Appendix B1: Notes on Functionals

The theory of functionals is an obvious generalization of the idea of an ordinary function. Recall that we can have a function $f(\mathbf{x}) = f(x_1, \ldots, x_n)$, such that

$$y = f(x_1, \ldots, x_n) \tag{1}$$

maps the set of variables $\{x_j\}$ to a single number y; we have a "many-to-one" mapping.

A *functional* maps a set of functions $\phi_j(x)$ to a single number, i.e.,

$$y = F\left[\phi_1(x), \ldots, \phi_n(x)\right] \tag{2}$$

with a mapping now from a space of functions to the field of real or complex numbers. Now, we can typically represent a function $\phi(x)$ as an infinite set of numbers, either

(a) as the infinite set of numbers $\phi_1 = \phi(x_1),\ \phi_2 = \phi(x_2), \ldots,$ where the $\{x_j\}$ take all possible values of x, or

(b) by a sum over orthonormal functions, as

$$\phi(x) = \sum_n \phi_n \chi_n(x) \tag{3}$$

where $\int \mathrm{d}x\ \chi_n(x)\chi_m(x) = \delta_{nm}$, defining $\phi(x)$ by the infinite set of numbers $\{\phi_n\}$,

Thus in a well-defined sense, a functional is like a generalization of (1) to an infinite set of variables. It is useful to give a few examples for orientation:

(i) Energy or free energy functionals in physics; for example

$$\mathcal{H}[\phi] \;=\; \int \mathrm{d}^D\mathbf{r}\,\big(-\frac{\hbar^2}{2m}\phi(\mathbf{r})\nabla^2\phi(\mathbf{r})\big) \;+\; \int \mathrm{d}^D\mathbf{r} \int \mathrm{d}^D\mathbf{r}'\ \phi^2(\mathbf{r})V(\mathbf{r}-\mathbf{r}')\phi^2(\mathbf{r}') \tag{4}$$

(ii) The action functional in field theory or ordinary classical mechanics:

$$\begin{aligned} S[q,\dot{q}] \;&=\; \int \mathrm{d}t\ \mathcal{L}(q,\dot{q};t) \qquad \text{(classical mechanics)} \\ S[\phi] \;&=\; \int \mathrm{d}^D x\, \mathcal{L}\big(\phi(x), \partial^\mu x\big) \qquad \text{(field theory)} \end{aligned} \tag{5}$$

(iii) The propagator in quantum mechanics; one has

$$\psi(\mathbf{r},t) \;=\; \int \mathrm{d}^D\mathbf{r}'\, G(\mathbf{r},\mathbf{r}';t,t')\psi(\mathbf{r}',t) \;\equiv\; F[\psi] \tag{6}$$

defining the wave-function $\psi(\mathbf{r},t)$ as a functional of the function $\psi(\mathbf{r}',t')$ at an earlier time; moreover we have

$$G(\mathbf{r},\mathbf{r}';t,t') \;=\; \int_{q(t')=\mathbf{r}'}^{q(t)=\mathbf{r}} \mathcal{D}q(\tau)\, e^{\frac{i}{\hbar}\int \mathrm{d}t\,\mathcal{L}(q,\dot{q};\tau)} \tag{7}$$

which defines $G(\mathbf{r}, \mathbf{r}'; t, t')$ as a *functional integral* over the set of all paths $q(\tau)$ between the end-points of the path integral at $(\mathbf{r}', t')$ and $(\mathbf{r}, t)$. Functional integrals will be defined more generally below.

(iv) Probability theory deals with probability functionals - the generalization of ordinary probability functions to "processes". Thus, the probability function $\mathcal{P}(x)$ describes the "outcome" x (a number) in some random sampling. But suppose the outcome is now some "process" $\phi(x)$, now a function of a variable x. We then deal with a functional $\mathcal{P}[\phi]$, assigning a probability to each possible process $\phi(x)$. Likewise, just as the expectation value $A(x)$, depending on the random variable x, is given by $\langle A \rangle = \int \mathrm{d}x\, \mathcal{P}(x) A(x)$, we have

$$\langle A \rangle \;=\; \int \mathcal{D}\phi(x)\, \mathcal{P}[\phi] A[\phi] \tag{8}$$

for the expectation value of some variable $A[\phi(x)]$ depending now on a process $\phi(x)$. The most common probability functional $\mathcal{P}[\phi]$ is that for a "Gaussian random process", for which

$$\mathcal{P}[\phi] \;\longrightarrow\; \left|\det K(x, x')\right|^{1/2} e^{-\frac{1}{2}\int \mathrm{d}x \int \mathrm{d}x'\, \phi(x) K(x-x') \phi(x')} \tag{9}$$

where the determinant, discussed below, is defined by

$$\int \mathcal{D}\phi(x)\, e^{-\frac{1}{2}\int \mathrm{d}x \int \mathrm{d}x'\, \phi(x) K(x-x') \phi(x')} \;=\; \left|\det K(x, x')\right|^{-1/2} \tag{10}$$

so that we have a normalized $\mathcal{P}[\phi]$:

$$\int \mathcal{D}\phi(x)\, \mathcal{P}[\phi] \;=\; 1 \tag{11}$$

In what follows we outline the theory of functionals as it applies to simple problems in quantum mechanics, statistical mechanics, and field theory (for probability theory, see App. B). The presentation will not be mathematically sophisticated, nor pretend to generality. In applications to physics, the functions $\phi(x)$, $q(t)$, etc., will often be assumed smooth.

App. B.1.1: FUNCTIONAL INTEGRATION

This will be considered as a simple generalization of ordinary integration over a finite set of variables, in the limit as the number of variables goes to infinity. To see what is involved, let's consider the example of a simple Gaussian integral. In one dimension this is just

$$I_0 \;=\; \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{\sqrt{2\pi}}\, e^{-\frac{1}{2}Kx^2 + Jx} \;=\; \frac{1}{\sqrt{K}}\, e^{\frac{1}{2}J^2/K} \tag{12}$$

and we want to generalize this to N dimensions, and then let $N \to \infty$, Let's first redefine the integration variable to get rid of the $\sqrt{2\pi}$ factor, i.e., let $x \to \tilde{x} = x/\sqrt{2\pi}$, and now consider the integral

$$I \;=\; \int \mathrm{d}^n\tilde{x}\; e^{-\frac{1}{2}\sum_{ij}\tilde{x}_i K_{ij}\tilde{x}_j + \sum_j J_j\tilde{x}_j} \;=\; \int \mathrm{d}\tilde{\mathbf{x}}\; e^{-\frac{1}{2}\tilde{\mathbf{x}}\mathbf{K}\tilde{\mathbf{x}} + \mathbf{J}\tilde{\mathbf{x}}} \tag{13}$$

for $\tilde{\mathbf{x}} = (\tilde{x}_1, \ldots, \tilde{x}_N)$. For $\mathbf{J} = (J_1, \ldots, J_N) = 0$, this is easily done, for we simply diagonalize $\mathbf{K} = K_{ij}$, to find

$$I_0 \;=\; \int \mathrm{d}^n\tilde{x}\; e^{-\frac{1}{2}\sum_{ij}\tilde{x}_i K_{ij}\tilde{x}_j} \;=\; |\det K_{ij}|^{-1/2} \tag{14}$$

If we now add back the term $\mathbf{J}\tilde{\mathbf{x}}$ in the exponent, we see we can make the same manoeuvre by "completing the square", i.e., writing (now suppressing the tilde over $\tilde{\mathbf{x}}$):

$$\begin{aligned} S(\mathbf{x}) \;&=\; \frac{1}{2}\mathbf{x}\mathbf{K}\mathbf{x} - \mathbf{J}\mathbf{x} \;=\; S(\mathbf{x}^0) + \frac{1}{2}(\mathbf{x}-\mathbf{x}^0)\mathbf{K}(\mathbf{x}-\mathbf{x}^0) \\ \text{where} \qquad & \mathbf{x}^0 = \mathbf{J}\mathbf{K}^{-1} \qquad\qquad (\text{i.e., } x^0_j = K^{-1}_{ij}J_j\;) \end{aligned} \tag{15}$$

and then redoing the Gaussian integration with $\mathbf{x}^0$ as the new "origin". Thus we get the result

$$I \;=\; \int d\mathbf{x}\; e^{-S(\mathbf{x})} \;\equiv\; \int d\mathbf{x}\; e^{-\frac{1}{2}\tilde{\mathbf{x}}\mathbf{K}\tilde{\mathbf{x}} + \mathbf{J}\tilde{\mathbf{x}}} \;=\; \frac{1}{|\mathbf{K}|^{1/2}}\; e^{\frac{1}{2}\mathbf{J}\mathbf{K}^{-1}\mathbf{J}} \tag{16}$$

Now this allows us to jump to the limit $N \to \infty$. The determinant $|\mathbf{K}| = \det K_{ij}$ is well-defined when N is finite. What we will suppose is that in the limit as $N \to \infty$, we can still sensibly define quantities like $S(\mathbf{x})$ and $|\mathbf{K}|$. Whether this is possible is a subtle mathematical question (it is certainly not possible in general!), but in physical applications, one typically always returns back to a case where N is finite - in any such application, there will typically be IR and UV cut-offs that make it so (and smooth all the functions concerned). Thus we now define the functional generalization of (16), to be

$$\begin{aligned} I \;&=\; \int \mathcal{D}x(t)\; e^{-S[x]} \\ &=\; \int \mathcal{D}x(t)\; e^{-\frac{1}{2}\int \mathrm{d}t \int \mathrm{d}t'\; x(t)K(t,t')x(t') + \int \mathrm{d}t\; J(t)x(t)} \end{aligned} \tag{17}$$

where the continuously varying parameter t is now introduced as a proxy for the index j; the functional integral is then

$$\int \mathcal{D}x(t) \;=\; \lim_{N\to\infty} \int \mathrm{d}\tilde{\mathbf{x}} \;=\; \lim_{N\to\infty} \frac{1}{(2\pi)^{N/2}} \prod_{j=1}^{N} \int_{-\infty}^{\infty} \mathrm{d}x(t_j) \tag{18}$$

where the times t_j are spaced by infinitesimal intervals, i.e., we let $\mathrm{d}t = t_{j+1} - t_j = T/N$, where T is the time interval involved (we now call t the "time").

Then the answer we get for the functional integral is

$$I = \int \mathcal{D}x(t)\, e^{-S[x]} \;=\; \frac{1}{|\det K(t,t')|^{1/2}} \exp\left\{ \frac{1}{2} \int \mathrm{d}t \int \mathrm{d}t'\; J(t) K^{-1}(t,t') J(t') \right\} \tag{19}$$

where the inverse function is defined as the obvious generalization of the inverse of a finite matrix, i.e.,

$$\int \mathrm{d}t'\; K(t_1,t') K^{-1}(t',t_2) \;=\; \delta(t_1 - t_2) \tag{20}$$

Again, we note that objects like $\det K$, or the integral itself, will be infinite when $N \to \infty$. However in physical applications we will see that these infinite quantities divide out, by normalization. This was already obvious in eqs. (9)-(11) above, where we had to divide out the determinant; but this determinant simply normalized the probability distribution.

We also notice that there is no need to work with a specific basis when defining these functional integrals. Just as we can make a similarity transformation in an expression like (13) or (16), i.e., rotate to a new orthonormal basis $\mathbf{y}$, where $\mathbf{y} = (y_1, \ldots, y_N)$, we can rotate in functional space (i.e., in the space of basis functions) to rewrite a functional integral. Thus, suppose we Fourier transform $x(t)$, such that

$$x(t) \;=\; \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\, e^{-i\omega t} x(\omega) \tag{21}$$

Then we can Fourier transform the functional integral in the same way - we will then have

$$I \;=\; \int \mathcal{D}x(\omega)\, e^{-S[x]} \tag{22}$$

with a corresponding change in the measure in (18).

App. B.1.2: FUNCTIONAL DIFFERENTIATION

We now want to define the inverse operation to functional integration. Just as functional integration is supposed to a generalization to a function space of ordinary integration, over an infinite set of functions, we can see functional differentiation as an infinite-dimensional generalization of ordinary partial differentiation for a finite set of variables. Recall that, where differentiation is well-defined, we can write for a function $f(x)$ of a single variable x, that

$$f(x_0 + \delta x) \;=\; f(x_0) \;+\; \sum_{n=1}^{\infty} \frac{1}{n!} \left. \frac{\mathrm{d}^n f(x)}{\mathrm{d}x^n} \right|_{x=x_0} (\mathrm{d}x)^n \tag{23}$$

and for an function $f(x_1, \ldots, x_N)$ of N variables, we have

$$f(\mathbf{x^0} + \delta\mathbf{x}) \;\equiv\; f(x_j^0 + \delta x_j) \;=\; f(\mathbf{x^0}) \;+\; \sum_{n=1}^{\infty} \frac{1}{n!} \left. \frac{\partial^n f(x)}{\partial x_{\alpha_1} \cdots \partial x_{\alpha_N}} \right|_{\mathbf{x}=\mathbf{x^0}} \mathrm{d}x_{\alpha_1} \cdots \mathrm{d}x_{\alpha_N} \tag{24}$$

Clearly these Taylor expressions don't work around singularities, but we are only going to discuss here cases where the functional differentials are well defined.

Now let's consider a variation of a function $\phi(x)$; we will call this variation $\delta\phi(x)$. The idea is that we start from some well-defined function $\phi_0(x)$, and vary it infinitesimally, so that

$$\phi_0(x) \longrightarrow \phi_0(x) + \delta\phi(x) \tag{25}$$

in the same way that, in (23) and (24) above, we let the variable $\mathbf{x}$ be varied, so that $\mathbf{x_0} \to \mathbf{x_0} + \delta\mathbf{x}$. We now want to know how some functional $F[\phi]$ changes under the change $\delta\phi(x)$. Clearly the appropriate generalization of (24) is just

$$\begin{aligned} \delta F[\phi] &= F[\phi_0 + \delta\phi] - F[\phi_0] \\ &= \sum_{n=1}^{\infty} \frac{1}{n!} \left. \frac{\delta^n F[\phi]}{\delta\phi(x_1)\cdots\delta\phi(x_n)} \right|_{\phi(x)=\phi_0(x)} \delta\phi(x_1)\cdots\phi(x_n) \end{aligned} \tag{26}$$

where if we wish to make sense of this expression by relating it back to (24), we should write $\phi(x)$ in terms of a set of orthonormal function $\chi_n(x)$ (cf. eq. (3)), write the variation as

$$\delta\phi(x) = \sum_n \chi_n(x)\delta\phi_n \tag{27}$$

in terms of the coefficients $\delta\phi_n$, and then expand in powers of the $\delta\phi_n$, just we expanded in powers of the $\mathrm{d}x_{\alpha_n}$ in (24). For the functional differentials to be well-defined, they must be independent of which basis set χ_n we use for the expansion in (27).

App. B.1.2 (a) BASIC RESULTS

Let's first establish some basic results for functional differentiation, and consider a few examples. We have already defined the n-th functional differential in eq. (26) above, but it is a little abstract, since we have not fixed the form of $\delta\phi(x)$. To do this we make a particularly simple choice in (27), viz., we write

$$\left. \begin{array}{lll} \chi_n(x) & \to & \chi_z(x) = \delta(x-z) \\ \delta\phi_n & \to & \delta\phi_z = \epsilon \end{array} \right| \qquad \text{ie.,} \qquad \delta\phi(x) = \epsilon\delta(x-z) \tag{28}$$

In functional language, this amounts to choosing as basis functions the infinite set of δ-functions which pick out different values of x; the function picks out $x = z$. Note that in QM, these are nothing but position eigenstates $|z\rangle$, so that

$$\langle x|z\rangle = \delta(x-z) \qquad \text{and} \qquad \int \mathrm{d}x\langle x|z\rangle = 1 \tag{29}$$

Now let's define the derivative $\delta F/\delta\phi(x)$ using this form for $\delta\phi(x)$. We have, under a variation $\delta\phi(x)$, a change

$$\delta F[\phi] = F[\phi(x) + \delta\phi(x)] - F[\phi(x)] \tag{30}$$

and by definition

$$\delta F[\phi] \;=\; \int \mathrm{d}x' \, \frac{\delta F[\phi]}{\delta\phi(x')}\delta\phi(x') \tag{31}$$

Then, with the assumption that $\delta\phi(x) = \epsilon\delta(x - x')$, as in (28), we get

$$\delta F[\phi] \;\longrightarrow\; \epsilon\int \mathrm{d}x' \, \frac{\delta F[\phi]}{\delta\phi(x')}\delta(x' - x) \;=\; \epsilon\frac{\delta F[\phi]}{\delta\phi(x)} \tag{32}$$

so that we have

$$\frac{\delta F[\phi(x)]}{\delta\phi(x')} \;=\; \frac{1}{\epsilon}\Big(F[\phi + \epsilon\delta(x - x')] - F[\phi]\Big) \tag{33}$$

This result is of practical use when it comes to calculating functional derivatives, or at least justifying results obtained by more heuristic means. We can use it derive a number of useful results; for example

<u>*Product Rule*</u>: For some product of functionals, we have

$$\frac{\delta}{\delta\phi(x)}\left\{F[\phi]G[\phi]\right\} \;=\; F[\phi]\frac{\delta G}{\delta\phi(x)} + G[\phi]\frac{\delta F}{\delta\phi(x)} \tag{34}$$

<u>*Chain Rule*</u> : Suppose we have a functional $G\left[F[\phi]\right]$ of a functional $F[\phi]$ of the function $\phi(x)$. Then the functional differential $\delta G/\delta\phi$ of the functional $G\left[F[\phi]\right]$ is

$$\frac{G\left[F[\phi]\right]}{\delta\phi(x)} \;=\; \int \mathrm{d}x' \, \frac{\delta G}{\delta\phi(x')}\,\frac{\delta F[\phi(x)']}{\delta\phi(x)} \tag{35}$$

If the functional $F[\phi]$ is just an ordinary function, $f\big(\phi(x)\big) = f(x)$, then (35) reduces to

$$\frac{\delta G[f]}{\delta\phi(x)} \;=\; \frac{\delta G[f]}{\delta f\big(\phi(x)\big)}\,\frac{\mathrm{d}f}{\mathrm{d}\phi(x)} \tag{36}$$

<u>$Functional\ \ Self-differentiation$</u>: The simplest functional $F[\phi]$ of $\phi(x)$ is the unit functional $F[\phi] = \phi(x)$. Then since

$$\delta\phi(x) \;=\; \int \mathrm{d}x' \, \frac{\delta\phi(x)}{\delta\phi(x')}\delta\phi(x') \qquad \text{and} \qquad \delta\phi(x) \;=\; \int \mathrm{d}x' \, \delta(x - x')\delta\phi(x') \tag{37}$$

we have

$$\frac{\delta\phi(x)}{\delta\phi(x')} \;=\; \delta(x - x') \tag{38}$$

Then, using the product rule, we have for any function $f\big(\phi(x)\big)$ that is differentiable, and so can be written as $f\big(\phi(x)\big) \;=\; \sum_n f_n\phi^n(x)$, that the functional

$$F[\phi] \;=\; \int \mathrm{d}x' \, f\big(\phi(x')\big) \tag{39}$$

has differential

$$\frac{F[\phi]}{\phi(x)} \;=\; \frac{f\big(\phi(x)\big)}{\phi(x)} \tag{40}$$

which follows from the simple result that

$$\frac{\delta\phi^n(x)}{\delta\phi(x')} \;=\; n\phi^{n-1}(x)\delta(x-x') \tag{41}$$

derived directly from (34) and (38).

From all these general results it is then fairly straightforward to derive some more specific results.

App. B.1.2 (b) SIMPLE EXAMPLES

In may applications we do not need to understand more than a few simple results. So in what follows I give a few of these, with remarks on how to get them. In another section we discuss a set of results that are crucial in quantum field theory.

(i) Derivatives of $\phi(x)$: We can imagine simple functionals involving derivatives of a function $\phi(x)$. The simplest example is the functional

$$F[\phi] \;=\; \int \mathrm{d}x \big(\phi'(x)\big)^n \;\equiv\; \int \mathrm{d}x \left(\frac{\mathrm{d}\phi(x)}{\mathrm{d}x}\right)^n \tag{42}$$

It is simple to then derive the result (starting as usual from (33))

$$\begin{aligned}\frac{\delta F[\phi]}{\delta\phi(x)} \;&=\; \int \mathrm{d}x'\, n\big(\phi'(x')\big)^{n-1}\frac{\mathrm{d}\delta(x'-x)}{\mathrm{d}x'} \\ &\xrightarrow[\text{integration by parts}]{} \; -n\,\frac{\mathrm{d}}{\mathrm{d}x'}\big(\phi'(x')\big)^{n-1}\Big|_{x'=x}\end{aligned} \tag{43}$$

where in the last step we assume that $\phi'(x')$ and its derivatives can be ignored at the end points of the integral.

Now, by writing some arbitrary function $f\big(\phi'(x)\big)$ as a power series in $\phi'(x)$, i.e., write $f\big(\phi'(x)\big) \;=\; \sum_n f_n(\phi')^n$, we can immediately derive the result for a functional

$$F[\phi] \;=\; \int \mathrm{d}x\; f\big(\phi'(x)\big) \tag{44}$$

that

$$\frac{\delta F[\phi]}{\delta\phi(x)} \;=\; -\frac{\mathrm{d}}{\mathrm{d}x'}\left(\frac{\mathrm{d}f(\phi')}{\mathrm{d}\phi'(x')}\right)\Big|_{x'=x} \tag{45}$$

These results can be easily extended to encompass higher derivatives $\phi^{(n)}(x) \;=\; \mathrm{d}^n\phi(x)/\mathrm{d}x^n$, or to multiple integrals over functional of $\phi'(x)$, or to functionals of $\phi'(\mathbf{r})$, where $\mathbf{r}$ exists in n-dimensional space; and so on.

(ii) <u>*Simple exponential functionals*</u>: In many applications, ranging from physics to economics, one has to deal with exponential functionals - the most important reason for this being in generating functionals used in probability theory and quantum field theory. Then, we need to look at

$$F(\phi) \;=\; \exp\left\{ \int \mathrm{d}x\; J(x)\phi(x) \right\} \tag{46}$$

which we write as

$$F[\phi] \;=\; \sum_{n=0}^{\infty} \frac{1}{n!} \left(\int \mathrm{d}x\; J(x)\phi(x) \right)^n \tag{47}$$

and then we easily find

$$\frac{\delta F[\phi]}{\delta \phi(x)} \;=\; J(x)\; e^{\int \mathrm{d}x\; J(x)\phi(x)} \;=\; J(x)F[\phi] \tag{48}$$

Notice that we can also write $F[\phi]$ as

$$F[J] \;=\; e^{\int \mathrm{d}x\; J(x)\phi(x)} \tag{49}$$

i.e., $J(x)$ and $\phi(x)$ appear symmetrically, and we have

$$\frac{\delta F[J]}{\delta J(x)} \;=\; \phi(x)\; e^{\int \mathrm{d}x\; J(x)\phi(x)} \;=\; \phi(x)F[J] \tag{50}$$

We can also consider Gaussian functionals of these variables. These are central in both probability theory and in field theory and statistical mechanics. Thus, in quantum field theory one deals with

$$F[J] \;=\; e^{\frac{i}{2}\int \mathrm{d}x_1 \int \mathrm{d}x_2\; J(x_1)\Delta(x_1,x_2)J(x_2)} \tag{51}$$

(here I have put $\hbar = 1$), and then one easily finds that

$$\begin{aligned} \frac{\delta F[J]}{\delta J(x)} \;&=\; i \int \mathrm{d}x'\; \Delta(x,x')J(x')\; e^{\frac{i}{2}\int \mathrm{d}x_1 \int \mathrm{d}x_2\; J(x_1)\Delta(x_1,x_2)J(x_2)} \\ &=\; i \int \mathrm{d}x'\; \Delta(x,x')J(x')\; F[J] \end{aligned} \tag{52}$$

and one can continue in this vein with more complicated exponential functionals.

(iii) <u>*Functional of "Correlator" form*</u>: Often, in classical physics (e.g., in E& M theory, or in ordinary mechanical systems), and in quantum mechanics and quantum field theory, or in condensed matter physics, one deals with "response functions", in which one looks at some "correlator" $K(x,x')$ between events at 2 different spacetime positions. One then deals with functionals like

$$F[\phi(z)] \;=\; \int \mathrm{d}z'\; K(z,z')\; \phi(z') \tag{53}$$

and we already saw a simple example of this in eq. (6). It is easy to then establish that

$$\frac{\delta F[\phi(z)]}{\delta\phi(x)} \;=\; K(z,x) \tag{54}$$

and we easily generalize this to the functional

$$F[\phi(z)] \;=\; \int \mathrm{d}z'\; K(z,z')\;\phi^n(z') \tag{55}$$

to find

$$\begin{aligned}\frac{\delta F[\phi(z)]}{\delta\phi(x)} \;&=\; \int \mathrm{d}z'\; n\phi^{n-1}(z')K(z,z')\delta(x-z') \\ &=\; nK(z,x)\;\phi^{n-1}(x)\end{aligned} \tag{56}$$

and from this we easily find that for a function $f\big(\phi(z)\big)$ expandable as a polynomial in $\phi(z)$, the functional

$$F[\phi] \;=\; \int \mathrm{d}z'\; K(z,z')f\big(\phi(z')\big) \tag{57}$$

has derivative

$$\frac{\delta F[\phi(z)]}{\delta\phi(x)} \;=\; K(z,x)\,\frac{\mathrm{d}f(\phi)}{\mathrm{d}\phi(x)} \tag{58}$$

Finally, we can consider correlators of form

$$F[\phi] \;=\; \int \mathrm{d}x_1 \int \mathrm{d}x_2\; \phi(x_1)K(x_1,x_2)\phi(x_2) \tag{59}$$

and it is clear that

$$\frac{\delta F[\phi]}{\delta\phi(x)} \;=\; \int \mathrm{d}x'\;\big(K(x,x')+K(x',x)\big)\phi(x') \tag{60}$$

and that

$$\frac{\delta^2 F[\phi]}{\delta\phi(x_1)\delta\phi(x_2)} \;=\; K(x_1,x_2)\;+\;K(x_2,x_1) \tag{61}$$

and one may continue in this vein with higher correlators involving integrals over n different ϕ-functions with different arguments $\{x_j\}$.

App. B.1.3: SHIFT OPERATORS

In field theory, and also elsewhere, it is important to be apply to apply different transformations to functional integrals that have come to be known as "shift operations", after they were used extensively by Schwinger in his work on QED in the early 1950's.

The simplest kind of "shift" or translation operation is that which generalizes the simple Taylor expansion beyond an infinitesimal translation $\mathrm{d}x$ (cf. eq. (23)). Thus for an ordinary function we have

$$e^{a_0 \frac{\mathrm{d}}{\mathrm{d}x}} f(x) \quad = \quad f(x+a_0) \tag{62}$$

again by power series expansion, now in powers of a_0 (as opposed to $\mathrm{d}x$).

The functional generalization of this is just

$$\hat{Q}_1 F[\phi] \quad = \quad e^{\int \mathrm{d}x \; A(x) \frac{\delta}{\delta\phi(x)}} F[\phi] \quad = \quad F[\phi(x) + A(x)] \tag{63}$$

There are various ways of demonstrating this - one of the fastest is to use the functional generalization of the usual definition of a delta-function, viz.,

$$\delta[f(x) - g(x)] \;=\; \int \mathcal{D}\phi(x) \; e^{i \int \mathrm{d}x \; \phi(x) \; [f(x) - g(x)]} \tag{64}$$

and to write a general functional $F[\phi(x)]$ in the form of a functional power series, i.e., write:

$$F[\phi] \quad = \quad \sum_{n=0}^{\infty} \frac{1}{n!} \prod_{j=1}^{n} \int \mathrm{d}x_j \; f_n(x_1 \ldots x_n)\phi(x_1)\ldots\phi(x_n) \tag{65}$$

which can also be written in the form

$$F[\phi] \quad = \quad \sum_{n=0}^{\infty} \frac{1}{n!} \prod_{j=1}^{n} \int \mathrm{d}x_j \left[f_n(x_1 \ldots x_n)\big(-i\frac{\delta}{\delta J(x_1)}\big) \cdots \big(-i\frac{\delta}{\delta J(x_n)}\big) \right] e^{i \int \mathrm{d}x \phi(x) J(x)} \Big|_{J=0} \tag{66}$$

and where we note that the coefficients $f_n(x_1 \ldots x_n)$ are just the functional derivatives of $F[\phi]$, i.e., that

$$f_n(x_1 \ldots x_n) \quad = \quad (-i)^n \; \frac{\delta^n F[\phi]}{\delta\phi(x_1)\cdots\delta\phi(x_n)}\Big|_{\phi=0} \tag{67}$$

The formula (66) and (67) are just the functional generalizations of what is written down in ordinary probability theory for the generating function and the moments of a probability distribution. Notice also that the "functional δ-function" in (64) is a special case of the "functional Fourier transform", viz.,

$$F[J] \;=\; \int \mathcal{D}\phi(x) \; e^{i \int \mathrm{d}x \; \phi(x) J(x)} F[\phi] \tag{68}$$

which defines the characteristic functional in probability theory.

Now let's look at some more complicated shift operators. The next one up is the "quadratic shift operator", which we write as

$$\hat{Q}_2 \;\equiv\; e^{i\hat{K}_\phi} \quad = \quad e^{\frac{i}{2} \int \mathrm{d}x_1 \int \mathrm{d}x_2 \; \frac{\delta}{\delta\phi(x_1)} K(x_1,x_2) \frac{\delta}{\delta\phi(x_2)}} \tag{69}$$

which is central in quantum field theory. Let's apply this to the simple exponential functional (being in mind we can write any functional using (68)); then we have

$$\begin{aligned} \hat{Q}_2\, e^{i\int \mathrm{d}x\, \phi(x)J(x)} &= e^{\frac{i}{2}\int \mathrm{d}x_1 \int \mathrm{d}x_2\, \frac{\delta}{\delta\phi(x_1)} K(x_1,x_2) \frac{\delta}{\delta\phi(x_2)}}\, e^{i\int \mathrm{d}x\, \phi(x)J(x)} \\ &= e^{\frac{-i}{2}\int \mathrm{d}x_1 \int \mathrm{d}x_2\, J(x_1)K(x_1,x_2)J(x_2)}\, e^{i\int \mathrm{d}x\, \phi(x)J(x)} \end{aligned} \quad (70)$$

and by using the Fourier transform we can extend this to any functional in place of this exponential.

The quadratic shift operators plays a particular role in field theory, when it is applied to more than one functional (representing, e.g., some n-point functional is a product of 2 functionals: let

$$F[\phi] \;=\; G_1[\phi]G_2[\phi] \quad (71)$$

Then we have

$$\hat{Q}_2\, G_1[\phi]\, G_2[\phi] \;=\; e^{\frac{i}{2}\int \mathrm{d}x_1 \int \mathrm{d}x_2\, \frac{\delta}{\delta\phi(x_1)} K(x_1,x_2) \frac{\delta}{\delta\phi(x_2)}}\; G_1[\phi]\; G_2[\phi] \quad (72)$$

and if we work this out, we get

$$\hat{Q}_2\, G_1[\phi]\, G_2[\phi] \;=\; e^{i\hat{K}^{\phi}_{12}} \left\{ e^{i\hat{K}^{\phi_1}_{11}} G_1[\phi] \;\; e^{i\hat{K}^{\phi_2}_{22}} G_2[\phi] \right\}\Big|_{\phi_1=\phi_2\,=\,\phi} \quad (73)$$

where the operators are

$$K^{\phi}_{ij} \;=\; \frac{1}{2}\int \mathrm{d}x \int \mathrm{d}x'\; \frac{\delta}{\delta\phi_i(x)} K(x,x') \frac{\delta}{\delta\phi_j(x')} \quad (74)$$

and the result in (73) acquires, in field theory, a clear diagrammatic interpretation. The operator K^{ϕ}_{jj} is a "linking" operator for the field $\phi_j(x)$, which joins together pairs of ϕ_j-factors (i.e., the "ϕ_j-field"); the exponentiation then includes all possible pairings between $\phi_j(x)$ and $\phi_j(x')$, repeated an arbitrary number of times between different values of x, x', x'', etc., as we go to higher order in the expansion of the exponential. These are then linked in all possible ways between the 2 different functionals $G_1[\phi]$ and $G_2[\phi]$ (ie., between the 2 fields $\phi_1(x)$ and $\phi_2(x')$), by the operator K^{ϕ}_{12}.

This can be generalized to a product $F[\phi] = \prod_{j=1}^{n} G_j[\phi]$ quite easily, and all possible linkings are then generated.

As a final example, let's look at the action of $\hat{Q}_2$ on a simple Gaussian functional. We can solve this starting from (70), or otherwise. We consider the form

$$\begin{aligned} \hat{Q}_2 F[\phi] &\equiv \hat{Q}_2\, e^{\frac{i}{2}\int \mathrm{d}x_1 \int \mathrm{d}x_2\, \phi(x_1)A(x_1,x_2)\phi(x_2) + i\int \mathrm{d}x\, J(x)\phi(x)} \\ &= e^{\frac{i}{2}\int \mathrm{d}x_1 \int \mathrm{d}x_2\, \frac{\delta}{\delta\phi(x_1)} K(x_1,x_2) \frac{\delta}{\delta\phi(x_2)}} \left[e^{\frac{i}{2}\int \mathrm{d}x_1 \int \mathrm{d}x_2\, \phi(x_1)A(x_1,x_2)\phi(x_2) + i\int \mathrm{d}x\, J(x)\phi(x)} \right] \end{aligned} \quad (75)$$

If we work this out, we get a key result, viz.,

$$\begin{aligned} \hat{Q}_2 F[\phi] &= \Omega_o \exp\left\{ \frac{i}{2}\int \mathrm{d}x_1 \int \mathrm{d}x_2 \right. \\ &\quad \left. \left[\phi(x)G^{\phi\phi}(x,x')\phi(x') \;+\; 2\phi(x)G^{\phi J}(x,x')J(x') \;-\; J(x)G^{JJ}(x,x')J(x') \right] \right\} \end{aligned} \quad (76)$$

where the correlators are

$$
\begin{aligned}
G^{\phi\phi}(x,x') &= \left(\frac{A}{1+KA}\right)_{xx'} \\
G^{\phi J}(x,x') &= \left(1+KA\right)^{-1}_{xx'} \\
G^{JJ}(x,x') &= \left(\frac{K}{1+KA}\right)_{xx'}
\end{aligned}
\tag{77}
$$

and the prefactor is

$$
\Omega_o = \exp\left\{-\frac{1}{2}\mathrm{Tr}\ \ln(1+KA)_{xx'}\right\} \tag{78}
$$

where by KA we mean the convolution of the functions $K(x,x')$ and $A(x,x')$. This a result much used in field theory.