Hamiltonian mechanics - Poisson brackets and canonical transformations

Last updated: January 10, 2024

As we saw in the first chapter on Hamiltonian mechanics, the Hamiltonian formalism is often more useful than the Lagrangian formalism for addressing theoretical questions. Liouville's theorem has been the first evidence of this. Here, we introduce new theoretical insights that can be obtained from the Hamiltonian approach, including those offered by Poisson brackets (leading, among others, to powerful new ways of identifying conserved quantities from Hamiltonians) and by canonical transformations (leading to the Hamilton-Jacobi equation, the entry door to quantum mechanics).

Poisson brackets

Let's start from where we left the previous chapter, namely, Liouville's theorem¹

$$\frac{d\rho}{dt} = 0.$$

Undoing some of the work we did to arrive to this equation, we can expand the total time derivative as

$$\begin{split} \frac{d\rho}{dt} &= \sum_{k} \left(\frac{\partial \rho}{\partial q_{k}} q_{k}' + \frac{\partial \rho}{\partial p_{k}} p_{k}' \right) + \frac{\partial \rho}{\partial t} \\ &= \sum_{k} \left(\frac{\partial \rho}{\partial q_{k}} \frac{\partial H}{\partial p_{k}} - \frac{\partial \rho}{\partial p_{k}} \frac{\partial H}{\partial q_{k}} \right) + \frac{\partial \rho}{\partial t} \\ &\equiv \left[\rho, H \right] + \frac{\partial \rho}{\partial t} \,, \end{split}$$

where we have introduced the **Poisson bracket** $[\rho, H]$, which is defined, in general, as

$$F,G] = \sum_{k} \left(\frac{\partial F}{\partial q_{k}} \frac{\partial G}{\partial p_{k}} - \frac{\partial F}{\partial p_{k}} \frac{\partial G}{\partial q_{k}} \right).$$

Poisson brackets turn out to be very useful, as we will see next.

Properties of Poisson brackets

From the definition of Poisson bracket, one can prove the following properties:²

- [F,G] = -[G,F], that is, the Poisson bracket is antisymmetric.³
- [F, F] = 0.

¹ This is just an excuse. As we will see, Poisson brackets can be defined without any mention to Liouville's theorem! This is just one context in which they are convenient.

² Exercise: Do it!

³ Poisson brackets have a direct connection to commutators in quantum mechanics, which are at the root of, for example, Heisenberg's uncertainty principle.

- If a is a constant, [a, F] = 0.
- $[F_1 + F_2, G] = [F_1, G] + [F_2, G].$
- $[F_1F_2, G] = F_1[F_2, G] + F_2[F_1, G].$
- $[F_1, [F_2, F_3]] + [F_2, [F_3, F_1]] + [F_3, [F_1, F_2]] = 0$. This property is known as Jacobi's identity.

Poisson brackets and time evolution

We have seen, from Liouville's theorem, that the total time derivative of the density ρ is given by $d\rho/dt = [\rho, H] + \partial \rho/\partial t$, where H is the Hamiltonian of the system. However, it is immediate to see from the derivation above that there is nothing special about ρ , in there. Indeed, for any function $F(\mathbf{q}, \mathbf{p}, t)$, we can write its equation of motion

$$\frac{d}{dt}F(\mathbf{q},\mathbf{p},t) = [F,H] + \frac{\partial F}{\partial t}.$$

Additionally, if $F = F(\mathbf{q}, \mathbf{p})$ does *not* depend explicitly on time

$$\frac{d}{dt}F(\mathbf{q},\mathbf{p})=\left[F,H\right],$$

which means that the time evolution of any function that depends only on the position in phase space (but not time) is given, simply, by the Poisson bracket of the function with the Hamiltonian. In other words, the Hamiltonian is the generator of time evolution.

This is true, in particular, for positions and momenta themselves, namely,

$$q_i' = \frac{dq_i}{dt} = [q_i, H]$$
 and $p_i' = \frac{dp_i}{dt} = [p_i, H]$,

which are, precisely, Hamilton's canonical equations.⁴ So, by taking as axioms the properties of Poisson brackets enumerated above, Hamiltonian mechanics (and, therefore, Lagrangian and Newtonian mechanics) can be fully formulated in terms of Poisson brackets alone!

⁴ Note that the sign difference is buried into the definition of the Poisson bracket.

Poisson brackets and generators: Symmetry and conservation

We have already seen that, with the help of Poisson brackets, we can regard the Hamiltonian as a generator of change in time⁵

$$\frac{d}{dt}F(\mathbf{q},\mathbf{p})=[F,H],$$

which means that the Poisson bracket of $F(\mathbf{q}, \mathbf{p})$ with the Hamiltonian gives the time variation of *F*.

Now note that, loosely speaking, time is the "conjugate coordinate" of the Hamiltonian (or, even more loosely, energy). For example, we saw that H is conserved when t does not appear in the

⁵ Let us insist that this is true if, and only if, F is does not depend explicitly on time.

Lagrangian, much in the same way that the generalized momentum p_i is conserved when q_i does not appear in the Lagrangian. So could it be that, in general, the Poisson bracket of a function with a coordinate/momentum gives the variation along the conjugate momentum/coordinate? Indeed from the definition of Poisson bracket, one can easily prove that

$$[F, q_i] = -\frac{\partial F}{\partial p_i}$$
 and $[F, p_i] = \frac{\partial F}{\partial q_i}$.

Fantastic! Let's see what this means: Consider how momenta act on coordinates in general

$$[q_j, p_i] = \frac{\partial q_j}{\partial q_i} = \delta_{ij}.$$

This means that momentum in the i "direction" does not do anything to coordinates in the $j \neq i$ direction, but it *moves* the *i* coordinate by 1 unit. This is true for any generalized coordinate. In Cartesian coordinates, the linear momentum p_x moves the x coordinate but leaves the others unchanged. In polar coordinates, angular momentum moves the corresponding angle. Less obviously, let's see what angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ and, in particular, its z component $L_z = xp_y - yp_x$, does to Cartesian coordinates:6

$$[x, L_z] = [x, xp_y - yp_x] = -y$$

 $[y, L_z] = [y, xp_y - yp_x] = x$
 $[z, L_z] = [z, xp_y - yp_x] = 0$

But, what is this? This is just (proportional to) the first order of a rotation in the xy plane!7

Therefore, we can regard generalized momenta as generators of translations of the generalized coordinates.⁸ From this perspective, what is the meaning of $[H, p_i]$? It is the change in the Hamiltonian due to the change in the coordinates q_i generated by p_i

$$[H, p_i] = \frac{\partial H}{\partial q_i}$$

When this is $[H, p_i] = 0$, it means that the Hamiltonian does not depend on q_i , that is, that the Hamiltonian is symmetric. At the same time $dp_i/dt = [p_i, H_i] = -[H, p_i] = 0$ means that p_i does not change in time, namely, that it is conserved. In this way, the connection between symmetries and conservation appears as an immediate consequence of the properties of Poisson brackets. In general, for an arbitrary generator G, [G, H] tells us both how G changes in time, and about how H changes under the transformation generated by G.

⁶ Do it from the definition of Poisson brackets and from the properties of Poisson brackets!

⁷ Remember, for small angles ϵ , in a rotation we have $x \to x \cos \epsilon - y \sin \epsilon \approx$ $-y\epsilon$ and $y \to x \sin \epsilon + y \cos \epsilon \approx x\epsilon$.

⁸ Mutatis mutandi, we can regard coordinates as generators of changes in momenta.

Poisson brackets and constants of motion

The considerations above lead us to realize that the properties of Poisson brackets allow us to **immediately identify constants of motion** of a system from its Hamiltonian. Let's see:

• As we have seen (and as we already knew from Lagrangian mechanics), if a coordinate does not appear in the Hamiltonian, the corresponding momentum is conserved because

$$\frac{dp_i}{dt} = [p_i, H] = -[H, p_i] = -\frac{\partial H}{\partial q_i} = 0.$$

• If all the dependencies of the Hamiltonian on q_1 and p_1 can be grouped in a single function $g(q_1, p_1)$ that does not depend explicitly on time

$$H = H(g(q_1, p_1), q_2, \dots, p_N, t)$$

then g is also a constant of motion. Indeed,

$$\frac{dg}{dt} = [g, H] = \frac{\partial g}{\partial q_1} \frac{\partial H}{\partial p_1} - \frac{\partial g}{\partial p_1} \frac{\partial H}{\partial q_1} = \frac{\partial g}{\partial q_1} \frac{\partial H}{\partial g} \frac{\partial g}{\partial p_1} - \frac{\partial g}{\partial p_1} \frac{\partial H}{\partial g} \frac{\partial g}{\partial q_1} = 0.$$

 As an extension to the previous property, if k coordinates and momenta are contained in a function g

$$H = H(g(q_1, ..., p_k, p_1, ..., p_k), q_{k+1}, ..., p_N, t)$$

then g is also a constant of motion.

Additionally, Poisson brackets can be used to **generate new constants of motion from known ones**. In particular, so-called **Poisson's theorem** states that if F and G are constants of motion, then [F,G] is also a constant of motion. The new constant could be trivial, like $[p_i,q_i]=1$ or a combination such as F+G, but sometimes it is a genuinely new constant of motion.

Poisson's theorem holds both for functions (F and G) that depend explicitly on time and those that do not. The proof for functions that do not depend explicitly on time is particularly beautiful because it can be carried out using the properties of Poisson brackets alone. Indeed, for $F(\mathbf{q}, \mathbf{p})$ and $Q(\mathbf{q}, \mathbf{p})$ (without explicit time dependence), the fact that F and G are constants of motion implies that [F, H] = 0 and [G, H] = 0. Additionally, proving that [F, G] is also a constant of motion amounts to proving that [F, G], H] = 0. But using the antisymmetric property of Poisson brackets and Jacobi's identity this is easy:

$$[[F,G],H] = -[H,[F,G]] = [F,[G,H]] + [G,[H,F]] = [F,0] + [G,0] = 0$$

⁹ Do the proof for functions that depend explicitly on time.

Canonical transformations

From a theoretical point of view, the Poisson bracket formalism emphasizes the symmetric roles played by coordinates and momenta in Hamiltonian mechanics. This suggests that the elementary identification of generalized coordinates with positions and generalized momenta with velocities is not essential in the formulation of mechanics. In view of this, it is natural to consider general transformations of phase space coordinates (q, p) to new coordinates (Q, P). Indeed, whereas in Lagrangian mechanics we only considered changes of coordinates of the form $Q_i = Q_i(\mathbf{q}, t)$, called **point transformations**, we are now led to consider more general transformations, known as contact transformations

$$Q_i = Q_i(\mathbf{q}, \mathbf{p}, t)$$
 and $P_i = P_i(\mathbf{q}, \mathbf{p}, t)$.

We interpret this transformation in passive way, as a relabeling of each and all points in phase space.

We now aim to derive the conditions for this general transformation to ensure that it leaves Hamilton's equations of motion invariant for all possible Hamiltonians. That is, we seek transformations that guarantee that there exists a new Hamiltonian $\tilde{H}(Q, P)$ such that

$$Q_i' = \frac{\partial \tilde{H}}{\partial P_i}$$
 and $P_i' = -\frac{\partial \tilde{H}}{\partial Q_i}$.

We call the transformations satisfying this condition canonical transformations.

Let's now see what conditions need to be fulfilled for a transformation to be canonical, and how can we generate them. Considering the variational principle that leads to the Euler-Lagrange and Hamilton's equations, written in terms of (q, p) and (Q, P), respectively, we have that 10

$$\delta \int_{t_1}^{t_2} dt \left[\sum_i p_i q_i' - H(q, p, t) \right] = 0$$

$$\delta \int_{t_1}^{t_2} dt \left[\sum_i P_i Q_i' - \tilde{H}(Q, P, t) \right] = 0.$$

If this variational principle is to hold for all trajectories, we have that in general the two integrands can differ only by the total time derivative of a function *F*, that is

$$\sum_{i} p_{i} q'_{i} - H(q, p, t) = \sum_{i} P_{i} Q'_{i} - \tilde{H}(Q, P, t) + \frac{dF}{dt}.$$
 (1)

This is a sufficient condition for form invariance of the Hamiltonian equations of motion; as we will see, it will also tell us how to define the new Hamiltonian \tilde{H} .

¹⁰ There is a non-trivial subtlety here, related to the fact that Hamilton's principle applies to variations that leave trajectories invariant at the endpoints t_1 and t_2 , something that cannot be guaranteed here. So rather than Hamilton's principle, here we are really using the Weiss action principle. In any case, being a bit cavalier about this subtlety leads to the correct results, so...

We call F the **generating function** of the transformation.¹¹ It generates a new but equivalent Hamiltonian (or Lagrangian) from the original one, but we think of a canonical transformation as associated with a given form of *F*, rather than to a particular physical system. Generating functions must mix some of the old phase space coordinates (q, p) with some of the new (Q, P). Based on this, we define four types of generating function¹²

$$F_{1} = F_{1}(q, Q, t),$$

$$F_{2} = F_{2}(q, P, t),$$

$$F_{3} = F_{3}(p, Q, t),$$

$$F_{4} = F_{4}(p, P, t).$$

Let's consider $F = F_1(q, Q, t)$ first. Take Eq. (1) and expand the total time derivative of $F_1(q, Q, t)$

$$\sum_{i} p_{i} q_{i}' - H(q, p, t) = \sum_{i} P_{i} Q_{i}' - \tilde{H}(Q, P, t) + \sum_{i} \frac{\partial F_{1}}{\partial q_{i}} q_{i}' + \sum_{i} \frac{\partial F_{1}}{\partial Q_{i}} Q_{i}' + \frac{\partial F_{1}}{\partial t}.$$

Now, because the Hamiltonians do not depend explicitly on velocities, the terms on q'_i and Q'_i must cancel out, which gives

$$p_i = \frac{\partial F_1}{\partial q_i}$$
 and $P_i = -\frac{\partial F_1}{\partial Q_i}$,

with the remaining terms giving the equation that specifies how the Hamiltonian must be transformed

$$\tilde{H}(Q,P,t) = H(p(Q,P),q(Q,P),t) + \frac{\partial}{\partial t}F_1(q(Q,P),Q,t).$$

Notice that this amounts to just replacing q(Q, P) and p(Q, P) in the original Hamiltonian and, if F_1 depends explicitly on time, adding the partial $\partial F_1/\partial t$.

From the previous derivation we see that the fact that F_1 is a function of q_i and Q_i is crucial for canceling the terms with q'_i and Q'_i in the Lagrangian. Therefore, we obtain the equations for the remaining types of generating functions by regarding F = F(q, Q, t) as a Legendre transform of $F_{i\neq 1}$.

FOR
$$F_2 = F_2(q, P, t)$$
 we use $F = F_2(q, P, t) - \sum_i Q_i P_i$. Then

$$\frac{dF}{dt} = \sum_{i} \frac{\partial F_2}{\partial q_i} q_i' + \sum_{i} \frac{\partial F_2}{\partial P_i} P_i' + \frac{\partial F_2}{\partial t} - \sum_{i} P_i' Q_i - \sum_{i} P_i Q_i'$$

and, plugging this into Eq. (1) and identifying terms, we get

$$p_i = \frac{\partial F_2}{\partial q_i}$$
 , $Q_i = \frac{\partial F_2}{\partial P_i}$ and $\tilde{H} = H + \frac{\partial F_2}{\partial t}$.

11 Important: Many, but not all, functions F are acceptable generating functions. A necessary and sufficient condition for the generating function to be valid is that its crossed second derivatives do not vanish. For example, if F = F(q, Q, t), then we must have $\partial^2 F/\partial q\partial Q \neq 0$.

12 For simplicity, from now on we consider a system with one degree of freedom.

¹³ Note that we choose a minus sign for the $\sum_{i} Q_{i} P_{i}$ term so that, once we take the time derivative, it cancels the $\sum_{i} P_{i} Q'_{i}$ term in the Lagrangian.

For $F_3 = F_3(p, Q, t)$ we use $F = F_3(p, Q, t) + \sum_i p_i q_i$.¹⁴ Then

$$\frac{dF}{dt} = \sum_{i} \frac{\partial F_3}{\partial p_i} p_i' + \sum_{i} \frac{\partial F_3}{\partial Q_i} Q_i' + \frac{\partial F_3}{\partial t} + \sum_{i} p_i' q_i + \sum_{i} p_i q_i'$$

and, again plugging this into Eq. (1) and identifying terms, we get

$$q_i = -rac{\partial F_3}{\partial p_i}$$
 , $P_i = -rac{\partial F_3}{\partial Q_i}$ and $\tilde{H} = H + rac{\partial F_3}{\partial t}$.

Finally, for $F_4 = F_4(p, P, t)$ we use $F = F_4(p, P, t) + \sum_i p_i q_i$ $\sum_{i} P_{i}Q_{i}$. Then

$$\frac{dF}{dt} = \sum_{i} \frac{\partial F_4}{\partial p_i} p_i' + \sum_{i} \frac{\partial F_4}{\partial P_i} P_i' + \frac{\partial F_4}{\partial t} + \sum_{i} p_i' q_i + \sum_{i} p_i q_i' - \sum_{i} P_i' Q_i - \sum_{i} P_i Q_i'$$

and, plugging this one last time into Eq. (1) and identifying terms, we get

$$q_i = -\frac{\partial F_4}{\partial p_i}$$
 , $Q_i = \frac{\partial F_4}{\partial P_i}$ and $\tilde{H} = H + \frac{\partial F_4}{\partial t}$.

In Table 1, we summarize the above results for easy access.

Generating function	Implicit transformation equations		
$F_1(q,Q,t)$	$p_i = \frac{\partial F_1}{\partial q_i}$	$P_i = -\frac{\partial F_1}{\partial Q_i}$	$\tilde{H} = H + \frac{\partial F_1}{\partial t}$
$F_2(q, P, t)$	$p_i = \frac{\partial F_2}{\partial q_i}$	$Q_i = \frac{\partial F_2}{\partial P_i}$	$\tilde{H} = H + \frac{\partial F_2}{\partial t}$
$F_3(p,Q,t)$	$q_i = -\frac{\partial F_3}{\partial p_i}$	$P_i = -\frac{\partial F_3}{\partial Q_i}$	$\tilde{H} = H + \frac{\partial F_3}{\partial t}$
$F_4(p, P, t)$	$q_i = -\frac{\partial F_4}{\partial p_i}$	$Q_i = \frac{\partial F_4}{\partial P_i}$	$\tilde{H} = H + \frac{\partial F_4}{\partial t}$

Example: Permutation transformation. Consider the canonical transformation given by the generating function

$$F_1 = q_i Q_i$$

Then, by applying the implicit transformation equations in Table 1, we get

$$p_i = \frac{\partial F_1}{\partial q_i} = Q_i$$
 and $P_i = -\frac{\partial F_1}{\partial Q_i} = -q_i$,

which means that, except for a minus sign, the roles of coordinates and momenta are exchanged by this canonical transformation. Now, this will not be useful at all in terms of integrating the equations of motion (of course, the resulting Hamiltonian will have the same form as before!), but it is useful to emphasize that coordinates and momenta loose their meaning as "positions" and "velocities."

14 Here we need a plus sign in front of the $\sum_i p_i q_i$ term because it has to cancel the $\sum_i p_i q_i'$ in the left hand side of the equation.

Table 1: Lookup table of possible generating functions for canonical transformations.

This may all seem very convoluted but, as shown in the previous example, in practice transforming a problem using a Canonical transformation is quite straightforward:

- 1. Specify a generating function (or, often, take a generating function that is given to you).
- 2. Use the Implicit transformations in Table 1 to solve for $q_i(Q, P, t)$ and $p_i(Q, P, t)$.
- 3. Obtain \tilde{H} by replacing in H (and, if necessary, adding the explicit temporal dependency in the generating function).

Example: Harmonic oscillator. We use the canonical transformation generated by the F_1 -type function¹⁵

$$F(q,Q) = \frac{1}{2}\omega q^2 \cot 2\pi Q$$

to find the equations of motion for the harmonic oscillator, whose Hamiltonian is

$$H(q,p) = \frac{1}{2} \left(p^2 + \omega^2 q^2 \right) .$$

By applying the transformation equations we get¹⁶

$$p = \frac{\partial F}{\partial q} = \omega q \cot 2\pi Q,$$

$$P = -\frac{\partial F}{\partial Q} = \frac{\pi \omega q^2}{\sin^2 2\pi O}.$$

From here, we solve for q(Q, P) and p(Q, P) to get¹⁷

$$q=\sqrt{\frac{P}{\pi\omega}}\sin 2\pi Q\,,$$

$$p = \sqrt{\frac{\omega P}{\pi}} \cos 2\pi Q.$$

Finally, by replacing in H(q, p) we obtain ¹⁸

$$\tilde{H} = \frac{\omega}{2\pi} P.$$

Isn't this Hamiltonian beautiful?! Of course, since Q is a cyclical coordinate, P is a constant of motion. For Q, Hamilton's equation tells us that

$$Q' = \frac{\partial \tilde{H}}{\partial P} = \frac{\omega}{2\pi},$$

which, aside from integration constants, gives

$$Q = \frac{\omega}{2\pi}t.$$

¹⁵ Which we obtained by careful analysis of a crystal ball.

16 Exercise: Do it!

¹⁷ Exercise: Do it!

18 Exercise: Do it!

Last, we can replace into p(Q, P) to obtain, in terms of the constant of motion P,

$$q = \sqrt{\frac{P}{\pi\omega}} \sin \omega t.$$

Canonical transformations and Poisson brackets

We are finally ready to provide another important and practical property of Poisson brackets, in relation to canonical transformations. It turns out that, if (Q, P) are a set of variables related by a canonical transformation to (q, p), then

$$[\tilde{F}, \tilde{G}]_{Q,P} = [F, G]_{q,p}$$
.

In particular,

$$[Q_i, Q_j]_{q,p} = 0$$
, $[P_i, P_j]_{q,p} = 0$, $[Q_i, P_j]_{q,p} = \delta_{ij}$.

These turn out to be necessary and sufficient conditions for the **transformation** $(q, p) \rightarrow (Q, P)$ **being canonical**. When we doubt about a transformation being canonical, verifying this property is a conclusive proof.

Hamilton-Jacobi equation

To conclude, we consider one very special canonical transformation that leads to yet another formulation of classical mechanics (besides the Newtonian, Lagrangian, and Hamiltonian). This new formulation is important because it is the one that leads more naturally to the Schrödinger equation and quantum mechanics.

Assume that there exists a canonical transformation for which the transformed Hamiltonian is identically zero, $\tilde{H} = 0$. Then, we have that

$$\tilde{H}(Q_1,\ldots,Q_n,P_1,\ldots,P_n)=0=H(q_1,\ldots,q_n,p_1,\ldots,p_n)+\frac{\partial F}{\partial t}$$

or

$$H(q_1,\ldots,q_n,p_1,\ldots,p_n)=-\frac{\partial F}{\partial t}.$$

Since the transformed variables Q_i and P_i are all constants (because Q'=0 and P'=0), the information about the time evolution of the system is contained in the transformation itself. Assume that there is a generating function of the second type

 $S \equiv F_2(q_1, \dots, q_n, P_1, \dots, P_n, t)$ that generates the desired canonical transformation.¹⁹ Then²⁰ $p_i = \partial S/\partial q_i$ and we arrive to the

Hamilton-Jacobi equation

$$H\left(q_1,\ldots,q_n,\frac{\partial S}{\partial q_1},\ldots,\frac{\partial S}{\partial q_n}\right)=-\frac{\partial S}{\partial t}.$$

¹⁹ This special generating function *S* is called Hamilton's principal function.

²⁰ See Table. 1.

The Lagrangian formulation leads to a system of *n* second-order differential equations, the Euler-Lagrange equations; the Hamiltonian formulation leads to a system of 2n first-order differential equations, Hamilton's canonical equations. Now, the Hamilton-Jacobi equation is a single differential equation in n+1 independent variables (q_i and t) and their derivatives. Learning how to solve this equation is beyond the scope of this course, but one example may help to give some key ideas.

Example: Hamilton-Jacobi for a falling mass. The Hamiltonian of a free falling mass *m* is

$$H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + mgz,$$

where p_i is the conjugate momentum of the particle in the *i*th direction. Then, the corresponding Hamilton-Jacobi equation is

$$\frac{1}{2m}\left(\left(\frac{\partial S}{\partial x}\right)^2 + \left(\frac{\partial S}{\partial y}\right)^2 + \left(\frac{\partial S}{\partial z}\right)^2\right) + mgz = -\frac{\partial S}{\partial t}.$$

This equation can be integrated easily by noting that *S* can be separated into terms, each depending only on one direction

$$S = W_1(x) + W_2(y) + W_3(z) - Et$$
,

where E is a constant.²¹

We finish with the promised connection to quantum MECHANICS. The special generating function $S(\mathbf{q},t)$ is a function of the coordinates q_i and time. The surfaces $S(\mathbf{q}, t) = \text{constant}$ can be regarded as wave fronts that move in coordinate space because of the time dependency of S.^{22,23} The historical motivation for the Hamilton-Jacobi equation was precisely to exploit this analogy between optics and mechanics.²⁴ Indeed, the propagation of light through a medium with variable index of refraction is described by an equation exactly like the Hamilton-Jacobi equation.²⁵ In this analogy, S can be regarded as the phase of the wave.

Now, consider the Schrödinger equation, which describes the quantum evolution of the wave function ψ of a particle in 1D under an arbitrary potential V(x)

$$H\psi = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = i\hbar\frac{\partial\psi}{\partial t}.$$

Assuming, based on the analogy, that *S* is proportional to the phase of the wave function

$$\psi = \sqrt{\rho(x,t)} \exp \left[\frac{iS(x,t)}{\hbar}\right],$$

21 Go ahead and solve the Hamilton-Jacobi equation in this case!

- 22 As we have seen in the example of the falling particle, if the Hamiltonian is conserved, then surfaces of constant S move due to the term Et.
- ²³ Momenta are proportional to the gradient of S in configuration space, so trajectories are perpendicular to wave fronts.
- ²⁴ Classical mechanics is to quantum mechanics as geometric optics is to wave optics.
- ²⁵ In the study of wave propagation, an eikonal equation is an equation of the form $H(\mathbf{x}, \nabla u(\mathbf{x})) = 0$.

replacing into the Schrödinger equation, and taking the limit $\hbar \to 0$, we get the Hamilton-Jacobi equation

$$\frac{1}{2m} \left(\frac{\partial S}{\partial x} \right)^2 + V(x) = -\frac{\partial S}{\partial t}.$$