

Chapter 10. A Bit More of Analytical Mechanics

In this chapter I will briefly discuss two alternative approaches to analytical mechanics, whose main advantage is a closer parallel to quantum mechanics in general and to its quasiclassical (WKB) approximation in particular. The Hamiltonian formalism will also be used to derive a very important result (the “adiabatic invariance”) for classical systems with slowly changing parameters.

10.1. Hamiltonian equations

Throughout this course we have seen how useful the analytical mechanics, in its Lagrangian form, may be for solving various problems. We will now discuss several alternative formulations,¹ which may not be more useful for the solution of most practical problems of classical mechanics, but shed light on its possible extensions, most importantly to quantum mechanics.

As was already discussed in Sec. 2.3, derivatives $p_j \equiv \partial L / \partial \dot{q}_j$, participating in the Lagrange equations (2.19)

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_j} - \frac{\partial L}{\partial q_j} = 0, \quad (10.1)$$

may be considered as generalized momenta, and used to define the Hamiltonian function

$$H \equiv \sum_j p_j \dot{q}_j - L. \quad (10.2)$$

Now let us rewrite its differential (which was, actually, already used in Eq. (2.33)), in the following form:

$$\begin{aligned} dH &= d\left(\sum_j p_j \dot{q}_j - L\right) = \sum_j \left(d(p_j) \dot{q}_j + p_j d(\dot{q}_j)\right) - dL \\ &= \sum_j \left(d(p_j) \dot{q}_j + p_j d(\dot{q}_j)\right) - \left[\frac{\partial L}{\partial t} dt + \sum_j \left(\frac{\partial L}{\partial q_j} dq_j + \frac{\partial L}{\partial \dot{q}_j} d(\dot{q}_j)\right)\right]. \end{aligned} \quad (10.3)$$

According to the definition of the generalized momentum, second terms in each sum over j cancel, while according to the Lagrange equation (1), the derivative $\partial L / \partial q_j$ is just \dot{p}_j , so that

$$dH = -\frac{\partial L}{\partial t} dt + \sum_j \left[\dot{q}_j dp_j - \dot{p}_j dq_j\right] \quad (10.4)$$

So far, this is just an identity. Now comes the main trick of the Hamiltonian approach: let us consider H a function of the following independent arguments: time t , the generalized coordinates q_j , and the generalized momenta p_j (rather than generalized velocities). Then the general rule of differentiation of a function of several arguments gives:

¹ Due mostly to W. Hamilton (1805-1865) and C. Jacobi (1804-1851).

$$dH = \frac{\partial H}{\partial t} dt + \sum_j \left(\frac{\partial H}{\partial q_j} dq_j + \frac{\partial H}{\partial p_j} dp_j \right). \quad (10.5)$$

With our new agreement, dt , dq_j , and dp_j should be considered independent differentials, and Eq. (5) should be valid for any choice of them, in particular if they correspond to the real trajectory of motion, on which Eq. (4) is valid as well. This requirement gives us three relations:

$$\frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}. \quad (10.6)$$

$$\dot{q}_j = \frac{\partial H}{\partial p_j}, \quad (10.7a)$$

$$\dot{p}_j = -\frac{\partial H}{\partial q_j}. \quad (10.7b)$$

Comparing the first of them with Eq. (2.35), we see that

$$\frac{dH}{dt} = \frac{\partial H}{\partial t}, \quad (10.8)$$

meaning that (only at our new convention!) the Hamiltonian can change in time only via its explicit dependence on t .

Equations (7) are even more substantial: provided that the function $H(t, q_j, p_j)$ has been calculated, they give us two first-order differential equations (called *Hamiltonian equations*) for the time evolution of the generalized coordinate and generalized momentum of each degree of freedom of the system.² Let us have a look at these equations for the simplest case of a system with one degree of freedom with the Lagrangian function (3.3):

$$L = \frac{m_{\text{ef}}}{2} \dot{q}^2 - U_{\text{ef}}(q, t). \quad (10.9)$$

In this case, $p \equiv \partial L / \partial \dot{q} = m_{\text{ef}} \dot{q}$, and $H \equiv p\dot{q} - L = m_{\text{ef}} \dot{q}^2 / 2 + U_{\text{ef}}(q, t)$. In order to honor our new commitment, we need to express the Hamiltonian function explicitly via t , q and p (rather than \dot{q} !):

$$H = \frac{p^2}{2m_{\text{ef}}} + U_{\text{ef}}(q, t). \quad (10.10)$$

Now we can substantiate Eqs. (7):

$$\dot{q} = \frac{\partial H}{\partial p} = \frac{p}{m_{\text{ef}}}, \quad (10.11)$$

$$\dot{p} = -\frac{\partial H}{\partial q} = -\frac{\partial U_{\text{ef}}}{\partial q}. \quad (10.12)$$

² Of course, the right-hand part of each equation (7) generally can include the coordinates and momenta of other degrees of freedom as well, so that the equations for different j are generally coupled.

While the first of these equations just repeats the definition of the generalized momentum corresponding to coordinate q , the second one gives the equation of momentum change. Differentiating Eq. (11) over time, and plugging Eq. (12) into the result, we get:

$$\ddot{q} = \frac{\dot{p}}{m_{\text{ef}}} = -\frac{1}{m_{\text{ef}}} \frac{\partial U_{\text{ef}}}{\partial x}. \quad (10.13)$$

So, we have returned to the same equation (3.4) which had been derived from the Lagrangian approach.

Thus, the Hamiltonian formalism does not give much new for the solution of most problems of classical mechanics. (This is why its discussion has been postponed until the end of this course.) Moreover, since the Hamiltonian function $H(t, q_j, p_j)$ does not include generalized velocities explicitly, the phenomenological introduction of dissipation in this approach is less straightforward than that in the Lagrangian formalism.

However, the Hamiltonian equations (7), which treat the generalized coordinates and momenta in a manifestly symmetric way, are intellectually very appealing and heuristically fruitful. This is especially true in the cases where these arguments participate in H in a similar way. For example, for the important case of dissipation-free harmonic oscillator, for which $U_{\text{ef}} = \kappa_{\text{ef}} q^2/2$, Eq. (10) gives the famous symmetric form

$$H = \frac{p^2}{2m_{\text{ef}}} + \frac{\kappa_{\text{ef}} x^2}{2} = \frac{p^2}{2m_{\text{ef}}} + \frac{m_{\text{ef}} \omega_0^2 x^2}{2}, \quad \omega_0^2 \equiv \frac{\kappa_{\text{ef}}}{m_{\text{ef}}}. \quad (10.14)$$

and the Hamiltonian equations (7) preserve this symmetry, especially evident if we use normalized momentum $\rho \equiv p/m_{\text{ef}}\omega_0$ (already used in Sec. 4.3 – see Fig. 4.9 and its discussion) and time $\tau \equiv \omega_0 t$:

$$\frac{dq}{d\tau} = \rho, \quad \frac{d\rho}{d\tau} = -q. \quad (10.15)$$

Second, the Hamiltonian approach gives additional tools for the search for the integrals of motion. In order to see that, let us consider the full time derivative of an arbitrary function $f(t, q_j, p_j)$:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_j \left(\frac{\partial f}{\partial q_j} \dot{q}_j + \frac{\partial f}{\partial p_j} \dot{p}_j \right). \quad (10.16)$$

Plugging in \dot{q}_j and \dot{p}_j from the Hamiltonian equations (7), we get

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \sum_j \left(\frac{\partial H}{\partial p_j} \frac{\partial f}{\partial q_j} - \frac{\partial H}{\partial q_j} \frac{\partial f}{\partial p_j} \right) = \frac{\partial f}{\partial t} + \{H, f\}, \quad (10.17)$$

where the last term is the so-called *Poisson bracket* which is defined, for two arbitrary functions $f(t, q_j, p_j)$ and $g(t, q_j, p_j)$, as

$$\{g, f\} \equiv \sum_j \left(\frac{\partial g}{\partial p_j} \frac{\partial f}{\partial q_j} - \frac{\partial g}{\partial q_j} \frac{\partial f}{\partial p_j} \right). \quad (10.18)$$

Using this definition, one can readily verify that besides evident relations (such as $\{f, g\} = -\{g, f\}$), the Poisson brackets satisfy the important *Jacobi identity*:

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0. \quad (10.19)$$

Now let us use these relations for a hunt for integrals of motion. First, equation (16) shows that if a function f does not depend on time explicitly, and

$$\{H, f\} = 0, \quad (10.20)$$

then $df/dt = 0$, i.e. function f is an integral of motion.

Moreover, if we already know two integrals of motion, f and g , then function

$$F = \{f, g\} \quad (10.21)$$

is also an integral of motion – the so-called *Poisson theorem*. In order to prove it, we may use the Jacobi identity (19) with $h = H$. Using Eq. (17) to express the Poisson brackets $\{g, H\}$, $\{H, g\}$, and $\{H, \{f, g\}\} = \{H, F\}$ via the full and partial time derivatives of functions f , g , and F , we get

$$\left\{f, \frac{\partial g}{\partial t} - \frac{dg}{dt}\right\} + \left\{g, \frac{df}{dt} - \frac{\partial f}{\partial t}\right\} + \frac{dF}{dt} - \frac{\partial F}{\partial t} = 0, \quad (10.22)$$

so that if $df/dt = dg/dt = 0$, then

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \left\{g, \frac{\partial f}{\partial t}\right\} - \left\{f, \frac{\partial g}{\partial t}\right\} = \frac{\partial F}{\partial t} - \left[\left\{ \frac{\partial f}{\partial t}, g \right\} + \left\{ f, \frac{\partial g}{\partial t} \right\} \right]. \quad (10.23)$$

Plugging Eq. (21) into the first term of the right-hand part of this equation, and differentiating it by parts, we get $dF/dt = 0$, i.e. F is indeed an integral of motion.

Finally, one more important role of the Hamiltonian formalism is that it allows one to trace the close connection between the classical and quantum mechanics. Indeed, using Eq. (18) to calculate the Poisson brackets of generalized coordinates and momenta, we readily get

$$\{q_j, q_{j'}\} = 0, \quad \{p_j, p_{j'}\} = 0, \quad \{q_j, p_{j'}\} = -\delta_{jj'}. \quad (10.24)$$

In quantum mechanics, operators of these quantities obey commutation relations

$$[\hat{q}_j, \hat{q}_{j'}] = 0, \quad [\hat{p}_j, \hat{p}_{j'}] = 0, \quad [\hat{q}_j, \hat{p}_{j'}] = i\hbar\delta_{jj'}, \quad (10.25)$$

where the definition of the commutator, $[\hat{g}, \hat{f}] \equiv \hat{g}\hat{f} - \hat{f}\hat{g}$, is to a certain extent³ similar to that (18) of the Poisson bracket. We see that the classical relations (24) are similar to quantum-mechanical relations (25) if we following parallel has been made:

$$\{g, f\} \leftrightarrow \frac{i}{\hbar} [\hat{g}, \hat{f}]. \quad (10.26)$$

This analogy extends well beyond Eqs. (24), (25). For example, making the replacement (26) in Eq. (17), we get

³ I would like to emphasize the conceptual difference between the “usual” products of function derivatives, participating in the Poisson brackets, and the operator products forming the commutator.

$$\frac{d\hat{f}}{dt} = \frac{\partial \hat{f}}{\partial t} + \frac{i}{\hbar} [\hat{H}, \hat{f}], \quad (10.27)$$

which is the correct equation of the operator dynamics in the Heisenberg picture of quantum mechanics.⁴

10.2. Adiabatic invariance

The Hamiltonian formalism also has several applications in classical mechanics, perhaps most importantly, for the solution of the following problem. Earlier in the course, we already studied some effects of time variation of parameters of a single oscillator (Sec. 4.5 and Problems 4.9 – 4.12) and coupled oscillators (Sec. 5.5 and Problem 5.4). However, those discussions were limited to the case when the parameter variation speed is comparable with the initial oscillation frequency (or frequencies) of the system. Another practically important case is when a parameter (let us call it λ) is changed much more slowly (“*adiabatically*”),⁵

$$\left| \frac{\dot{\lambda}}{\lambda} \right| \ll \frac{1}{T}, \quad (10.28)$$

where T is the typical period of oscillations in the system. Let us consider a 1D system whose Hamiltonian $H(q, p, \lambda)$ depends on time only via the slow (28) evolution of $\lambda = \lambda(t)$, and whose initial energy restricts system’s motion to a finite coordinate interval – see Fig. 3.2c.

Then, as we know from Sec. 3.3, if parameter λ is constant, system performs periodic (though not necessarily sinusoidal) motion back and forth axis q , or, in a different language, along a closed trajectory on the phase plane $[q, p]$ – see Fig. 1.⁶ According to Eq. (8), in this case H is constant on the trajectory. (In order to distinguish this particular *value* from the Hamilton *function* as such, I will assume that this constant coincides with energy E , like is does for Hamiltonian (10), though this assumption is not necessary for the calculation made below.)

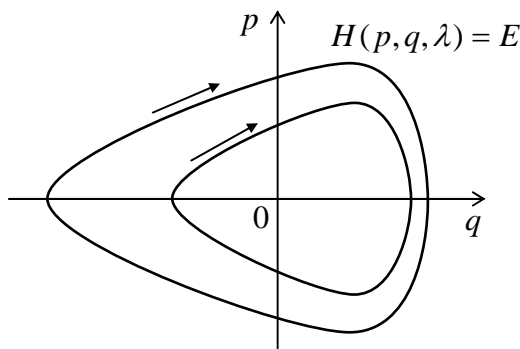


Fig. 10.1. The phase-plane presentation of periodic oscillations of a 1D Hamiltonian system, for two values of energy (schematically).

The oscillation period T may be calculated as a contour integral along this closed trajectory:

⁴ See, e.g., QM Sec. 4.6.

⁵ This term has come from thermodynamics (see, e.g., SM Sec. 1.3) where it implies not only a slow parameter variation, but also thermal insulation. Evidently, the latter condition is irrelevant in our current context.

⁶ In Sec. 4.6, we discussed this plane for the particular case of sinusoidal oscillations – see Fig. 9

$$T \equiv \int_0^T dt = \oint \frac{dt}{dq} dq. \quad (10.29)$$

Using the Hamiltonian equation (7a), we may now present this integral as

$$T = \oint \frac{1}{\partial H / \partial p} dq. \quad (10.30)$$

At each given point q of the trajectory, $H = E$ is a function of p alone, so that we may flip the partial derivative in the denominator just as a full derivative, and rewrite Eq. (30) as

$$T = \oint \frac{\partial p}{\partial E} dq. \quad (10.31)$$

For the particular Hamiltonian (10), this relation is immediately reduced to Eq. (3.27) in the form of a contour integral:

$$T = \left(\frac{m_{\text{ef}}}{2} \right)^{1/2} \oint \frac{1}{[E - U_{\text{ef}}(q)]^{1/2}} dq. \quad (10.32)$$

Superficially, it might look that these formulas may be also used to find the motion period change when parameter λ is being changed adiabatically (28), for example, by plugging known functions $m_{\text{ef}}(\lambda)$ and $U_{\text{ef}}(q, \lambda)$ into Eq. (31). However, there is no guarantee that energy E would stay constant as the parameter change, and indeed we will see below that this is not the case. Even more interestingly, in the most important case of the harmonic oscillator ($U_{\text{ef}} = \kappa_{\text{ef}} q^2 / 2$), whose oscillation period T does not depend on E (see Eq. (3.29) and its discussion), its variation in the adiabatic limit may be readily predicted: $T(\lambda) = 2\pi / \omega_0(\lambda) = 2\pi [m_{\text{ef}}(\lambda) / \kappa_{\text{ef}}(\lambda)]^{1/2}$, but the dependence of the oscillation energy E (and hence amplitude) on λ is not immediately obvious.

In order to address this problem, let us use Eq. (8) (with $E = H$) to present the energy change with $\lambda(t)$, i.e. in time, as

$$\frac{dE}{dt} = \frac{\partial H}{\partial t} = \frac{\partial H}{\partial \lambda} \frac{d\lambda}{dt}. \quad (10.33)$$

We are actually interested in slow (adiabatic) time evolution of energy, so we can average Eq. (32) over fast oscillations in the system. Moreover, if we look only for the energy change proportional to small $\dot{\lambda}$, we may (similarly to what we did it in Sec. 4.3 for weakly nonlinear oscillations) limit ourselves to averaging $\partial H / \partial t$ over one period T .⁷ This yields

$$\overline{\frac{dE}{dt}} = \overline{\frac{\partial H}{\partial \lambda}} = \frac{d\lambda}{dt} \frac{1}{T} \int_0^T \frac{\partial H}{\partial \lambda} dt. \quad (10.34)$$

Transforming the time integral to the contour one, just as we did in Eq. (30), and using Eq. (31) for T , we get

⁷ This is the most critical point of reasoning, because at any finite rate of the parameter change the oscillations are, strictly speaking, non-periodic. This is why more strict (but also much more cumbersome) proofs are still being offered in literature – see, e.g., C. G. Wells and S. T. C. Siklos, *Eur. J. Phys.* **28**, 105 (2007).

$$\frac{\overline{dE}}{dt} = \frac{d\lambda}{dt} \frac{\oint \frac{\partial H / \partial \lambda}{\partial H / \partial p} dq}{\oint \frac{\partial p}{\partial E} dq}. \quad (10.35)$$

At each point q of the contour, H is a function of not only λ , but also of p which may be also λ -dependent, so that if E is fixed, *partial* (not full!) differentiation of relation $E = H$ yields

$$\frac{\partial H}{\partial \lambda} + \frac{\partial H}{\partial p} \frac{\partial p}{\partial \lambda} = 0, \quad \text{i.e.} \quad \frac{\partial H / \partial \lambda}{\partial H / \partial p} = -\frac{\partial p}{\partial \lambda}. \quad (10.36)$$

Plugging this relation, in its last form, into Eq.(34), we get

$$\frac{\overline{dE}}{dt} = -\frac{d\lambda}{dt} \frac{\oint \frac{\partial p}{\partial \lambda} dq}{\oint \frac{\partial p}{\partial E} dq}. \quad (10.37)$$

Since the left-hand part, and the derivative $d\lambda/dt$ do not depend on q , we may move them into the integrals over q as constants, and rewrite Eq. (37) as

$$\oint \left(\frac{\partial p}{\partial E} \frac{\overline{dE}}{dt} + \frac{\partial p}{\partial \lambda} \frac{d\lambda}{dt} \right) dq = 0. \quad (10.38)$$

Now let us consider the following integral over the same contour,

$$J \equiv \frac{1}{2\pi} \oint p dq, \quad (10.39)$$

called the *action variable*. Just to understand what it is, let us calculate J for a harmonic oscillator (14). As we know very well by now, for such oscillator, $q = A \cos \Psi$, $p = -m_{\text{ef}} \omega_0 A \sin \Psi$ (with $\Psi = \omega_0 t + \text{const}$), and J may be easily expressed either via the oscillation amplitude A , or their energy $E = H = m_{\text{ef}} \omega_0^2 A^2 / 2$:

$$J = \frac{1}{2\pi} \oint p dq = \frac{1}{2\pi} \int_{\Psi=0}^{\Psi=2\pi} (-m_{\text{ef}} \omega_0 A \sin \Psi) d(A \cos \Psi) = \frac{1}{2\pi} \frac{m_{\text{ef}} \omega_0}{2} A^2 = \frac{E}{\omega_0}. \quad (10.40)$$

Returning to the general oscillator with adiabatically changed parameter λ , let us calculate dJ/dt , again taking into account that at each point q of the trajectory, p is a function of E and λ :

$$\frac{dJ}{dt} = \frac{1}{2\pi} \oint \frac{dp}{dt} dq = \frac{1}{2\pi} \oint \left(\frac{\partial p}{\partial E} \frac{dE}{dt} + \frac{\partial p}{\partial \lambda} \frac{d\lambda}{dt} \right) dq. \quad (10.41)$$

Within the accuracy of our approximation, in which the contour integrals (38) and (41) are calculated along a closed trajectory, factor dE/dt is indistinguishable from its time average, and these integrals coincide. Hence, we have finally arrived at a very important result: at an adiabatically-slow parameter variation, the action variable remains constant:

$$J = \text{const}. \quad (10.42)$$

This is the famous *adiabatic invariance*. In particular, according to Eq. (43), in a harmonic oscillator, energy of oscillation changes proportionately to the (slowly changed) eigenfrequency.

Before moving on, let me briefly note that the adiabatic invariance is not the only application of the action variable J . By its definition (39), it is essentially a sum of several (formally, infinite number of) values of momentum p . Since the initial choice of generalized coordinates and velocities (and hence the generalized momenta) in analytical mechanics is arbitrary (see Sec. 2.1), it is almost evident that J may be taken as a new generalized momentum corresponding to a certain new generalized coordinate Θ ,⁸ and that pair $\{J, \Theta\}$ should satisfy Hamiltonian equations (7), in particular,

$$\frac{d\Theta}{dt} = \frac{\partial H}{\partial J}. \quad (10.43)$$

Following the commitment of Sec. 1 (made there for the “old” arguments q_j, p_j), before the differentiation in the right-hand part in Eq. (43), H should be expressed as a function of t, J , and Θ . For time-independent Hamiltonian systems, H is uniquely defined by J – see, e.g., Eq. (40). Hence the right-hand part of Eq. (43) does not depend on either t or Θ , so that according to that equation, Θ (called the *angle variable*) is a linear function of time:

$$\Theta = \frac{\partial H}{\partial J} t + \text{const}. \quad (10.44)$$

For a harmonic oscillator, according to Eq. (40), derivative $\partial H/\partial J = \partial E/\partial J = \omega_0 = 2\pi/T$, so that $\Theta = \omega_0 t + \text{const}$. It may be shown that the more general form of this relation,

$$\frac{\partial H}{\partial J} = \frac{2\pi}{T}, \quad (10.45)$$

is valid for an arbitrary oscillator described by Eq. (52). Thus, Eq. (57) becomes

$$\Theta = 2\pi \frac{t}{T} + \text{const}. \quad (10.46)$$

In other words, for a harmonic oscillator, Θ is just the total phase Ψ (which we used so much in Ch. 4), while for an arbitrary (nonlinear) 1D oscillator, this is a convenient generalization of that notion. Due to this reason, variables J and Θ present a convenient alternative tool for discussion of certain fine points of dynamics strongly nonlinear oscillators.⁹

10.3. The Hamilton principle

Let us show now that the Lagrangian equations of motion, which have been derived in Sec. 2.1 from the Newton laws, may be also obtained from the so-called *Hamilton principle*, namely the condition of a minimum (or rather an extremum) of the integral called *action*:

$$S \equiv \int_{t_{\text{ini}}}^{t_{\text{fin}}} L dt, \quad (10.47)$$

⁸ This is of course a plausible argument but not a strict proof. For more mathematical vigor, the reader is referred to Sec. 45 of *Mechanics* by Landau and Lifshitz, which discusses the general rules of the so-called *canonical transformation* from one set of Hamiltonian arguments to another, say from $\{p, q\}$ to $\{J, \Theta\}$.

⁹ See, e.g., Chapter 6 in J. V. Jose and E. J. Saletan, *Classical Dynamics*, Cambridge U. Press, 1998.

where t_{ini} and t_{fin} are, respectively, the initial and final moments of time, at which all generalized coordinates and velocities are considered fixed – see Fig. 2.

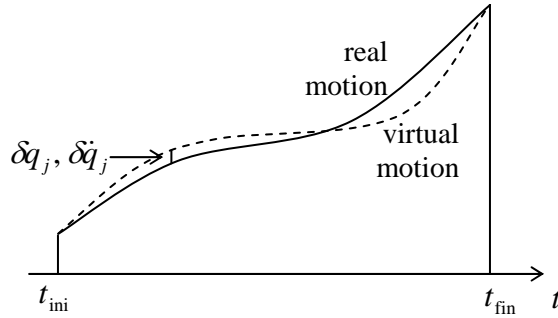


Fig. 10.2. Deriving the Hamilton principle.

The proof of that statement is rather simple. Considering, similarly to Sec. 2.1, a possible virtual variation of the motion, described by infinitesimal deviations $\{ \delta q_j(t), \delta \dot{q}_j(t) \}$ from the real motion, the requirement $S = \min$ may be presented as

$$\delta S \equiv \int_{t_{\text{ini}}}^{t_{\text{fin}}} \delta L dt, \quad (10.48)$$

where δS and δL are the variations of the action and the Lagrange function, corresponding to the set $\{ \delta q_j(t), \delta \dot{q}_j(t) \}$. As has been already discussed in Chapter 2, we can use the operation of variation just as the usual differentiation (but at fixed time, see Fig. 1), swapping these two operations if needed – see Fig. 2.1 and its discussion. Thus, we can write

$$\delta L = \sum_j \left[\frac{\partial L}{\partial q_j} \delta q_j + \frac{\partial L}{\partial \dot{q}_j} \delta \dot{q}_j \right] = \sum_j \frac{\partial L}{\partial q_j} \delta q_j + \sum_j \frac{\partial L}{\partial \dot{q}_j} \frac{d}{dt} \delta q_j. \quad (10.49)$$

Plugging the last expression into Eq. (29), we can integrate the second term by parts:

$$\delta S = \int_{t_{\text{ini}}}^{t_{\text{fin}}} \sum_j \frac{\partial L}{\partial q_j} \delta q_j dt + \int_{t_{\text{ini}}}^{t_{\text{fin}}} \frac{\partial L}{\partial \dot{q}_j} \frac{d}{dt} \delta q_j dt = \int_{t_{\text{ini}}}^{t_{\text{fin}}} \sum_j \frac{\partial L}{\partial q_j} \delta q_j dt + \sum_j \left[\frac{\partial L}{\partial \dot{q}_j} \delta q_j \right]_{t_{\text{ini}}}^{t_{\text{fin}}} - \sum_j \int_{t_{\text{ini}}}^{t_{\text{fin}}} \delta q_j d \left(\frac{\partial L}{\partial \dot{q}_j} \right). \quad (10.50)$$

Since the generalized coordinates in the initial and final points are considered fixed (not affected by the variation), all $\delta q_j(t_{\text{ini}}) = \delta q_j(t_{\text{fin}}) = 0$, so that the second term in the right-hand part vanishes. Multiplying and dividing the last term by dt , we finally get

$$\delta S = \int_{t_{\text{ini}}}^{t_{\text{fin}}} \sum_j \frac{\partial L}{\partial q_j} \delta q_j dt - \sum_j \int_{t_{\text{ini}}}^{t_{\text{fin}}} \delta q_j \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) dt = - \int_{t_{\text{ini}}}^{t_{\text{fin}}} dt \sum_j \left[\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} \right] \delta q_j = 0. \quad (10.51)$$

Since this equation should hold for an arbitrary set of functions $\delta q_j(t)$, it is only possible if the expressions in square brackets equal zero for all j , giving us the Lagrange equations.

In order to demystify action S , defined by Eq. (47), let us calculate it for the simple case of a single particle moving in a potential field which conserves its energy $E = T + U$. In this case the Lagrangian function $L = T - U$ may be presented as

$$L = T - U = 2T - (T + U) = 2K - E = mv^2 - E, \quad (10.52)$$

so that

$$S = \int L dt = \int mv^2 dt - Et + \text{const.} \quad (10.53)$$

Presenting the expression under the remaining integral as $m\mathbf{v} \cdot \mathbf{v} dt = \mathbf{p} \cdot (d\mathbf{r}/dt) dt = \mathbf{p} \cdot d\mathbf{r}$, we get finally:

$$S = S_0 - Et + \text{const.}, \quad (10.54)$$

where the time-independent integral

$$S_0 \equiv \int \mathbf{p} \cdot d\mathbf{r} \quad (10.55)$$

is called the *abbreviated action*.

This expression may be used to establish one more connection between the classical and quantum mechanics, now in the Schrödinger picture. Indeed, in the quasiclassical (WKB) approximation of that picture¹⁰ a particle of fixed energy is associated with a wave

$$\Psi(\mathbf{r}, t) \propto \exp\left[i\left(\int \mathbf{k} \cdot d\mathbf{r} - \omega t + \text{const}\right)\right], \quad (10.56)$$

where wavevector \mathbf{k} is proportional to the particle's momentum, while frequency ω , to its energy:

$$\mathbf{k} = \frac{\mathbf{p}}{\hbar}, \quad \omega = \frac{E}{\hbar}. \quad (10.57)$$

Plugging these expressions into Eq. (36) and comparing the result with Eq. (35), we see that the wavefunction may be presented as

$$\Psi \propto \exp\left(\frac{i}{\hbar} S\right). \quad (10.58)$$

Hence the Hamilton's principle means that the total phase of the quasiclassical wavefunction along the particle's trajectory should be minimal. But this is exactly the so-called *eikonal minimum principle* well known from the optics (though valid for any other waves as well), where it serves to define the ray paths in the geometric optics limit. Thus, S/\hbar may be considered as the eikonal, i.e. the total phase accumulation, of the de Broigle waves.

Also, comparing Eq. (55) with Eq. (33), we see that the action variable J is just the change of the abbreviated action S_0 on one phase plane contour (divided by 2π). This means that in the WKB approximation, J corresponds to the number of de Broigle waves along the classical trajectory of a particle, i.e. to an integer value of the corresponding quantum number. If system's parameters are changed slowly, the quantum number has to stay integer, and hence J cannot change, giving a quantum-mechanical interpretation of the adiabatic invariance. It is really fascinating that a fact of classical mechanics, may be "derived", or at least understood more easily from the quantum mechanics standpoint. (As a reminder, we have run into a similar case during our discussion of the non-degenerate parametric excitation in Sec. 5.5.)

¹⁰ See, e.g., QM Sec. 2.3.

10.4. The Hamilton-Jacobi equation

Action S , defined by Eq. (47), may be used for one more formulation of classical mechanics.¹¹ For that, we need a new convention: S is considered a function of the final time point t_{fin} (which we will, for brevity, denote t in this section), and the set of generalized coordinates (by not generalized velocities!) at that point:

$$S = S[t, q_j(t)] = \int_{t_{\text{ini}}}^t L dt. \quad (10.59)$$

For this function, we may repeat the variation calculations described by Eqs. (49)-(52), besides that now variations δq_j at the finite point (t) do not necessarily equal zero. As a result, we get

$$\delta S = \sum_j \frac{\partial L}{\partial \dot{q}_j} \delta q_j \Big|_t - \int_{t_{\text{ini}}}^t dt \sum_j \left[\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} \right] \delta q_j. \quad (10.60)$$

For the motion along the real trajectory, i.e. satisfying the Lagrange equations of motion, the second term of this expression equals zero. Hence Eq. (60) shows that, for (any) fixed time t ,

$$\frac{\partial S}{\partial q_j} = \frac{\partial L}{\partial \dot{q}_j}. \quad (10.61)$$

But the last derivative is of course nothing else than the generalized momentum p_j . As a result, the full derivative of action $S(t, q_j)$ over time takes the form

$$\frac{dS}{dt} = \frac{\partial S}{\partial t} + \sum_j \frac{\partial S}{\partial q_j} \dot{q}_j = \frac{\partial S}{\partial t} + \sum_j p_j \dot{q}_j. \quad (10.62)$$

Now, by the very definition (59), the full derivative dS/dt is nothing more than the Lagrange function L , so that Eq. (61) may be rewritten as

$$\frac{\partial S}{\partial t} = L - \sum_j p_j \dot{q}_j. \quad (10.63)$$

However, according to the definition (2.26) of the Hamiltonian function H , the right-hand part of Eq. (63) is just $(-H)$, so that we get an extremely simply-looking *Hamilton-Jacobi equation*

$$\frac{\partial S}{\partial t} = -H. \quad (10.64)$$

This simplicity is, however, rather deceiving, because in order to use this equation for the calculation of the function $S(t, q_j)$ for any particular problem, the Hamiltonian function has to be first expressed as a function of time t , generalized coordinates q_j , and the generalized momenta p_j (which may be, according to Eq. (61), presented just as derivatives $\partial S/\partial q_j$). Let us see how does this procedure

¹¹ It is curious that in the 1940s this approach has been extended (mostly by R. Bellman) to a completely different field – the optimal control theory, where it has become the basis of the so-called *dynamic programming* – see, e.g., T. P. Bertsekas, *Dynamic Programming and Optimal Control*, vols. 1 and 2, Aetna Scientific, 2005 and 2007.

work for the simplest case of a 1D system with Hamiltonian function (10). In this case, the only generalized momentum $p = \partial S/\partial q$, so that

$$H = \frac{p^2}{2m_{\text{ef}}} + U_{\text{ef}}(q, t) = \frac{1}{2m_{\text{ef}}} \left(\frac{\partial S}{\partial q} \right)^2 + U_{\text{ef}}(q, t), \quad (10.65)$$

and the Hamilton-Jacobi equation (44) is a partial differential equation,

$$\frac{\partial S}{\partial t} + \frac{1}{2m_{\text{ef}}} \left(\frac{\partial S}{\partial q} \right)^2 + U_{\text{ef}}(q, t) = 0, \quad (10.66)$$

whose solution is easy to find only in the case of time-independent potential energy $U_{\text{ef}} = U_{\text{ef}}(x)$. In this case, Eq. (66) is evidently satisfied by a variable-separated solution

$$S(t, q) = S_0(q) + \text{const} \times t. \quad (10.67)$$

Plugging this solution into Eq. (66), we see that since the two last terms of that equation present the full mechanical energy E , the constant in Eq. (67) is nothing but $(-E)$. Thus for function S_0 we get an ordinary differential equation

$$-E + \frac{1}{2m_{\text{ef}}} \left(\frac{dS_0}{dq} \right)^2 + U_{\text{ef}}(q) = 0. \quad (10.68)$$

Integrating it, we get

$$S_0 = \int \{2m_{\text{ef}} [E - U_{\text{ef}}(q)]\}^{1/2} dq + \text{const}, \quad (10.69)$$

so that, finally, the action is equal to

$$S = \int \{2m_{\text{ef}} [E - U_{\text{ef}}(q)]\}^{1/2} dq - Et + \text{const}. \quad (10.70)$$

For the case of 1D motion of a single particle ($q = x$, $m_{\text{ef}} = m$, $U_{\text{ef}}(q) = U(x)$), this solution is just the 1D case of the more general Eqs. (54)-(55) which was obtained by much more simple way. (In particular, S_0 is just the abbreviated action.) Thus the Hamilton-Jacobi equation is not the most efficient way for solution of most practical problems, though it may be useful for studies of some mathematical aspects of dynamics.¹²

¹² See, e.g., Chapters 6-9 in I. C. Percival and D. Richards, *Introduction to Dynamics*, Cambridge U. Press, 1983.