

The nuclear Energy Density Functional formalism

Preliminary document

Functional and functional derivatives

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We introduce the notions of functional and functional derivative.

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I. FUNCTIONAL

A function maps a number onto another number. A functional assigns a number to a function. In other words, a functional is an application that takes a vector as its argument or input and returns a scalar. Its use goes back to the calculus of variations where one searches for a function which minimizes a certain functional. A particularly important application in physics is the search for the state of a system that minimizes its energy.

For example, let us consider all periodic functions $r(\theta)$, $0 \leq \theta \leq 2\pi$, i.e. $r(\theta + 2\pi) = r(\theta)$. For such a curve, one can define P as its length and A as the area it encloses. P and A are functionals of $r(\theta)$, in the sense that, for a given curve, such as the ellipse

$$r(\theta) = \frac{1}{\sqrt{\sin^2(\theta) + 4 \cos^2(\theta)}} , \quad (1)$$

there is a single well-defined value of P and A . We use $P[r]$ and $A[r]$ as a notation to indicate such functional dependencies. A second example is the Coulomb potential at position \vec{r} that is a functional of the local charge density $\rho(\vec{r})$

$$F[\rho] \equiv V(\vec{r}) = \frac{1}{4\pi\epsilon_0} \int d\vec{r}' \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} . \quad (2)$$

Given a particular charge-density function and a point in space, one can compute a number which represents the Coulomb potential created at that point by the specified charge-density function.

II. FUNCTIONAL DERIVATIVES

In the nuclear Energy Density Functional approach, one is led to minimize the energy with respect to (constrained) variations of neutron and proton density matrices. Consequently, it is necessary to specify how to differentiate a functional.

A. Definition

We consider the restrictive case where a functional F acts on a Banach space or even a Hilbert space that comes with the scalar product $\langle f, g \rangle$. The functional derivative of the functional F of ρ , denoted as $\frac{\delta F}{\delta \rho}$, is a distribution $\delta F[\rho]$ defined such that, for any test function φ , one has

$$\langle \frac{\delta F}{\delta \rho}, \varphi \rangle \equiv \frac{d}{d\epsilon} F[\rho + \epsilon\varphi] \Big|_{\epsilon=0} . \quad (3)$$

The functional derivative describes how the functional $F[\rho]$ changes as a result of an arbitrary small change $\delta\rho = \varphi$. Note that such a definition can be easily generalized to a functional of several functions by introducing the differential derivatives $\delta F[\rho]$ as in standard calculus.

B. Standard physics cases

We now consider the even more particular case of real *local* functionals F expressed as

$$F[\rho] \equiv \int d\vec{r} f[\vec{r}, \rho(\vec{r})] , \quad (4)$$

and acting on the space of square integrable real functions ρ whose associated scalar product is defined as

$$\langle f, g \rangle \equiv \int d\vec{r} f(\vec{r}) g(\vec{r}) . \quad (5)$$

The functional F is local in the sense that it is given by a single integral over a function that depends only on one position vector¹. The functional derivative of F is in this case

$$\frac{d}{d\epsilon} F[\rho + \epsilon\varphi] \Big|_{\epsilon=0} \equiv \frac{d}{d\epsilon} \int d\vec{r} f[\vec{r}, \rho(\vec{r}) + \epsilon\varphi(\vec{r})] \Big|_{\epsilon=0} = \int d\vec{r} \frac{\partial f}{\partial \rho(\vec{r})} \varphi(\vec{r}) , \quad (6)$$

such that

$$\frac{\delta F}{\delta \rho(\vec{r})} = \frac{\partial f}{\partial \rho(\vec{r})} . \quad (7)$$

All previous definitions can be easily extended to *non-local* functionals that depend on a function of several position vectors $(\vec{r}_1, \vec{r}_2, \dots)$ as well as to functionals of several functions. Also, it is easy to show that the standard chain-rule technique applies when the functional F is defined through a composition of functions.

In order to illustrate the above, let us come back to the example of the Coulomb potential (Eq. (2)) that is a functional of the local charge density $\rho(\vec{r})$. In such a case, one finds

$$\frac{d}{d\epsilon} F[\rho + \epsilon\varphi] \Big|_{\epsilon=0} = \frac{d}{d\epsilon} \frac{1}{4\pi\epsilon_0} \int d\vec{r}' \frac{\rho(\vec{r}') + \epsilon\varphi(\vec{r}')}{|\vec{r} - \vec{r}'|} \Big|_{\epsilon=0} = \frac{1}{4\pi\epsilon_0} \int d\vec{r}' \frac{\varphi(\vec{r}')}{|\vec{r} - \vec{r}'|} , \quad (8)$$

such that indeed

$$\frac{\delta V(\vec{r})}{\delta \rho(\vec{r}')} = \frac{\partial}{\partial \rho(\vec{r}')} \left[\frac{1}{4\pi\epsilon_0} \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} \right] = \frac{1}{4\pi\epsilon_0} \frac{1}{|\vec{r} - \vec{r}'|} . \quad (9)$$

¹ In that sense the input function already depends on three scalar variables but the common vocabulary in physics is to count the number of three-dimensional vectors as for characterizing the functional as being local or non-local.