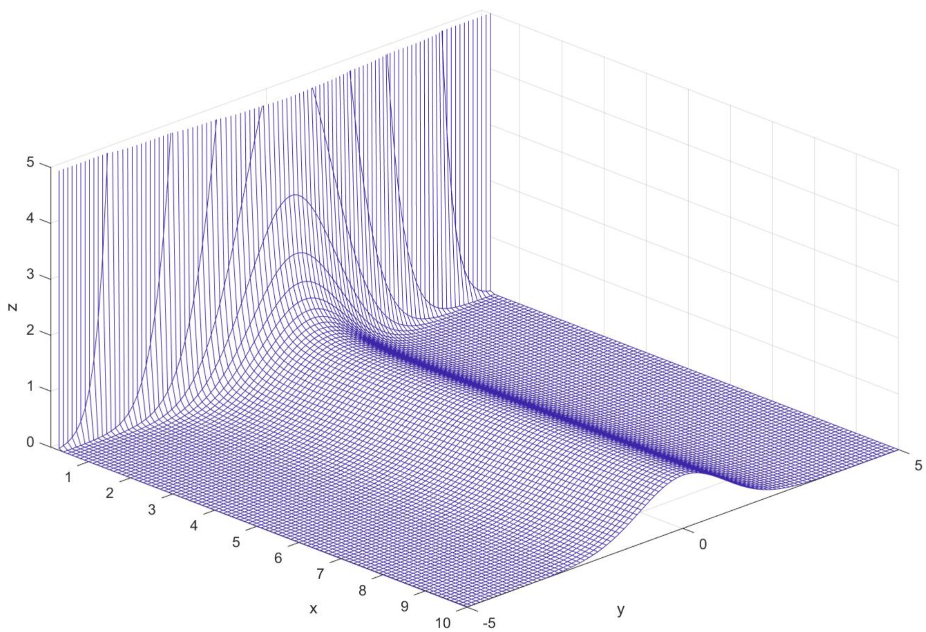

Figure 2: Stationary distribution of Keplerian motion

7 Conclusion

These results highlight the effectiveness of using Hamiltonian mechanics to understand the statistical behavior of mechanical systems. This approach provides valuable insights into the nature of stationary states and their stability under different conditions. The separable solutions obtained for the harmonic oscillator and Keplerian motion underscore the significance of symmetry in determining the form of stationary distributions.

References

[1] F. Reif, *Statistical Mechanics*, McGraw-Hill, 1965.

[2] L.D. Landau and E.M. Lifshitz, *Fluid Mechanics*, 2nd Edition, Pergamon Press, 1987.

[3] J.B. Marion and S.T. Thornton, *Classical Dynamics of Particles and Systems*, 5th Edition, Brooks Cole, 2003.