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Functional differentiation under conservation constraints

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Abstract
The formula for differentiation of functionals $A[\rho]$ under conservation constraints of the form $\int f(\rho(x))\,\mathrm{d}x = K$, and some essential properties of this K-conserving functional differentiation, are derived. A generalization to include treatment of time-evolution is also given.

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Functional differentiation plays an essential role in all branches of physics. One of its basic occurrences is in the determination of extrema of physical quantities A with respect to some distribution function $\rho(x)$, functional derivatives appearing in the Euler equation belonging to the given extremizing problem,

$$\frac{\delta A[\rho]}{\delta \rho(x)} = 0. \qquad (1)$$

In most cases, only certain kinds of variations of the variable $\rho(x)$ of A are allowed, due to the given physical laws or to a restricted domain of $\rho(x)$ in the definition of $A[\rho]$, that is, various constraints have to be taken into account while making variations, or differentiating. Restricting the domain on which differentiation of a functional is made may go with the modification of the differentiational rules. In the determination of extrema, the well-known Lagrange method is a satisfactory tool to take a constraint

$$C[\rho] = 0 \qquad (2)$$

into consideration by a multiplier λ,

$$\frac{\delta A[\rho]}{\delta \rho(x)} - \lambda \frac{\delta C[\rho]}{\delta \rho(x)} = 0 \qquad (3)$$

as the value of λ is determinable by adjusting it so that the solution $\rho(x;\lambda)$ of the Euler–Lagrange equation (3) satisfies the constraint. However, the method of Lagrange multipliers does not provide a general, full treatment of inclusion of constraints into functional differentiation, which can be especially relevant in physics in nonequilibrium or time-dependent problems, as was demonstrated recently in [1, 2] in the case of problems of the density-functional formulation of quantum mechanics [3].

In [1], the analytical formula that describes how the form of a functional derivative changes due to the constraint of norm conservation of the functional variable,

$$\int \rho(x)\,\mathrm{d}x = N \tag{4}$$

has been derived:

$$\frac{\delta A[\rho]}{\delta_N \rho(x)} = \frac{\delta A[\rho]}{\delta\rho(x)} - \frac{1}{N}\int \rho(x')\frac{\delta A[\rho]}{\delta\rho(x')}\,\mathrm{d}x' \tag{5}$$

showing how the functional and the constraint together explicitly determine an additive term modifying the unconstrained functional derivative. The substantial property of this so-called number-conserving functional differentiation that it ruins the symmetry of multiple functional derivatives $\frac{\delta}{\delta\rho(x)}$ in their x arguments has been proved [1] to be crucial for the requirement of causality [4] in the time-dependent density-functional theory [3, 4]. The effect on functional differentiation of a more restricting and more complicated constraint on the domain of wavefunctions, namely, the restriction of the domain to wavefunctions that correspond to some density via the density–wavefunction map of density-functional theory, has also been pointed out to be unignorable [2], its neglect being pointed out to be the source of error in the derivation of incorrect results in density-functional theory.

Here, the formula for functional differentiation under a general (local) 'integral-conserving' constraint

$$\int f(\rho(x))\,\mathrm{d}x = K \tag{6}$$

will be presented, together with an extension to include a parameter in which the constraint is pointwise,

$$\int f(\rho(x,t))\,\mathrm{d}x = K(t) \tag{7}$$

to treat time-evolution.

To get the desired formula, the idea of [1] leading to equation (5) will be utilized. For this, as a starting point, finding an appropriate decomposition of $\rho(x)$ is necessary. It is important to recognize that two essential properties of the decomposition

$$\rho(x) = N\frac{g(x)}{\int g(x')\,\mathrm{d}x'} \tag{8}$$

make it the right choice to be the basis for the derivation of equation (5): (i) for arbitrary $g(x)$ it gives a $\rho(x)$ of norm N, (ii) it holds for $g = \rho$. In the case of a constraint of, e.g., $f(\rho) = \rho^n$, the appropriate decomposition,

$$\rho(x) = \sqrt[n]{\frac{K}{\int g^n(x')\,\mathrm{d}x'}}\,g(x) \tag{9}$$

arises quite trivially, but not for a general case including entropy conservation, with $f(\rho) = -k\rho\ln\rho$, for example. The general way of decomposing $\rho(x)$ so that the above-mentioned criteria are fulfilled is

$$\rho(x) = f^{-1}\left(\frac{K}{\int f(g(x'))\,\mathrm{d}x'}f(g(x))\right) \tag{10}$$

with $K = \int f(\rho(x))\,\mathrm{d}x$, which, indeed, gives equation (6) for any $g(x)$, and holds for $g = \rho$. Having equation (10), the K-conserving differentiation of a functional can be traced back to an unconstrained partial functional differentiation, similar to the case of N-conserving differentiation [1], as

$$\left(\frac{\delta\rho(x')[g,K]}{\delta g(x)}\right)_K\bigg|_{g=\rho} = \frac{\delta\rho(x')}{\delta_K\rho(x)} \tag{11}$$

or more generally,

$$\left(\frac{\delta A[\rho[g,K]]}{\delta g(x)}\right)_K\bigg|_{g=\rho} = \frac{\delta A[\rho]}{\delta_K\rho(x)} \tag{12}$$

since any variation of $g(x)$ at $\rho(x)$ conserves $\int f(\rho(x))\,\mathrm{d}x$ and $g(x)$ can run on $\rho(x)$ (of K). Thus, as

$$\left(\frac{\delta\rho(x')}{\delta g(x)}\right)_K = \frac{1}{f^{(1)}(\rho(x'))}\frac{K}{\int f(g(x''))\,\mathrm{d}x''}\Bigg(f^{(1)}(g(x'))\delta(x'-x) - \frac{f^{(1)}(g(x))}{\int f(g(x''))\,\mathrm{d}x''}f(g(x'))\Bigg) \tag{13}$$

$f^{(1)}$ denoting the first derivative of f, and

$$\left(\frac{\delta A[\rho[g,K]]}{\delta g(x)}\right)_K = \int \frac{\delta A[\rho]}{\delta\rho(x')}\left(\frac{\delta\rho(x')}{\delta g(x)}\right)_K \mathrm{d}x' \tag{14}$$

$$\frac{\delta\rho(x')}{\delta_K\rho(x)} = \delta(x'-x) - \frac{f^{(1)}(\rho(x))}{K}\frac{f(\rho(x'))}{f^{(1)}(\rho(x'))} \tag{15}$$

and

$$\frac{\delta A[\rho]}{\delta_K\rho(x)} = \int \frac{\delta A[\rho]}{\delta\rho(x')}\frac{\delta\rho(x')}{\delta_K\rho(x)}\,\mathrm{d}x' \tag{16}$$

emerge, from which finally

$$\frac{\delta A[\rho]}{\delta_K\rho(x)} = \frac{\delta A[\rho]}{\delta\rho(x)} - \frac{f^{(1)}(\rho(x))}{K}\int \frac{f(\rho(x'))}{f^{(1)}(\rho(x'))}\frac{\delta A[\rho]}{\delta\rho(x')}\,\mathrm{d}x'. \tag{17}$$

Following are some essential properties of K-conserving functional differentiation, arising from equation (17) (or simply from equation (16) in some cases):

(i) For any K-conserving derivative,

$$\int \frac{f(\rho(x))}{f^{(1)}(\rho(x))}\frac{\delta A[\rho]}{\delta_K\rho(x)}\,\mathrm{d}x = 0. \tag{18}$$

(ii) Besides equation (16),

$$\frac{\delta A[\rho]}{\delta_K\rho(x)} = \int \frac{\delta A[\rho]}{\delta_K\rho(x')}\frac{\delta\rho(x')}{\delta_K\rho(x)}\,\mathrm{d}x' \tag{19}$$

is also true, which can be considered as the analogue of

$$\frac{\delta A[\rho]}{\delta\rho(x)} = \int \frac{\delta A[\rho]}{\delta\rho(x')}\frac{\delta\rho(x')}{\delta\rho(x)}\,\mathrm{d}x'. \tag{20}$$

(iii) It is closely related to the nature of K-conserving functional differentiation that

$$\frac{\delta\{f(\rho(x'))/\int f(\rho(x''))\,\mathrm{d}x''\}}{\delta_K\rho(x)} = \frac{\delta\{f(\rho(x'))/\int f(\rho(x''))\,\mathrm{d}x''\}}{\delta\rho(x)}. \tag{21}$$

(iv) Two (unconstrained) $\frac{\delta}{\delta\rho(x)}$ derivatives yield the same $\frac{\delta}{\delta_K\rho(x)}$ derivative if and only if they differ only by some $f^{(1)}(\rho(x))B[\rho]$,

$$\frac{\delta A'[\rho]}{\delta\rho(x)} - \frac{\delta A[\rho]}{\delta\rho(x)} = f^{(1)}(\rho(x))B[\rho] \tag{22}$$

with $B[\rho]$ not depending on x, that is, a $\frac{\delta}{\delta_K\rho(x)}$ derivative determines the $\frac{\delta}{\delta\rho(x)}$ derivative only up to an additive $f^{(1)}(\rho(x))B[\rho]$. Equation (22) is true if

$$A'[\rho] = A[\rho] + h(K). \tag{23}$$

(v) K conservation spoils the symmetry of second $\frac{\delta}{\delta\rho(x)}$ derivatives in their x arguments, which can be exhibited well by the commutator

$$\begin{aligned}\left[\frac{\delta}{\delta_K\rho(x)}, \frac{\delta}{\delta_K\rho(x')}\right] = &-\frac{f^{(1)}(\rho(x'))}{K}\left(1 - \frac{f(\rho(x))f^{(2)}(\rho(x))}{f^{(1)^2}(\rho(x))}\right)\frac{\delta}{\delta\rho(x)} \\ &+ \frac{f^{(1)}(\rho(x))}{K}\left(1 - \frac{f(\rho(x'))f^{(2)}(\rho(x'))}{f^{(1)^2}(\rho(x'))}\right)\frac{\delta}{\delta\rho(x')} \\ &+ \frac{1}{K^2}\left(f^{(1)}(\rho(x))\frac{f(\rho(x'))f^{(2)}(\rho(x'))}{f^{(1)}(\rho(x'))}\right. \\ &\left. - f^{(1)}(\rho(x'))\frac{f(\rho(x))f^{(2)}(\rho(x))}{f^{(1)}(\rho(x))}\right)\int \mathrm{d}x''\frac{f(\rho(x''))}{f^{(1)}(\rho(x''))}\frac{\delta}{\delta\rho(x'')}.\end{aligned} \tag{24}$$

Note that the symmetry is also broken if only one of the functional differentiations is constrained, as was shown in [1] with the exchange-correlation kernel of time-dependent density-functional theory.

(vi) For functionals composed from two functionals there are rules similar to those of unconstrained functional differentiation, namely,

$$\frac{\delta(A+B)}{\delta_K\rho(x)} = \frac{\delta A}{\delta_K\rho(x)} + \frac{\delta B}{\delta_K\rho(x)} \tag{25}$$

$$\frac{\delta(AB)}{\delta_K\rho(x)} = \frac{\delta A}{\delta_K\rho(x)}B + A\frac{\delta B}{\delta_K\rho(x)} \tag{26}$$

and the chain rule

$$\frac{\delta A[b(x')]}{\delta_K\rho(x)} = \int \frac{\delta A}{\delta b(x')}\frac{\delta b(x')}{\delta_K\rho(x)}\,\mathrm{d}x'. \tag{27}$$

Giving an alternative possibility for the definition of a K-conserving functional derivative, it can be shown that a $\frac{\delta}{\delta_K\rho(x)}$ derivative is that part of a $\frac{\delta}{\delta\rho(x)}$ derivative that gives, for any variation $\delta\rho(x)$, the (K-conserving) variation of a functional that is due to the K-conserving part of $\delta\rho(x)$, $\delta_K\rho(x)$, via

$$\delta_K A[\rho] = \int \frac{\delta A[\rho]}{\delta_K\rho(x)}\delta\rho(x)\,\mathrm{d}x \tag{28}$$

where $\delta_K A[\rho] = A[\rho + \delta_K\rho] - A[\rho]$. Considering that arbitrary variations of $\rho(x)$ are allowed in the integrand in equation (28), equation (28) can be a definition for the K-conserving derivative of a functional, analogous to

$$\delta A[\rho] = \int \frac{\delta A[\rho]}{\delta\rho(x)}\delta\rho(x)\,\mathrm{d}x \tag{29}$$

for unconstrained derivatives. The basis for the justification of equation (28) is the decomposition of a variation $\delta\rho(x)$ into a K-conserving and a remaining part,

$$\delta\rho(x) = \delta_K\rho(x) + \delta_{\bar{K}}\rho(x). \tag{30}$$

This can be achieved with the help of the two-variable functional $\rho[g, K]$ defined by equation (10), the full variation of which is given by

$$\delta\rho[g, K] = \int \left(\frac{\delta\rho[g, K]}{\delta g(x')}\right)_K \delta g(x')\,\mathrm{d}x' + \left(\frac{\partial\rho\,[g, K]}{\partial K}\right)_g \partial K \tag{31}$$

for $g = \rho$, yielding the desired decomposition equation (30); that is,

$$\begin{aligned}\delta_K\rho(x) &= \int \left(\frac{\delta\rho(x)[g, K]}{\delta g(x')}\right)_K \delta g(x')\,\mathrm{d}x'\bigg|_{g=\rho} \\ &= \int \left\{\delta(x - x') - \frac{f^{(1)}(\rho(x'))}{K}\,\frac{f(\rho(x))}{f^{(1)}(\rho(x))}\right\} \delta\rho(x')\,\mathrm{d}x' \end{aligned}\tag{32}$$

and

$$\delta_{\bar{K}}\rho(x) = \left(\frac{\partial\rho(x)\,[g, K]}{\partial K}\right)_g \partial K\bigg|_{g=\rho} = \frac{1}{K}\,\frac{f(\rho(x))}{f^{(1)}(\rho(x))}\partial K \tag{33}$$

the sum of which, of course, gives $\delta\rho(x)$ identically. Inserting equation (32) into

$$\delta_K A[\rho] = \int \frac{\delta A[\rho]}{\delta\rho(x)}\delta_K\rho(x)\,\mathrm{d}x \tag{34}$$

implied by equation (29), and taking equation (11) and (16) (that is equation (12)) into consideration, then leads to equation (28). Similarly, with the use of equation (33),

$$\delta_{\bar{K}} A[\rho] = \int \frac{\delta A[\rho]}{\delta_{\bar{K}}\rho(x)}\delta\rho(x)\,\mathrm{d}x \tag{35}$$

with

$$\frac{\delta A[\rho]}{\delta_{\bar{K}}\rho(x)} = \frac{f^{(1)}(\rho(x))}{K}\int \frac{f(\rho(x'))}{f^{(1)}(\rho(x'))}\,\frac{\delta A[\rho]}{\delta\rho(x')}\,\mathrm{d}x' \tag{36}$$

which is the other component of an unconstrained, that is, full derivative,

$$\frac{\delta A[\rho]}{\delta\rho(x)} = \frac{\delta A[\rho]}{\delta_K\rho(x)} + \frac{\delta A[\rho]}{\delta_{\bar{K}}\rho(x)}. \tag{37}$$

From equation (28), for the case of $\delta_K A[\rho] = 0$ for any variation $\delta_K\rho(x)$ of $\rho(x)$, the Euler equation

$$\frac{\delta A[\rho]}{\delta_K\rho(x)} = 0 \tag{38}$$

follows straight away, yielding, if $A[\rho]$ has an unconstrained derivative,

$$\frac{\delta A[\rho]}{\delta\rho(x)} = \lambda f^{(1)}(\rho(x)) \tag{39}$$

(with equation (6)), which can be obtained via equation (34) as well, considering

$$\int f^{(1)}(\rho(x))\,\delta\rho(x)\,\mathrm{d}x = 0. \tag{40}$$

That equation (38) gives back just the usual Lagrange method, equation (39) with equation (6), if $A[\rho]$ has an unconstrained derivative, can be seen in the following way: from equation (38), utilizing equation (17),

$$\frac{\delta A[\rho]}{\delta\rho(x)} = f^{(1)}(\rho(x))\frac{1}{K}\int \frac{f(\rho(x'))}{f^{(1)}(\rho(x'))}\,\frac{\delta A[\rho]}{\delta\rho(x')}\,\mathrm{d}x' \tag{41}$$

arises, giving equation (39), the substitution of which for $\frac{\delta A[\rho]}{\delta\rho(x)}$ into equation (41) to determine the $\rho(x)$ with the proper K,

$$\lambda f^{(1)}(\rho(x)) = f^{(1)}(\rho(x))\frac{1}{K}\int \frac{f(\rho(x'))}{f^{(1)}(\rho(x'))}\lambda f^{(1)}(\rho(x'))\,\mathrm{d}x' \tag{42}$$

gives the (K-conserving) constraint (6). Equation (39) also gives back equation (38), as K-conserving differentiation cancels a $c\,f^{(1)}(\rho(x))$ out (see property (iv) above).

Besides the simplest case of constraint (6), that is, number conservation, considered in [1], the conservation of the entropy

$$S = \int -k\,\rho(x)\,\ln\rho(x)\,\mathrm{d}x \tag{43}$$

gives another important example of constraint on functional differentiation. For this case equation (17) yields

$$\frac{\delta A[\rho]}{\delta_S\rho(x)} = \frac{\delta A[\rho]}{\delta\rho(x)} - \frac{\ln\rho(x)+1}{S}\int \frac{-k\,\rho(x')\ln\rho(x')}{\ln\rho(x')+1}\frac{\delta A[\rho]}{\delta\rho(x')}\,\mathrm{d}x' \tag{44}$$

the formula of entropy-conserving functional differentiation. (Note that x in the above formulae can denote a set of variables, e.g., phase-space coordinates, as well.) To treat the 'reverse' problem in statistical physics [5], namely, differentiation of the entropy under conservation constraints of statistical averages of dynamical functions, however, a slight generalization of the derived formulae is necessary to include constraints of the form

$$\int f(\rho(x), x)\,\mathrm{d}x = K \tag{45}$$

where f has a direct dependence on x, as in $\int \rho(x)H(x)\,\mathrm{d}x = E$, for example. To do this, the x variable of $f(\rho, x)$ can be handled as a parameter in the decomposition equation (10), that is,

$$f(\rho, x) = f_x(\rho) \tag{46}$$

with which

$$\rho(x) = f_x^{-1}\left(\frac{K}{\int f_{x'}(g(x'))\,\mathrm{d}x'}f_x(g(x))\right) \tag{47}$$

giving

$$\frac{\delta A[\rho]}{\delta_K\rho(x)} = \frac{\delta A[\rho]}{\delta\rho(x)} - \frac{f_x^{(1)}(\rho(x))}{K}\int \frac{f_{x'}(\rho(x'))}{f_{x'}^{(1)}(\rho(x'))}\frac{\delta A[\rho]}{\delta\rho(x')}\mathrm{d}x'. \tag{48}$$

For time-dependent problems, an extension of equation (17) is needed to include constraints with an external parameter, equation (7). In this case, the starting point in the derivation is the decomposition

$$\rho(x,t) = f^{-1}\left(\frac{K(t)}{\int f(g(x',t))\,\mathrm{d}x'}f(g(x,t))\right) \tag{49}$$

of $\rho(x,t)$, with the use of which

$$\frac{\delta A[\rho]}{\delta_K\rho(x,t)} = \frac{\delta A[\rho]}{\delta\rho(x,t)} - \frac{f^{(1)}(\rho(x,t))}{K(t)}\int \frac{f(\rho(x',t))}{f^{(1)}(\rho(x',t))}\frac{\delta A[\rho]}{\delta\rho(x',t)}\mathrm{d}x' \tag{50}$$

emerges as the formula for $K(t)$-conserving functional differentiation.

In summary, formula (17) for differentiation of functionals under conserving constraints of the form (6), 'K-conserving' constraints, has been derived, together with the essential properties (18)–(27) and an alternative definition for a K-conserving derivative, equation (28), that is not related to an unconstrained derivative (and may be general for arbitrary constraints).

Two extensions of equation (17), equations (48) and (50), have also been presented to include important cases, for example, for statistical physics and to handle time-evolution.

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