IP326. Lecture 21. Thursday, March 14, 2019

● Mathematical interlude: A non-rigorous introduction to functional calculus

As our earlier discussions have shown, a dynamical variable A under thermal equilibrium conditions is effectively a random variable that can fluctuate across a range of possible values. The distribution of these values at some time t, $P(A,t)$, contains considerably more information about the dynamics of A than just its mean or variance, which are the quantities one typically determines from an equation for the evolution of A. What we'd like to do now is use this evolution equation to determine $P(A,t)$, or at least to set up an equation for it that could in principle be solved. To make the connection between $A(t)$ and $P(A,t)$, we'll adopt an approach based on an exact result known as Novikov's theorem. This theorem is formulated in terms of mathematical objects referred to as functionals, and in this section, we'll discuss a few of their relevant properties.

Let's first recall that a quantity f is said to be a function of a variable x if given a value for x, the value of f is determined. In the equation below, for example,

$$f(x) = x^2$$

f is said to be a function of x because its value is specified once a value is assigned to x.

In general, f can depend on more than one variable, as in the equation below

$$f(x_1,\ldots,x_2) = \sum_{i=1}^{n} x_i^2$$

where f is said to be a function of x_1, x_2, …, x_n. A function that depends on an effectively infinite number of independent variables can be said to be a *functional*. Somewhat more precisely, a quantity F is said to be a functional of a function $y(x)$ (for some range of x) if given $y(x)$ in the chosen interval of x, the value of F is determined. The dependence of F on $y(x)$ is denoted $F[y]$ (note the square brackets and the omission of the argument of y.) Here are some examples of functionals

$$F_1[y] = \int_a^b dx G(x) y(x), \quad G(x) \text{ being some function of } x,$$

$$F_2[y] = \int_a^b dx \exp[y(x)]$$

There are several things about the functional F that must be borne in mind: 1) F is not a function of x, 2) F is not a function of a function (contrary to the definition in the glossary of Chaikin and Lubensky's textbook on condensed matter physics.) What we generally understand by the term "function of a function" can illustrated by the following example: let $f(x) = x+1$ be some function of x and $g(x) = x^2$ be another. Both $g(f(x)) = (x+1)^2$ and $f(g(x)) = x^2 + 1$ are functions of functions; their values are specified once the value of *x* is specified. For the value of a functional *F* to be specified, however, an effectively infinite number of variable values must be specified. Which is why *F* cannot be described as a function of a function.

Functional derivatives

If *f* is a function of *x*, the derivative of *f* with respect to *x*, *df*/*dx*, is defined as

$$\frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

Thus, *df*/*dx* can be identified from the relation

$$\Delta f = \frac{df}{dx} \Delta x$$

in the limit of small Δx. If *f* is a function of many variables, the corresponding relation is

$$\Delta f = \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} \Delta x_i$$

By analogy, we identify the functional derivative of a functional *F* with respect to a function *y* at the point *x*, which we denote, $\delta F[y]/\delta y(x)$, from the equation

$$\delta F = F[y+\delta y] - F[y] \equiv \int_a^b dx \frac{\delta F}{\delta y(x)} \delta y(x)$$

where δy is some arbitrary change in the function *y* at the point *x* that can be defined as $\delta y(x) = \lim_{\varepsilon \to 0} \varepsilon Y(x)$, *Y*(*x*) being some other arbitrary function of *x*.

Examples

1. If $F[y] = \int_a^b dx G(x) y(x)$, find $\delta F[y]/\delta y(x)$.

Answer

$$\delta F = F[y+\delta y] - F[y] \equiv \int_a^b dx G(x)(y(x)+\delta y(x)) - \int_a^b dx G(x) y(x)$$

$$= \int_a^b dx G(x) \delta y(x)$$

Hence,

$$\frac{\delta F[y]}{\delta y(x)} = G(x)$$

2. If $F[y] = \int_a^b dx \exp[\beta y(x)]$, where β is a constant, find $\delta F[y]/\delta y(x)$.

<u>Answer</u>

$$\delta F = F[y+\delta y] - F[y] \equiv \int_a^b dx e^{\beta(y(x)+\delta y(x))} - \int_a^b dx e^{\beta y(x)}$$

$$= \int_a^b dx e^{\beta y(x)} \left(1 + \beta \delta y(x) + \cdots\right) - \int_a^b dx e^{\beta y(x)}$$

$$= \beta \int_a^b dx e^{\beta y(x)} \delta y(x)$$

And so,

$$\frac{\delta F[y]}{\delta y(x)} = \beta e^{\beta y(x)}$$

3. If $F[y] = y(x)$, find $\delta F[y]/\delta y(x)$.

<u>Answer</u> Strictly speaking, the given equation for F does not define a functional, but it can be recast so that it does, at least in terms of appearance. The way to do this is to rewrite the equation as

$$F[y] = \int_{-\infty}^{\infty} dx' y(x') \delta(x - x')$$

Then,

$$\delta F = F[y+\delta y]-F[y] \equiv \int_{-\infty}^{\infty} dx'(y(x')+\delta y(x'))\delta(x-x') - \int_{-\infty}^{\infty} dx' y(x')\delta(x-x')$$

$$= \int_{-\infty}^{\infty} dx' \delta(x-x')\delta y(x')$$

Therefore,

$$\frac{\delta F[y]}{\delta y(x')} = \frac{\delta y(x)}{\delta y(x')} = \delta(x-x')$$

Higher order functional derivatives are defined much the way they are in discrete variable calculus. For instance, if $F[y]$ is a functional of $y(x)$, then the functional derivative of $\delta F[y]/\delta y(x)$ with respect to a function y at the point x' can be regarded as the second order functional derivative of F, and denoted $\delta^2 F[y]/\delta y(x')\delta y(x)$.

Examples

1. Let

$$F[y] = \int_a^b dx y^2(x)$$

Then,

$$\frac{\delta F[y]}{\delta y(x)} = 2y(x)$$

and

$$\frac{\delta^2 F[y]}{\delta y(x')\delta y(x)} = 2\delta(x-x')$$

2. Suppose

$$F[y] = y(x)$$

Then,

$$\frac{\delta F[y]}{\delta y(x')} = \delta(x - x')$$

and

$$\frac{\delta^2 F[y]}{\delta y(x'')\delta y(x')} = 0$$

3. Similarly, if

$$F[y] = \int_a^b dx'' G(x'') y(x'')$$

then

$$\frac{\delta^2 F[y]}{\delta y(x)\delta y(x')} = \frac{\delta}{\delta y(x)} G(x') = 0$$

Functional Calculus

Most rules of ordinary differential calculus – such as the chain rule and the product rule – apply, in generalized form, to functional derivatives as well.

1. The Chain Rule

Suppose $H[y] = e^{F[y]}$. Then $\frac{\delta H[y]}{\delta y(x)} = e^{F[y]} \frac{\delta F[y]}{\delta y(x)}$.

Proof

$$H[y + \delta y] - H[y] = e^{F[y+\delta y]} - e^{F[y]}$$

Now $$F[y + \delta y] = F[y] + \int dx \frac{\delta F[y]}{\delta y(x)} \delta y(x)$$

Therefore,

$$H[y+\delta y]-H[y]=e^{F[y]}\left(1+\int dx\,\frac{\delta F[y]}{\delta y(x)}\delta y(x)+\cdots\right)-e^{F[y]}$$

$$=\int dx e^{F[y]}\frac{\delta F[y]}{\delta y(x)}\delta y(x)$$

Hence, $\frac{\delta H[y]}{\delta y(x)}=e^{F[y]}\frac{\delta F[y]}{\delta y(x)}$, as asserted.

2. The Product Rule

Suppose $H[y]=F_1[y]F_2[y]$. Then $\frac{\delta H[y]}{\delta y(x)}=F_2\frac{\delta F_1[y]}{\delta y(x)}+F_1\frac{\delta F_2[y]}{\delta y(x)}$

Proof

$$\delta H[y]=F_1[y+\delta y]F_2[y+\delta y]-F_1[y]F_2[y]$$

$$=\left(F_1[y]+\int dx\,\frac{\delta F_1[y]}{\delta y(x)}\delta y(x)\right)\left(F_2[y]+\int dx\,\frac{\delta F_2[y]}{\delta y(x)}\delta y(x)\right)-F_1[y]F_2[y]$$

$$=\int dx\left(F_2[y]\frac{\delta F_1[y]}{\delta y(x)}+F_1[y]\frac{\delta F_2[y]}{\delta y(x)}\right)\delta y(x)$$

So $\frac{\delta H[y]}{\delta y(x)}=F_2\frac{\delta F_1[y]}{\delta y(x)}+F_1\frac{\delta F_2[y]}{\delta y(x)}$, as asserted.

Once the notion of multiple derivatives of a functional is formalized, it becomes possible to extend other useful results from ordinary calculus to the functional realm. One such result is the Taylor's series, which for a functional is defined as

$$F[y]=\sum_{k=0}^{\infty}\frac{1}{k!}\int dx_1\cdots\int dx_k\,\left.\frac{\delta^k F[y]}{\delta y(x_1)\cdots\delta y(x_k)}\right|_{y=0}y(x_1)\cdots y(x_k)$$

in analogy with the Taylor's series expansion of a function of several variables. (N.B. In the equation above, the $k=0$ term in the sum is understood to mean just $F[0]$.)