

# Week 11

PHY 305 Classical Mechanics

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*These notes are provided for the students of the class above only. There is no guarantee for correctness, please contact me if you spot a mistake.*

## 4.5 Canonical transformations

We had stated in section 2.5 that Lagrange's equations take the same form for any choice of coordinates, which is essentially because the statement on which they are founded, "that the action is stationary at the physical path", does not care about in which coordinates we express the action.

Hamilton's equation now allow us to make this powerful feature even more powerful, but placing  $\mathbf{q}$  and  $\mathbf{p}$  on the same footing. We can then define a

**Canonical transformation** of our phase-space variables  $\mathbf{q}$  and  $\mathbf{p}$ , into new coordinates  $\mathbf{Q}$  and  $\mathbf{P}$

$$\begin{aligned}\mathbf{Q} &= \mathbf{Q}(\mathbf{q}, \mathbf{p}, t), \\ \mathbf{P} &= \mathbf{P}(\mathbf{q}, \mathbf{p}, t),\end{aligned}\tag{4.30}$$

which must be such that they leave Hamilton's equations invariant, i.e. they should still be

$$\dot{Q}_k = \frac{\partial \mathcal{K}}{\partial P_k}, \quad \dot{P}_k = -\frac{\partial \mathcal{K}}{\partial Q_k},\tag{4.31}$$

where  $\mathcal{K}(Q, P)$  is a new Hamiltonian.

- Importantly, this goes beyond your usual concept of "co-ordinate transformations", by allowing one to mix momentum and position coordinates. While the new ones are still segregated into "positions  $Q$ " and "momenta  $P$ " depending on their evolution equation (plus or minus), they no longer need to have a clear interpretation as positions or momenta.
- The reason we want the transformation to preserve the form of Hamilton's equations, is that then all earlier conclusions, for example about the structure of phase-space in section 4.4 and many you see later in week11 remain unchanged.
- A possible use for canonical transformations is reach a simpler Hamiltonian. We could for example try to render all new coordinates  $Q$  cyclic. According to section 4.3 we then know that all their associated momenta  $P$  are conserved. This, in turn, according to section 4.4.2 implies that the system is integrable and its dynamics regular (see later).

- Finding out which transformations (4.30) are canonical is tricky. There are two main approaches discussed in the books, for which it is useful that you have heard the names: (i) Finding the transformation via so-called generating functions. (ii) Identifying the right transformation by their need to be symplectic, which means that their Jacobian leave a certain high dimensional matrix invariant. We list some more optional info on item (i) in section 4.5.1, but lets first look at an example that illustrates a possible use of canonical transformations, and how they can mix positions and momenta.

**Example 43, Canonical transformation of the simple harmonic oscillator:**

Let's consider the simple harmonic oscillator with Hamiltonian  $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2$ . Let us define

$$\begin{aligned} p &= \sqrt{2Pm\omega} \cos Q, \\ q &= \sqrt{\frac{2P}{m\omega}} \sin Q. \end{aligned} \quad (4.32)$$

Inserting these into the Hamiltonian we get

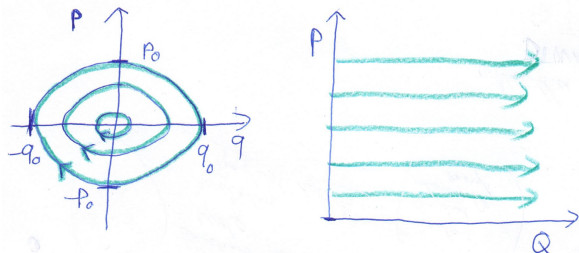
$$\mathcal{K} = \mathcal{H} = \frac{2m\omega P}{2m} (\cos^2 Q + \sin^2 Q) = \omega P, \quad (4.33)$$

hence this has made all coordinates cyclic.

Hence trivially  $\dot{P} = -\frac{\partial \mathcal{K}}{\partial Q} = 0$  and  $\dot{Q} = \omega$ , which is solved by  $Q(t) = Q(0) + \omega t$ . Let's pick  $Q(0) = 0$  and insert back into Eq. (4.32), then we have reached

$$\begin{aligned} p(t) &= \sqrt{2P(0)m\omega} \cos(\omega t), \\ q(t) &= \sqrt{\frac{2P(0)}{m\omega}} \sin(\omega t). \end{aligned} \quad (4.34)$$

which is the correct solution of the SHO for energy  $E = \omega P(0)$ . We hence now know that Eq. (4.32) was a valid canonical transformation, which we had skipped to show. All statements regarding Hamiltonian systems remain valid in the new coordinates, e.g. phase-space trajectories do not cross.



**left:** Phase space of the harmonic oscillator in the usual coordinates  $(p, q)$  on the left and the new coordinates  $(P, Q)$ . The phase space flow has been made super easy in the new ones, which was the whole point of defining them.

To draw the contour lines in the old coordinates, we use  $1 = (p/p_0)^2 + (q/q_0)^2$  with  $p_0 = \sqrt{2mE}$  and  $q_0 = \sqrt{2E/m/\omega^2}$ , which tells us the trajectory must look elliptical. The equation follows from energy conservation.

**Example continued:** This is an example of what are called action-angle variables, since  $Q = \omega t$  is an angle (argument of  $\cos$ ) and  $P$  has dimensions of an action as seen from Eq. (4.33). It can be a general strategy for the solution of mechanical problems to use a canonical transformation to make all variables action-angle variables.

### 4.5.1 Generating functions

In the above, we have not yet really discussed how one would actually make sure a given transformation is canonical. Since the requirement is for them to leave Hamilton's equations structurally unchanged, Hamilton's equations are based on Lagrange's equations, and Lagrange's equations are based on a stationary action (2.22), we know that we should get Hamilton's equations in terms of new canonical coordinates  $Q, P$  as long as these also fulfill the same variational principle:

$$\begin{aligned}
 0 = \delta S &= \delta \int_{t_1}^{t_2} \mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}, t) dt \Leftrightarrow \\
 0 = \delta S &= \delta \int_{t_1}^{t_2} [\mathbf{p} \cdot \dot{\mathbf{q}} - \mathcal{H}(\mathbf{p}, \mathbf{q}, t)] dt \\
 0 = \delta \bar{S} &= \delta \int_{t_1}^{t_2} [\mathbf{P} \cdot \dot{\mathbf{Q}} - \mathcal{K}(\mathbf{P}, \dot{\mathbf{Q}}, t)] dt
 \end{aligned} \tag{4.35}$$

Clearly the third line would follow from the second, if  $\mathbf{p} \cdot \dot{\mathbf{q}} - \mathcal{H}(\mathbf{p}, \mathbf{q}, t) = \mathbf{P} \cdot \dot{\mathbf{Q}} - \mathcal{K}(\mathbf{P}, \dot{\mathbf{Q}}, t)$ , however it turns out that would be a too strong constraint: You can see that we can add the time-derivative of a function  $F(\mathbf{q}, \mathbf{Q})$  into the varied integrand without changing the statement:

$$0 = \delta \bar{S} = \delta \int_{t_1}^{t_2} [\mathbf{P} \cdot \dot{\mathbf{Q}} - \mathcal{K}(\mathbf{P}, \dot{\mathbf{Q}}, t) + \frac{dF(\mathbf{q}, \mathbf{Q})}{dt}] dt. \tag{4.36}$$

Since time derivative and integration cancel each other, variation of the last term amounts to  $\delta[F(\mathbf{q}(t_2), \mathbf{Q}(t_2)) - F(\mathbf{q}(t_1), \mathbf{Q}(t_1))]$ . However in section 2.5.1 we have kept the variation of the path zero at the endpoint (endpoints are fixed), so this expression vanishes. We hence require

$$\begin{aligned}
 \mathbf{p} \cdot \dot{\mathbf{q}} - \mathcal{H}(\mathbf{p}, \mathbf{q}, t) &= \mathbf{P} \cdot \dot{\mathbf{Q}} - \mathcal{K}(\mathbf{P}, \dot{\mathbf{Q}}, t) + \frac{dF(\mathbf{q}, \mathbf{Q})}{dt} \\
 \mathbf{p} \cdot \dot{\mathbf{q}} - \mathcal{H}(\mathbf{p}, \mathbf{q}, t) &= \mathbf{P} \cdot \dot{\mathbf{Q}} - \mathcal{K}(\mathbf{P}, \dot{\mathbf{Q}}, t) + \frac{\partial F(\mathbf{q}, \mathbf{Q})}{\partial \mathbf{q}} \dot{\mathbf{q}} + \frac{\partial F(\mathbf{q}, \mathbf{Q})}{\partial \mathbf{Q}} \dot{\mathbf{Q}} + \frac{\partial F(\mathbf{q}, \mathbf{Q})}{\partial t} \Leftrightarrow \\
 (\mathbf{p} - \frac{\partial F(\mathbf{q}, \mathbf{Q})}{\partial \mathbf{q}}) \dot{\mathbf{q}} - (\mathbf{P} + \frac{\partial F(\mathbf{q}, \mathbf{Q})}{\partial \mathbf{Q}}) \dot{\mathbf{Q}} &= \mathcal{H} - \mathcal{K} + \frac{\partial F(\mathbf{q}, \mathbf{Q})}{\partial t}.
 \end{aligned} \tag{4.37}$$

This equation is true if  $\mathbf{p} = \frac{\partial F(\mathbf{q}, \mathbf{Q})}{\partial \mathbf{q}}$  and  $\mathbf{P} = -\frac{\partial F(\mathbf{q}, \mathbf{Q})}{\partial \mathbf{Q}}$  and  $\mathcal{K} = \mathcal{H} + \frac{\partial F(\mathbf{q}, \mathbf{Q})}{\partial t}$ .

Now it turns out, for the right of choice of  $F$  this function provides a very useful trick in establishing canonical transformations, hence it gets a name:

**Generating function** The function  $F(\mathbf{q}, \mathbf{Q})$  that depends on the new and old coordinates in a canonical transformation is called generating function of the transformation. It is specific for one transformation, makes sure the transformation is canonical, and provides us with a formal (not necessarily practical) recipe to find  $\mathbf{Q}$  and  $\mathbf{P}$  in terms of  $\mathbf{q}$   $\mathbf{p}$  and the new Hamiltonian through

$$\mathbf{p} = \frac{\partial F(\mathbf{q}, \mathbf{Q})}{\partial \mathbf{q}}, \quad \mathbf{P} = -\frac{\partial F(\mathbf{q}, \mathbf{Q})}{\partial \mathbf{Q}}, \quad \mathcal{K} = \mathcal{H} + \frac{\partial F(\mathbf{q}, \mathbf{Q})}{\partial t}. \quad (4.38)$$

- The generating function  $F$  is useful, if we can invert Eq. (4.38) to provide the relations (4.30), i.e.  $P$  and  $Q$  in terms of  $p$  and  $q$ .
- There is much more technical details on generating functions to be found in many books, we attempt to by-pass them here mostly, but require them for the presentation of Hamilton-Jacobi theory in week11.
- Here we have discussed only a generating function of the form  $F(\mathbf{q}, \mathbf{Q})$ . It turns out one can also find ones of the form  $F(\mathbf{q}, \mathbf{P})$ ,  $F(\mathbf{p}, \mathbf{Q})$ ,  $F(\mathbf{p}, \mathbf{P})$ . If these are need relations (4.38) get replaced by similar ones yielding the two missing variables.

**Example 44, Generating function:** for the simple harmonic oscillator transformation in example 43: We can use

$$F(q, Q) = \frac{m\omega}{2} q^2 \cot Q. \quad (4.39)$$

We can see based on Eq. (4.38) that we recover the same  $P$  and  $Q$  as used earlier. This adds nothing new to the earlier example, but justifies how we could know that it was a canonical transformation.

## 4.6 Classical foundations of quantum mechanics

Perhaps one of the most important uses of Hamiltonian mechanics, is that it provides the structural basis on which quantum mechanics was formulated. You of course know already that, the classical Hamiltonian function, e.g. (4.7) gets replaced in quantum theory by the corresponding Hamiltonian operator  $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q})$ . It looks deceptively similar, however now all classical canonical variables have been replaced by operators. In this section we see that there are many more directly analogous concepts.<sup>11</sup>

Besides an additional understanding of why quantum mechanics takes the mathematical structure it does, the material here also helps to work out how much of quantum mechanics is actually classical mechanics in disguise. This is true for many phenomena, while some others of course are genuine “quantum-only” phenomena based on particles being in fact waves.

<sup>11</sup>A lot of the material in this week was inspired so strongly by the lecture note of Prof. David Tong at Cambridge University, that I should acknowledge [the source](#) .

### 4.6.1 Poisson brackets

We start this exploration by returning to phase-space section 4.4 and investigating the following definition of a

**Poisson bracket** Suppose we have two functions  $f(\mathbf{q}, \mathbf{p})$  and  $g(\mathbf{q}, \mathbf{p})$  of the  $M$  dimensional phase space variables. We then define the “Poisson bracket of  $f$  and  $g$ ” as

$$\{f, g\} = \sum_n \frac{\partial f}{\partial q_n} \frac{\partial f}{\partial p_n} - \frac{\partial g}{\partial q_n} \frac{\partial g}{\partial p_n}. \quad (4.40)$$

- From the definition (4.40), you can show the following properties

- (i)  $\{f, g\} = -\{g, f\}$ .
- (ii) Linearity  $\{\alpha f + \beta h, g\} = \alpha\{f, g\} + \beta\{h, g\}$ , where  $\alpha, \beta$  are constants.
- (iii) Leibnitz rule:  $\{fg, h\} = f\{g, h\} + \{f, h\}g$ .
- (iv) Jacobi identity:  $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$ .

You realize that these are exactly the same algebraic properties as for the quantum-mechanical commutator  $[\hat{A}, \hat{B}]$  of two operators.

- Following the latter even further, we see that when we choose  $f$  and  $g$  as the coordinates themselves, we reach

$$\begin{aligned} \{q_n, q_m\} &= 0, \\ \{p_n, p_m\} &= 0, \\ \{q_n, p_m\} &= \delta_{nm}, \end{aligned} \quad (4.41)$$

which are strongly reminiscent of the commutation relations of position operators  $\hat{q}_m$  and momentum operators  $\hat{p}_k$ .

This is no co-incidence, but caused by the procedure of

**Canonical quantisation** When constructing a quantum theory from a classical theory we replace function  $f, g$  by operators such that the commutation relations follow the classical Poisson bracket relations

$$\{ \ , \ }_{\text{classical}} \leftrightarrow -\frac{i}{\hbar} [ \ , \ ]_{\text{quantum}}, \quad (4.42)$$

- You would have seen this for position and momentum, but it works for many other variables, e.g. the magnetic flux and charge in a superconducting circuit.

Let's push the above a little further, by calculating the total time derivative of a function  $f$  on phase space

$$\frac{df}{dt} = \sum_n \left( \frac{\partial f}{\partial q_n} \dot{q}_n + \frac{\partial f}{\partial p_n} \dot{p}_n \right) + \frac{\partial f}{\partial t} \stackrel{\text{Eq. (4.10)}}{=} \sum_n \left( \frac{\partial f}{\partial q_n} \frac{\partial \mathcal{H}}{\partial p_n} - \frac{\partial f}{\partial p_n} \frac{\partial \mathcal{H}}{\partial q_n} \right) + \frac{\partial f}{\partial t} = \{f, \mathcal{H}\} + \frac{\partial f}{\partial t}. \quad (4.43)$$

This has shown us that a function that “Poisson commutes” with the Hamiltonian and is time independent will be a constant of the motion. The exact same happens in quantum mechanics, where you can show (in what is called the Heisenberg picture) that  $\frac{d}{dt} \hat{A} = -\frac{i}{\hbar} [\hat{A}, \hat{H}] + \frac{\partial}{\partial t} \hat{A}$ .

**Example 45, Angular momentum Poisson brackets:** Let us consider the angular momentum of a single particle in 3D  $L_k = \sum_{nm} \epsilon_{knm} q_n p_m$ , using Eq. (2.96). As an exercise you can show that their Poisson brackets are

$$\{L_i, L_j\} = \epsilon_{ijk} L_k, \quad (4.44)$$

for  $ijk \in xyz$ . This is again exactly the same structure as the quantum-mechanical angular momentum algebra:  $[\hat{L}_i, \hat{L}_j] = (i\hbar)\epsilon_{ijk}\hat{L}_k$ . We can also show  $\{L^2, L_z\} = 0$ , again mimicking the corresponding quantum commutation relations.

- You can show that Poisson brackets are invariant under canonical transformations. That means if (4.41) is true, and you do a canonical transformations as in section 4.5, you end up with

$$\begin{aligned} \{Q_n, Q_m\} &= 0, \\ \{P_n, P_m\} &= 0, \\ \{Q_n, P_m\} &= \delta_{nm}. \end{aligned} \quad (4.45)$$

Even the reverse is true: If a transformation leaves the Poisson brackets invariant, you can know that it is canonical.

#### 4.6.2 Liouville equation

We had seen in section 4.4.1 that an ensemble of particles in a Hamiltonian phase-space evolves such that its phase-space volume is preserved. We can express the earlier results by some density of particles in phase space  $\rho(\mathbf{q}, \mathbf{p}, t)$ . In terms of Eq. (4.25)  $\rho = N/V$ , where  $V$  is the phase space volume occupied by these  $N$  particles or members of an ensemble. The density is thus normalized to give  $\int d^M \mathbf{q} d^M \mathbf{p} \rho(\mathbf{q}, \mathbf{p}, t) = N$ . From Eq. (4.28) we can thus also write

$$0 = \frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \sum_n \left( \frac{\partial \rho}{\partial q_n} \dot{q}_n + \frac{\partial \rho}{\partial p_n} \dot{p}_n \right). \quad (4.46)$$

Again using Eq. (4.10) and then the definition of (4.40) we then reach

### Liouville's equation

$$\frac{\partial \rho}{\partial t} = \{\mathcal{H}, \rho\} \quad (4.47)$$

- Again a very similar equation exists in quantum mechanics for the density operator  $\hat{\rho}$  for a quantum system. It is formally written as  $\hat{\rho} = |\Psi\rangle\langle\Psi|$  if you have a closed quantum system and fulfills, the von-Neumann equation

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] \quad (4.48)$$

which you can show from its definition and Schrödinger's equation.

- Even without invoking density matrices, there is a very thorough classical backbone in quantum time evolution. This is encoded in Ehrenfest's theorem, which states that, for Hamiltonian  $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{q})$

$$\begin{aligned} \frac{\partial}{\partial t} \langle \hat{p}(t) \rangle &= \left\langle \frac{\partial \hat{H}}{\partial q} \right\rangle, \\ \frac{\partial}{\partial t} \langle \hat{q}(t) \rangle &= -\left\langle \frac{\partial \hat{H}}{\partial p} \right\rangle. \end{aligned} \quad (4.49)$$

Compare these with Hamilton's equations (4.10).

### 4.6.3 Hamilton-Jacobi theory

We had already mentioned in section 4.5 that a possible use of canonical transformations, is to make the dynamics easier to solve, e.g. by making all coordinates cyclic. In this section, we follow an even more radical idea: Can we make the new Hamiltonian vanish, i.e.  $\mathcal{K} = 0$ ? If we can, then all coordinates are constant according to (4.31), so we don't even need to solve anything. Turns out we can, at least in principle.

The requirement for  $\mathcal{K} = 0$  can be re-cast into a requirement for the generating function of the transformation used, according to (4.38), we thus have  $0 = \mathcal{K} = \mathcal{H} + \frac{\partial F(\mathbf{q}, \mathbf{P})}{\partial t}$ . Using also  $\mathbf{p} = \frac{\partial F}{\partial \mathbf{q}}$ , we can re-write this as the

### Hamilton-Jacobi equation

$$\mathcal{H}(q_1, \dots, q_M, \frac{\partial F}{\partial q_1}, \dots, \frac{\partial F}{\partial q_M}) + \frac{\partial F}{\partial t} = 0. \quad (4.50)$$

- (4.50) is a partial differential equation (PDE, like a wave-equation or Schrödinger's equation, for the generating function  $F$ , in terms of the old coordinates  $q$ . While  $F$  also depends on  $P$ , these are constant per construction and can be identified with integration constants that anyway pop up in the solution of (4.50), see example below.

- One can show, that here the function  $F$  is actually the classical action  $S$  from (2.22) itself.
- The equation is more useful as a conceptual tool, as we shall see shortly, but can be the most powerful analytical technique for mechanics in certain cases.

**Example 46, Harmonic oscillator with Hamilton-Jacobi:** To see how (4.50) works, let us apply it to the simple harmonic oscillator. Inserting  $\frac{\partial F}{\partial q}$  instead of  $p$  into the Hamiltonian gives

$$\frac{1}{2m} \left( \frac{\partial F(q, P, t)}{\partial q} \right)^2 + \frac{1}{2} m \omega^2 q^2 = -\frac{\partial F(q, P, t)}{\partial t}. \quad (4.51)$$

We have written all dependencies of  $F$  for clarity. First we confirm that this is a PDE, containing partial derivatives wrt. time  $t$  and space  $q$ . We do not treat  $P$  as a variable here, since per construction at the outset it is a constant.

Since (except within  $F$ ), we have written all dependencies on  $q$  on the left-hand-side and all dependencies on  $t$  on the right hand side, we can attempt a separation of variables: This means we use the Ansatz  $F(q, P, t) = W(q) + V(t)$ . We have dropped  $P$  since it is just a constant parameter. If we find a solution in this way, that justifies the Ansatz afterwards. Inserting the new form for  $F$  into (4.50) we reach:

$$\frac{1}{2m} \left( \frac{\partial W(q)}{\partial q} \right)^2 + \frac{1}{2} m \omega^2 q^2 = C = -\frac{\partial V(t)}{\partial t}. \quad (4.52)$$

In the middle we have used the fact that, *since the lhs depends on  $q$  only, and the rhs on  $t$  only, they both must be equal to the same constant  $C$* . The rhs equality trivially gives  $V(t) = -Ct$  and since the lhs one says  $H = C$ , we can identify  $C$  with the total energy,  $C = E$ .

However now comes the crucial trick: Mathematics tells us that the general solution of a PDE of the kind (4.50) will contain  $M+1$  unknown constants (specified by initial conditions). One of them is an additive constant to  $F$  which is irrelevant. In the present example, that leaves just one constant. However we also know that  $P$  must be constant per construction, hence in addition we can write  $C = E = P$ .

Let us further reform the lhs equation into

$$\frac{\partial W(q)}{\partial q} = \sqrt{2mE - m^2\omega^2q^2}, \quad (4.53)$$

which has the formal solution  $W(q) = \int dq \sqrt{2mE - m^2\omega^2q^2}$ . We can now assemble  $F = -Pt + \int dq \sqrt{2mP - m^2\omega^2q^2}$ .



**Example continued:** We now use  $Q = \frac{\partial F}{\partial P}$ , which replaces (4.38) since we have a generating function of type  $F(q, P)$ , which gives

$$Q = -t + \int dq \frac{2m}{\sqrt{2mP - m^2\omega^2 q^2}} = -t + \frac{1}{\omega} \arcsin \left( q \sqrt{\frac{m\omega^2}{2P}} \right), \quad (4.54)$$

which gives us  $q(t) = \sqrt{\frac{2E}{m\omega^2}} \sin[\omega(t + Q)]$ . Similarly, using  $p = \frac{\partial F}{\partial q}$ , we arrive at an equation that can be reformed into  $p(t) = \sqrt{2mE} \cos[\omega(t + Q)]$ . At this point we have recovered the earlier solution, see e.g. example 43.

Since this “week” is devoted to connections to quantum mechanics, we are also interested in the following example:

**Example 47, Classical approximation of quantum mechanics:** Let’s start with Schrödinger’s equation in 1D with potential  $V(q)$

$$i\hbar \frac{\partial}{\partial t} \psi(q, t) = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + V(q) \right] \psi(q, t). \quad (4.55)$$

Now we split the complex  $\psi \in \mathbb{C}$  according to  $\psi(q, t) = R(q, t)e^{iF(q, t)}$  into real amplitude  $R(q, t)$  and real phase  $F(q, t)$ . Insertion into (4.55) and then dividing by  $e^{iF(q, t)}$  gives

$$i\hbar \left[ \frac{\partial R}{\partial t} + i \frac{R}{\hbar} \frac{\partial F}{\partial t} \right] = -\frac{\hbar^2}{2m} \left[ \frac{\partial^2 R}{\partial q^2} + \frac{2i}{\hbar} \frac{\partial R}{\partial q} \frac{\partial F}{\partial q} - \frac{R}{\hbar^2} \left( \frac{\partial F}{\partial q} \right)^2 + i \frac{R}{\hbar} \frac{\partial^2 F}{\partial q^2} \right] + VR \quad (4.56)$$

Now we take the limit  $\hbar \rightarrow 0$ , or more physically we assume that the de-Broglie wavelength of the particle is much shorter than every other length-scale of the problem. We reach

$$\frac{\partial F}{\partial t} + \frac{1}{2m} \left( \frac{\partial F}{\partial q} \right)^2 + V = \mathcal{O}(\hbar). \quad (4.57)$$

We can see that this corresponds to the Hamilton-Jacobi equation (4.50), using the Hamiltonian  $\mathcal{H} = \frac{p^2}{2m} + V(q)$ . Since we know that  $F$  is the classical action along the path, this now also gave us an additional interpretation of the phase of the quantum wave function.

#### 4.6.4 Action along paths in quantum dynamics

We had seen that classical mechanics can be based on the concept of variations of the action over possible paths, and the requirement that the classical path makes the action stationary. This is true for the Lagrange formalism, in (2.22) as well as for Hamilton, using an action such as in (4.35). While it is a bit advanced, we cannot resist to mention that the concept of “trying out different paths” seems to be even deeper rooted in quantum mechanics.

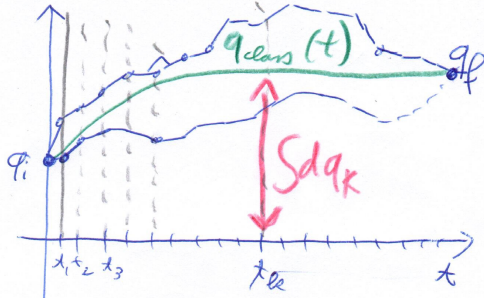
Sticking to the same one dimensional quantum wavefunction  $\psi$  as above, one can show the

**Feynman path integral formula** for the evolution of the wave function from an initial state  $\psi_0(q, t = 0)$  to a final state  $\psi(q, t)$

$$\psi(q, t) = \frac{1}{Z} \int dx \int \mathcal{D}[q(t)]_{q(0)=x} e^{i\frac{S(q,t)}{\hbar}} \psi_0(x, 0), \quad (4.58)$$

where  $S(q, t)$  is the action and  $\mathcal{D}[q(t)]$  denotes an integration over all possible paths from  $x$  to  $q$ , as discussed below, and  $Z$  is a normalisation constant

- The path integral is the biggest beast of an integration that we have. It seriously means to integrate over the value  $q(t_k)$  for every time  $0 < t_k < t$  between the beginning and the end. Formally we could write  $\mathcal{D}[q(t)] \sim \lim_{N \rightarrow \infty} \prod_{k=1}^N \int dq_k$ , where  $q_k = q(t_k)$ , so this is an infinite dimensional integration. It is probably better to understand this in the drawing below:



**left:** The Feynman path integral implies an integration over all possible paths, imagine slicing up the time axis in discrete intervals as a computer would do. Compare with the drawing in section 2.12.

- We can again see, that for  $\hbar \rightarrow 0$  only the classical path is being selected: For all other paths, the exponent  $S(q, t)/\hbar$  varies rapidly and thus the complex numbers average out. Only near the classical path, the variation is smaller since the path makes the action stationary.
- For finite  $\hbar$ , the equation (4.58) can be interpreted as the quantum system actually actively sampling all possible classical paths, each of which then contributes to the final wavefunction with a phase that depends on the action along the path (as seen also in section 4.6.3).