# Appendix A
# Functionals and the Functional Derivative

In this Appendix we provide a minimal introduction to the concept of functionals and the functional derivative. No attempt is made to maintain mathematical rigor. A more extended and mathematically more precise discussion of the material summarized here can be found in the books of Courant and Hilbert [728] and of Atkinson and Han [29] (for the special context of DFT see also [28]).

## A.1 Definition of the Functional

A functional is defined by a rule, which associates a number (real or complex) with a function of one or several variables,

$$f(x) \ \text{ or } \ f(\boldsymbol{r}_1,\ldots) \qquad \xrightarrow{\text{rule}} \qquad F[f]\,, \tag{A.1}$$

or, more generally, which associates a number with a set of functions,

$$f_1, f_2, \ldots \qquad \xrightarrow{\text{rule}} \qquad F[f_1,f_2,\ldots]\,. \tag{A.2}$$

This definition is quite well described by the designation as a function of a function. Some examples are:

- A definite integral over a continuous function $f(x)$

$$F[f] = \int_{x_1}^{x_2} f(x)dx \tag{A.3}$$

  (similarly one can have integrals with functions of several variables).
- A slightly more general form is

$$F_w[f] = \int_{x_1}^{x_2} w(x)f(x)dx\,, \tag{A.4}$$

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that is an integral over the function $f$ with a fixed weight function $w(x)$.

- A prescription which associates a function with the value of this function at a particular point in the interior of a given interval $[x_1, x_2]$

$$F[f] = f(x_0) \qquad x_0 \in (x_1, x_2) \; . \tag{A.5}$$

This functional can be represented in integral form with the aid of the $\delta$-function,

$$F_\delta[f] = \int_{x_1}^{x_2} \delta(x - x_0) f(x) dx \; , \tag{A.6}$$

that is with a weight function in the form of a generalized function (a distribution).

The examples (A.3) and (A.5) directly show that a functional can itself be a function of a variable, i.e. of one of the parameters in its definition, as the boundaries in the integral (A.3) or the point $x_0$ in the functional (A.5). The dependence on such a parameter $y$ is denoted as $F[f](y)$.

So far, all examples are characterized by the fact that they depend linearly on the function $f(x)$, so that they satisfy the relation

$$F[c_1 f_1 + c_2 f_2] = c_1 F[f_1] + c_2 F[f_2] \; , \tag{A.7}$$

with $c_1, c_2$ being complex numbers. Examples of nonlinear functionals are:

- The energy functional of the simplest DFT, the Thomas-Fermi kinetic energy,

$$F_{\rm TF}[n] \;\equiv\; T_{\rm s}^{\rm TF}[n] \;=\; C_{\rm TF} \int d^3 r\, n^{5/3}(\boldsymbol{r}) \; . \tag{A.8}$$

- A nonlocal functional of two functions,

$$F_w[f_1, f_2] \;=\; \int f_1(x_1) w(x_1, x_2) f_2(x_2) dx_1 dx_2 \; . \tag{A.9}$$

- The action integral of classical mechanics,

$$F[\boldsymbol{q}] \;\equiv\; A[\boldsymbol{q}] \;=\; \int_{t_1}^{t_2} dt\, L(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t), t) \; . \tag{A.10}$$

The abbreviation $\boldsymbol{q}(t)$ stands for a set of generalized coordinates, which depend on time.

- Any matrix element of quantum mechanics, e.g. the ground state energy and the $S$-matrix element of potential scattering theory,

$$F[\Psi_0, \Psi_0^*] \equiv E[\Psi_0, \Psi_0^*] \;=\; \int d^3 r\, \Psi_0^*(\boldsymbol{r}) \hat{H} \Psi_0(\boldsymbol{r})$$

$$F[\Psi_{\boldsymbol{k}}, \Psi_{\boldsymbol{q}}^*] \equiv S[\Psi_{\boldsymbol{k}}, \Psi_{\boldsymbol{q}}^*] \;=\; \int d^3 r\, \Psi_{\boldsymbol{q}}^*(\boldsymbol{r}) \hat{S} \Psi_{\boldsymbol{k}}(\boldsymbol{r}) \; .$$

It seems worthwhile to emphasize that the two functions $\Psi_0$ and $\Psi_0^*$ have to be considered as being independent, so that one is dealing with a functional of two functions. Alternatively, a dependence on the real and the imaginary part of the wavefunctions can be used to characterize the functional.

## A.2 Functional Derivative

Usually knowledge of the complete functional $F[f]$, as for example the classical action $A[\boldsymbol{q}]$ for all possible trajectories in phase space or the value of the integral (A.3) for all continuous functions, is not required. Rather it is the behavior of the functional in the vicinity of the function $f_0$, which makes $F[f]$ extremal or stationary, which is of interest.[1] The implementation of the search for $f_0$ involves the exploration of the space of functions in the vicinity of $f_0$ in a suitable fashion.

A variation of any function $f$ by an infinitesimal but arbitrary amount can be represented in the form

$$\begin{aligned} \delta f(x) &= \varepsilon\,\eta(x) && \text{for one variable} \\ \delta f(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots) &= \varepsilon\,\eta(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots) && \text{for several variables .} \end{aligned} \tag{A.11}$$

The quantity $\varepsilon$ is an infinitesimal number, $\eta$ is an arbitrary function. In order to explore the properties of the functionals a generalization of the (ordinary or partial) derivative (of first and higher order)—the functional derivative—is required. It can be defined via the variation $\delta F$ of the functional $F[f]$ which results from variation of $f$ by $\delta f$,

$$\delta F := F[f + \delta f] - F[f] \ . \tag{A.12}$$

The technique used to evaluate $\delta F$ is a Taylor expansion of the functional $F[f+\delta f] = F[f+\varepsilon\eta]$ in powers of $\delta f$, respectively of $\varepsilon$. The functional $F[f+\varepsilon\eta]$ is an ordinary function of $\varepsilon$. This implies that the expansion in terms of powers of $\varepsilon$ is a standard Taylor expansion,

$$F[f + \varepsilon\,\eta] = F[f] + \left.\frac{dF[f+\varepsilon\eta]}{d\varepsilon}\right|_{\varepsilon=0} \varepsilon + \frac{1}{2}\left.\frac{d^2F[f+\varepsilon\eta]}{d\varepsilon^2}\right|_{\varepsilon=0} \varepsilon^2 + \ldots \tag{A.13}$$

$$= \sum_{n=0}^{N} \frac{1}{n!} \left.\frac{d^nF[f+\varepsilon\eta]}{d\varepsilon^n}\right|_{\varepsilon=0} \varepsilon^n + \mathscr{O}\left(\varepsilon^{N+1}\right) \ . \tag{A.14}$$

As indicated, the sum in (A.14) can be finite or infinite. In the latter case, it has to be assumed that the function $F(\varepsilon)$ can be differentiated with respect to $\varepsilon$ any number of times.

[1] Often functionals are introduced to recast some equation(s) in the form of an extremum or stationarity principle.

The derivatives with respect to $\varepsilon$ now have to be related to the functional derivatives. This is achieved by a suitable definition. The definition of the functional derivative (also called variational derivative) is

$$\left.\frac{dF[f+\varepsilon\eta]}{d\varepsilon}\right|_{\varepsilon=0} =: \int dx_1\, \frac{\delta F[f]}{\delta f(x_1)}\,\eta(x_1)\,. \tag{A.15}$$

This definition implies that the left-hand side can be brought into the form on the right-hand side, i.e. the form of a linear functional with kernel $\delta F[f]/\delta f$ acting on the test function $\eta$. This is by no means guaranteed for arbitrary functionals and arbitrary $f$. It is exactly this point where rigorous mathematics sets in. A functional for which (A.15) is valid is called *differentiable*.[2] We will, however, not go into any details concerning the existence of the functional derivative, nor will we make any attempt to characterize the space of (test) functions which are allowed in (A.15) (as usual, the existence of all integrals involved is assumed, of course).

The definition (A.15) can be thought of as an extension of the first total differential of a function of several variables,

$$f(x_1,x_2,\ldots) \quad \longrightarrow \quad df = \sum_{n=1}^{N} \frac{\partial f}{\partial x_n}\,dx_n\,,$$

to the case of an infinite set of variables $f(x_1)$. The definition of the second order functional derivative corresponds to the second order total differential,

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[2] More precisely, a functional $F[f]$ which maps an open subset of some Banach space $\mathscr{X}$ (i.e. some complete normed vector space) of functions $f$ onto another Banach space $\mathscr{Y}$ (which could be the set of real or complex numbers) is called *Fréchet differentiable*, if there exists a linear continuous operator $\delta F_f^{\mathrm{F}} : \mathscr{X} \to \mathscr{Y}$ with the property

$$\lim_{\|\eta\|\to 0} \frac{\|F[f+\eta]-F[f]-\delta F_f^{\mathrm{F}}[\eta]\|_{\mathscr{Y}}}{\|\eta\|_{\mathscr{X}}} = 0\,.$$

Here $\|F\|_{\mathscr{Y}}$ and $\|\eta\|_{\mathscr{X}}$ denote the norms in the two Banach spaces. The Fréchet derivative has to be distinguished from the Gâteaux derivative, which exists if there is a linear continuous operator $\delta F_f^{\mathrm{G}} : \mathscr{X} \to \mathscr{Y}$ such that

$$\delta F_f^{\mathrm{G}}[\eta] = \lim_{\lambda\to 0} \frac{\|F[f+\lambda\eta]-F[f]\|_{\mathscr{Y}}}{\lambda}\,.$$

If the right-hand side of this relation exists, but does not yield a linear continuous operator, it is called the Gâteaux differential,

$$F'[f,\eta] = \lim_{\lambda\to 0} \frac{\|F[f+\lambda\eta]-F[f]\|_{\mathscr{Y}}}{\lambda}.$$

Thus any Fréchet differentiable functional is also Gâteaux differentiable, but the converse is not true. The existence of the Fréchet derivative is only ensured, if the Gâteaux derivative is continuous or if the Gâteaux differential is uniform with respect to $\eta$ with $\|\eta\| = 1$.

$$\left.\frac{d^2F[f+\varepsilon\eta]}{d\varepsilon^2}\right|_{\varepsilon=0} =: \int dx_1 dx_2 \, \frac{\delta^2 F[f]}{\delta f(x_1)\delta f(x_2)} \, \eta(x_1)\eta(x_2) \, . \tag{A.16}$$

The definition of the general derivative can be guessed at this stage. The functional derivative of $n$-th order is given by

$$\left.\frac{d^nF[f+\varepsilon\eta]}{d\varepsilon^n}\right|_{\varepsilon=0} =: \int dx_1 \dots dx_n \, \frac{\delta^n F[f]}{\delta f(x_1)\dots\delta f(x_n)} \, \eta(x_1)\dots\eta(x_n) \, . \tag{A.17}$$

This derivative constitutes the kernel of the Taylor expansion of a functional $F$ in terms of the variation $\delta f(x) = \varepsilon\eta(x)$,

$$\begin{aligned} F[f+\varepsilon\eta] = &\sum_{n=0}^{N} \frac{1}{n!} \int dx_1 \dots dx_n \, \frac{\delta^n F[f]}{\delta f(x_1)\dots\delta f(x_n)} \, \delta f(x_1)\dots\delta f(x_n) \\ &+\mathscr{O}\left(\varepsilon^{N+1}\right) \, , \end{aligned} \tag{A.18}$$

again with $N$ being either finite or infinite.

The actual calculation of the functional derivative relies on the evaluation of the difference (A.12). This will be illustrated with the aid of a few examples.

- According to Eq. (A.12), the variation of the functional (A.6) is

  $$\delta F_\delta = \int_{x_1}^{x_2} \delta(x-x_0)\varepsilon\eta(x)dx \, .$$

  Comparison with the definition (A.15) shows that

  $$\frac{\delta F_\delta}{\delta f(x)} = \delta(x-x_0) \, , \tag{A.19}$$

  as $\eta(x)$ can vary freely. A very useful formula is obtained if the definition

  $$F_\delta[f] = f(x_0)$$

  is used explicitly,

  $$\frac{\delta F_\delta}{\delta f(x)} = \frac{\delta f(x_0)}{\delta f(x)} = \delta(x-x_0) \, . \tag{A.20}$$

  All higher order functional derivatives of $F_\delta$ vanish.
- This example is readily extended to the functional

  $$f(x_0)^\alpha = \int dx \, \delta(x-x_0) \, f(x)^\alpha \, .$$

  Its variation can be evaluated by straightforward Taylor expansion,

  $$\delta f(x_0)^\alpha = \int dx \, \delta(x-x_0) \, [(f(x)+\varepsilon\eta(x))^\alpha - f(x)^\alpha]$$

$$= \int dx\, \delta(x-x_0) \Big[ \alpha f(x)^{\alpha-1} \varepsilon\eta(x) + \frac{\alpha(\alpha-1)}{2} f(x)^{\alpha-2} (\varepsilon\eta(x))^2 + \ldots \Big] .$$

The functional derivative is again identified by comparison with the definition (A.15),

$$\frac{\delta f(x_0)^\alpha}{\delta f(x)} = \delta(x-x_0)\, \alpha f(x)^{\alpha-1} . \tag{A.21}$$

In order to calculate the second functional derivative one can simply reuse Eq. (A.21),

$$\frac{\delta^2 f(x_0)^\alpha}{\delta f(x_1) \delta f(x_2)} = \delta(x_1-x_0)\, \delta(x_2-x_0)\, \alpha(\alpha-1) f(x)^{\alpha-2} . \tag{A.22}$$

- The variation of the Thomas-Fermi functional (A.8) is obtained from

$$\delta F_{\mathrm{TF}} = C_{\mathrm{TF}} \int d^3r \left[ (n(\boldsymbol{r}) + \varepsilon\eta(\boldsymbol{r}))^{5/3} - n(\boldsymbol{r})^{5/3} \right]$$

in the form of a binomial expansion

$$\delta F_{\mathrm{TF}} = C_{\mathrm{TF}} \int d^3r\, n(\boldsymbol{r})^{5/3} \sum_{k=1}^{\infty} \binom{5/3}{k} \left( \frac{\varepsilon\eta(\boldsymbol{r})}{n(\boldsymbol{r})} \right)^k .$$

The functional derivatives, which can be extracted from this expression, are

$$\frac{\delta F_{\mathrm{TF}}}{\delta n(\boldsymbol{r})} = \frac{5}{3} C_{\mathrm{TF}}\, n(\boldsymbol{r})^{2/3} \tag{A.23}$$

for the first derivative and, applying (A.21),

$$\frac{\delta^2 F_{\mathrm{TF}}}{\delta n(\boldsymbol{r}) \delta n(\boldsymbol{r}')} = \frac{10}{9} C_{\mathrm{TF}}\, n(\boldsymbol{r})^{-1/3}\, \delta^{(3)}(\boldsymbol{r}-\boldsymbol{r}')$$

for the second derivative.

- The variation of the nonlocal functional

$$F_w[f] = \int_{y_1}^{y_2} dx_1 \int_{y_1}^{y_2} dx_2\, f(x_1) w(x_1,x_2) f(x_2) \tag{A.24}$$

is

$$\delta F_w = \int_{y_1}^{y_2} dx_1 \int_{y_1}^{y_2} dx_2\, w(x_1,x_2) [f(x_1)\varepsilon\eta(x_2) + f(x_2)\varepsilon\eta(x_1) + \varepsilon\eta(x_1)\varepsilon\eta(x_2)] . \tag{A.25}$$

The variational derivatives are

$$\frac{\delta F_w}{\delta f(x)} = \int_{y_1}^{y_2} dx_2 \, [w(x,x_2) + w(x_2,x)] f(x_2) \tag{A.26}$$

and

$$\frac{\delta^2 F_w}{\delta f(x_1) f(x_2)} = w(x_1,x_2) + w(x_2,x_1) \; . \tag{A.27}$$

All derivatives with $n > 2$ vanish for this example.

## A.3 Calculational Rules

The calculation of the functional derivative can be abbreviated using a variation in terms of the $\delta$-function: for the functionals relevant in physics all local, $\delta$-type variations of $f(x)$ are equivalent to probing the functional with arbitrary general variations $\eta(x)$. The functional derivative can therefore be recast in the form of the (almost familiar) limiting value

$$\frac{\delta F}{\delta f(x_1)} = \lim_{\varepsilon \to 0} \frac{F[f(x) + \varepsilon \delta(x - x_1)] - F[f(x)]}{\varepsilon} \; . \tag{A.28}$$

The reader may check that this form follows from the definition (A.15) with the replacement $\eta(x) \longrightarrow \delta(x - x_1)$ and that it reproduces the results of the examples. When using the form (A.28), one has to remember that the variation $\delta f = \varepsilon \delta(x - x_1)$ should always be understood in the sense of a representation of the $\delta$-function via some sequence of regular functions, so that powers of the $\delta$-function are uncritical.

As the functional derivatives constitute an extension of the concept of the ordinary derivative, most of the rules for ordinary derivatives can be taken over. For example, the product rule of functional differentiation can be obtained directly with the argument

$$\begin{aligned}\left[\frac{d(F_1[f+\varepsilon\eta]F_2[f+\varepsilon\eta])}{d\varepsilon}\right]_{\varepsilon=0} &= \left[\frac{dF_1[f+\varepsilon\eta]}{d\varepsilon}F_2[f+\varepsilon\eta]\right]_{\varepsilon=0} \\ &\quad + \left[F_1[f+\varepsilon\eta]\frac{dF_2[f+\varepsilon\eta]}{d\varepsilon}\right]_{\varepsilon=0} \; ,\end{aligned}$$

which is valid as $F_1$ and $F_2$ are *functions* of $\varepsilon$. In the actual limit $\varepsilon \to 0$ there follows with (A.15)

$$\frac{\delta(F_1 F_2)}{\delta f(x)} = \frac{\delta F_1}{\delta f(x)} F_2 + F_1 \frac{\delta F_2}{\delta f(x)} \; . \tag{A.29}$$

Let us next extend the chain rule for functions to functionals. Consider a functional $F$ which depends on some function $G(y)$, which itself is a functional of $f(x)$, $G[f](y)$. The functional $F$ therefore is also a functional of $f(x)$. Its variation with $f$ is then given by

$$\begin{aligned}\delta F_f &= F[G[f(x)+\varepsilon\eta(x)](y)] - F[G[f(x)](y)] \\ &= \left.\frac{dF[G[f(x)+\varepsilon\eta(x)](y)]}{d\varepsilon}\right|_{\varepsilon=0} \varepsilon + \mathscr{O}(\varepsilon^2) \qquad \text{(A.30)} \\ &= \int \frac{\delta F[f]}{\delta f(x)}\, \varepsilon\eta(x)\, dx + \mathscr{O}(\varepsilon^2)\,, \qquad \text{(A.31)}\end{aligned}$$

where the last line simply represents the definition of the functional derivative of $F$ with respect to $f$, according to Eq. (A.15). Similarly, the variation of $G$ with $f$ is obtained as

$$\begin{aligned}\delta G(y) &= G[f(x)+\varepsilon\eta(x)](y) - G[f(x)](y) \\ &= \left.\frac{dG[f(x)+\varepsilon\eta(x)](y)}{d\varepsilon}\right|_{\varepsilon=0} \varepsilon + \mathscr{O}(\varepsilon^2) \qquad \text{(A.32)} \\ &= \int \frac{\delta G[f](y)}{\delta f(x)}\, \varepsilon\eta(x)\, dx + \mathscr{O}(\varepsilon^2)\,. \qquad \text{(A.33)}\end{aligned}$$

Now, to first order in $\varepsilon$ one can express $G[f(x)+\varepsilon\eta(x)](y)$ via Eq. (A.33),

$$G[f(x)+\varepsilon\eta(x)](y) = G[f(x)](y) + \int \frac{\delta G[f](y)}{\delta f(x)}\, \varepsilon\eta(x)\, dx + \mathscr{O}(\varepsilon^2)\,,$$

to obtain

$$\begin{aligned}\int \frac{\delta F[f]}{\delta f(x)}\, \eta(x)\, dx = &\left.\frac{dF[G[f(x)](y) + \int \frac{\delta G[f](y)}{\delta f(x)} \varepsilon\eta(x)dx + \mathscr{O}(\varepsilon^2)]}{d\varepsilon}\right|_{\varepsilon=0} \\ &+\mathscr{O}(\varepsilon)\,. \qquad \text{(A.34)}\end{aligned}$$

However, the derivative on the right-hand side has exactly the form of the variation of $F$ with $G$,

$$\begin{aligned}\delta F_G &= F[G(y)+\varepsilon\bar{\eta}(y)] - F[G(y)] \\ &= \left.\frac{dF[G(y)+\varepsilon\bar{\eta}(y)]}{d\varepsilon}\right|_{\varepsilon=0} \varepsilon + \mathscr{O}(\varepsilon^2)\,, \qquad \text{(A.35)}\end{aligned}$$

with $\bar{\eta}$ given by

$$\bar{\eta}(y) = \int \frac{\delta G[f](y)}{\delta f(x)} \eta(x) dx\,. \qquad \text{(A.36)}$$

Provided that $\bar{\eta}(y)$ probes the complete space around $G(y)$, in which $F[G]$ is defined, when $\eta(x)$ goes through all legitimate variations of $f(x)$, the expression (A.34) coincides with the corresponding functional derivative of $F$ with respect to $G(y)$,

$$\left.\frac{dF[G(y)+\varepsilon\bar{\eta}(y)]}{d\varepsilon}\right|_{\varepsilon=0} = \int \frac{\delta F[G]}{\delta G(y)}\,\bar{\eta}(y)\,dy + \mathscr{O}(\varepsilon)\,. \tag{A.37}$$

Combination of Eqs. (A.34), (A.36) and (A.37) finally yields

$$\int \frac{\delta F[f]}{\delta f(x)}\,\eta(x)\,dx = \int \frac{\delta F[G]}{\delta G(y)}\,\frac{\delta G[f](y)}{\delta f(x)}\,\eta(x)\,dxdy\,,$$

and thus, due to the arbitrary form of $\eta(x)$,

$$\frac{\delta F[f]}{\delta f(x)} = \int \frac{\delta F[G]}{\delta G(y)}\,\frac{\delta G[f](y)}{\delta f(x)}\,dy\,. \tag{A.38}$$

Equation (A.38) represents the chain rule of functional differentiation. It is valid, if the variation $\eta(x)$ generates all possible variations $\bar{\eta}(y)$ in the neighborhood of $G[f](y)$. This is guaranteed if there is a one-to-one correspondence between the admissible functions $f(x)$ and the corresponding functions $G(y)$ (at least locally) and both spaces of functions are sufficiently dense to define a functional derivative. The condition of a unique correspondence is satisfied in particular, if the kernel $\frac{\delta G[f](y)}{\delta f(x)}$ is invertible.

It is worthwhile to note a special case of the rule (A.38). If there is a unique relation between $f(x)$ and $G(y)$, i.e. if the form of the complete function $G(y)$ is uniquely determined by $f(x)$ and vice versa, one can consider the functional $F[G[f(x)](y)] \equiv f(x_0)$. Application of the chain rule (A.38) then leads to

$$\begin{aligned}\delta(x-x_0) = \frac{\delta f(x_0)}{\delta f(x)} &= \frac{\delta F[f]}{\delta f(x)} = \int \frac{\delta F[G]}{\delta G(y)}\,\frac{\delta G[f](y)}{\delta f(x)}\,dy \\ &= \int \frac{\delta f(x_0)}{\delta G(y)}\,\frac{\delta G(y)}{\delta f(x)}\,dy\,. \end{aligned} \tag{A.39}$$

This relation shows that one can always insert a complete set of variations in a variational derivative (here $\delta f(x_0)/\delta f(x)$), as long as there exists a one-to-one correspondence between the functions involved.

## A.4 Variational Principle

An apt example for the discussion of variational principles on the basis of functional calculus is the derivation of the Euler-Lagrange equations for the action functional (A.10). For the case of one degree of freedom,

$$A[q] = \int_{t_1}^{t_2} dt\, L(q, \dot{q}, t) \,, \tag{A.40}$$

which suffices to point out the main features, extrema are characterized by setting the first variation equal to zero. This implies

$$\delta A = \int_{t_1}^{t_2} dt\, [L(q + \delta q, \dot{q} + \delta \dot{q}, t) - L(q, \dot{q}, t)] = 0 \tag{A.41}$$

to first order in the variation of the variable and its derivative. Taylor expansion of the first term to first order gives

$$\delta A = \int_{t_1}^{t_2} dt\, \left[ \frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right] = 0 \,. \tag{A.42}$$

This is followed by partial integration of the second term with the result

$$\delta A = \int_{t_1}^{t_2} dt\, \left[ \frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right] \delta q + \left[ \frac{\partial L}{\partial \dot{q}} \delta q \right]_{t_1}^{t_2} = 0 \,. \tag{A.43}$$

For arbitrary variations $\delta q$ the Euler-Lagrange equations have to be satisfied,

$$\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} = 0 \,. \tag{A.44}$$

No further conditions apply, if the variation at the end points is restricted by boundary conditions,

$$\delta q(t_1) = \delta q(t_2) = 0 \,. \tag{A.45}$$

This restriction does not apply to the case of a free boundary, for which arbitrary variations at the points $t_1$ and $t_2$ are permitted. Therefore it is necessary to demand in addition the "natural boundary conditions" (see [728])

$$\left[ \frac{\partial L}{\partial \dot{q}} \right]_{t_1} = \left[ \frac{\partial L}{\partial \dot{q}} \right]_{t_2} = 0 \tag{A.46}$$

in this case.