汎関数の計算

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ここでは定義域が関数であるような関数を**汎関数** functional とする. 例えば, $F : (A \to B) \to C$ など. このとき, $\varphi : A \to B$ を用いて $F[\varphi(x)] \in C$ と書く. ただし表記中 $x \in A$ は「ダミー」であって, 汎関数の定義中で用いられる文字である. 単に $F[\varphi]$ とも略記される. この文章中では, ダミー変数を添字にした $F_x[\varphi], F_{x \in A}[\varphi]$ も用いる[*1]. $F[\varphi(x)]$ が汎関数であるとき, 通常の関数 $g : C \to D$ を用いた $g(F[\varphi(x)])$ もまた汎関数である.

以下では物理学において頻出する汎関数の基本的な計算方法についてまとめる. 数学的な厳密性は一切考慮していない. 高校微積分程度の理解を目指している[*2]. また, 勝手な解釈も多く含んでいるので参考程度に読んでほしい.

0.1　汎関数の考え方

例として関数 $\varphi : [a, b] \to \mathbb{R}$ の汎関数 $F[\varphi(x)]$ を考える. I の分割 $a = x_0 < \cdots < x_N = b$ に対し, 関数値を $\varphi_n := \varphi(x_n)$ として, 汎関数 $F[\varphi(x)]$ はある関数 $f_N(\varphi_0, \ldots, \varphi_N)$ の分割数 N を極限まで増やしたものと見做すことができる. たとえば積分 $F[\varphi(x)] = \displaystyle\int_a^b \mathrm{d}x\, \varphi(x)$ では, 分割幅を $\Delta x_n := x_n - x_{n-1}$ として, Riemann 積分の考え方を用いれば[*3],

$$
\begin{aligned}
f_N(\varphi_0, \ldots, \varphi_N) &= \sum_{n=1}^{N} \Delta x_n \times \varphi(x_n) \\
\xrightarrow{N \to \infty} \quad F[\varphi(x)] &= \int_a^b \mathrm{d}x\, \varphi(x).
\end{aligned}
$$

[*1] $F[\varphi(x)]$ という表記法は誤解を生む. たとえば, 十分に小さい x の関数 $\varepsilon : A \to A$ に対して $F[\varphi(x + \varepsilon(x))]$ を考える. このとき,

$$\varphi(x + \varepsilon(x)) = \varphi(x) + \varphi'(x)\varepsilon(x)$$

であるが,

$$F[\varphi(x + \varepsilon(x))] \neq F[\varphi(x) + \varphi'(x)\varepsilon(x)]$$

である. ダミー変数を添字にした $F_x[\varphi]$ という表記法を用いれば, 不等号の理由は明らかであろう:

$$F_{x+\varepsilon(x)}[\varphi] \neq F_x[\varphi + \varphi'\varepsilon].$$

[*2] それすら怪しいかもしれない. 気付いたことがあれば随時更新する.

[*3] これは Riemann 積分ではなく「区分求積法」である. Riemann 和を用いるならば $\varphi_n = \varphi(x_n)$ ではなく, 代表点 $x_{n-1} \leq \xi_n \leq x_n$ を用いて $\varphi_n := \varphi(\xi_n)$ とするべき. しかし, ここでは計算を主目的としているので, 細かいことは気にしない.

または, 等間隔な分割 $x_n := a + \dfrac{n(b-a)}{N}$, 分割幅 $\Delta x := \dfrac{b-a}{N}$ に対し, 例えば $\varphi(x) := x^2$ とすると,

$$
\begin{aligned}
f_N(x_0^2, \dots, x_N^2) &= \sum_{n=1}^{N} \Delta x \times x_n^2 \\
\xrightarrow{N\to\infty} \quad F[x^2] &= \int_a^b \mathrm{d}x\, x^2.
\end{aligned}
$$

このような汎関数の離散的な表現を考えることも重要である. 特に, 汎関数積分の計算においては離散表現が必須である.

0.1.1　汎関数の例

以下は汎関数である:

1. 積分
$$
\begin{aligned}
i_N(\varphi_0, \dots, \varphi_N) &= \sum_{n=1}^{N} \Delta x \times \mathrm{g}(\varphi_n) \\
\xrightarrow{N\to\infty} \quad I[\varphi(x)] &= \int \mathrm{d}x\, \mathrm{g}(\varphi(x)).
\end{aligned}
$$

2. 代入
$$
\begin{aligned}
s(\varphi_0, \dots, \varphi_N; x_m = x') &= \sum_{n=1}^{N} \Delta x \times \varphi_n \frac{\delta_{nm}}{\Delta x} = \varphi_m \\
\xrightarrow{N\to\infty} \quad S[\varphi(x)](x') &= \int \mathrm{d}x\, \varphi(x)\delta(x-x') = \varphi(x').
\end{aligned}
$$
汎関数中のデルタ関数 $\delta(x-x')$ は, 離散表現の $\dfrac{\delta_{nm}}{\Delta x}$ に対応している.

3. Fourier 変換
$$
\begin{aligned}
f_N(\varphi_0, \dots, \varphi_N; k_m) &= \sum_{n=1}^{N} \frac{\Delta x}{\sqrt{2\pi}} \times \varphi_n e^{-ik_m x_n} \\
\xrightarrow{N\to\infty} \quad \mathcal{F}[\varphi(x)](k) &= \int \frac{\mathrm{d}x}{\sqrt{2\pi}} \varphi(x) e^{-ikx}.
\end{aligned}
$$

4. Fourier 逆変換
$$
\begin{aligned}
f_N^{\text{“}-1\text{”}}(\tilde{\varphi}_0, \dots, \tilde{\varphi}_N; x_n) &= \sum_{m=1}^{N} \frac{\Delta k}{\sqrt{2\pi}} \times \tilde{\varphi}_m e^{ik_m x_n} \\
\xrightarrow{N\to\infty} \quad \mathcal{F}^{-1}[\tilde{\varphi}(k)](x) &= \int \frac{\mathrm{d}k}{\sqrt{2\pi}} \tilde{\varphi}(k) e^{ikx};
\end{aligned}
$$
実際, $\mathcal{F}^{-1}[\mathcal{F}[\varphi(\tilde{x})](k)](x) = \varphi(x)$.

5. 汎関数のダミー変数を関数にしたもの
$$
\begin{aligned}
g_N(x_0, \dots, x_N) &= f_N(\varphi_0, \dots, \varphi_N) \\
\xrightarrow{N\to\infty} \quad G_t[x] &:= F_{x(t)}[\varphi].
\end{aligned}
$$

ただし, $x_n = x(t_n)$. 例えば $F_x[\varphi] := \int \mathrm{d}x\, \varphi(x)$ に対して,

$$
\begin{aligned}
&g_N(x_0, \dots, x_N) = f_N(\varphi_0, \dots, \varphi_N) = \sum_{n=1}^{N} \Delta x \times \varphi_n = \sum_{n=1}^{N} \Delta t \times \frac{\Delta x}{\Delta t} \varphi(x_n) \\
\xrightarrow{N\to\infty} \quad &G_t[x] = F_{x(t)}[\varphi] = \int \mathrm{d}x(t)\, \varphi(x(t)) = \int \mathrm{d}t\, \frac{\mathrm{d}x}{\mathrm{d}t} \varphi(x(t)).
\end{aligned}
$$

0.2 汎関数微分

汎関数 $F[\varphi(x)]$ の点 y における**汎関数微分**functional derivative は, 以下で定義される:

$$
\frac{\delta F[\varphi(x)]}{\delta \varphi(y)} := \lim_{h\to 0} \frac{F[\varphi(x) + h\delta(x-y)] - F[\varphi(x)]}{h}.
$$

物理では汎関数微分を変分とも呼び, 単に $\dfrac{\delta F[\varphi]}{\delta \varphi}$ とも略記される.

汎関数微分の離散的な表現は, $y = x_m$ として, 定義から

$$
\begin{aligned}
&\lim_{h\to 0} \frac{f_N\left(\varphi_1 + h\dfrac{\delta_{1m}}{\Delta x}, \dots, \varphi_N + h\dfrac{\delta_{Nm}}{\Delta x}\right) - f_N(\varphi_1, \dots, \varphi_N)}{h} \\
&= \frac{1}{\Delta x} \lim_{h\to 0} \frac{f_N(\varphi_1, \dots, \varphi_m + h/\Delta x, \dots, \varphi_N) - f_N(\varphi_1, \dots, \varphi_N)}{h/\Delta x} \\
&= \frac{1}{\Delta x} \frac{\partial f_N}{\partial \varphi_m}.
\end{aligned}
$$

したがって, 汎関数微分演算子 $\dfrac{\delta}{\delta \varphi(y)}$ に対応する離散表現は $\dfrac{1}{\Delta x}\dfrac{\partial}{\partial \varphi_m}$ である.

0.2.1 汎関数微分の計算例

以下の汎関数 $F[\varphi(x)]$ について汎関数微分 $\dfrac{\delta F[\varphi(x)]}{\delta \varphi(y)}$ を計算する:

1. $F[\varphi(x)] = \int \mathrm{d}x\, g(x)\varphi(x)$:

$$
\begin{aligned}
&\frac{\delta}{\delta \varphi(y)} \int \mathrm{d}x\, g(x)\varphi(x) \\
&= \lim_{h\to 0} \frac{1}{h} \left[\int \mathrm{d}x\, g(x)(\varphi(x) + h\delta(x-y)) - \int \mathrm{d}x\, g(x)\varphi(x) \right] \\
&= \lim_{h\to 0} \frac{1}{h} \int \mathrm{d}x\, g(x) h\delta(x-y) \\
&= \int \mathrm{d}x\, g(x)\delta(x-y) = g(y).
\end{aligned}
$$

離散表現では, $y = x_m$ として,

$$
\frac{1}{\Delta x} \frac{\partial}{\partial \varphi_m} \sum_{n=1}^{N} \Delta x \times g(x_n)\varphi_n = g(x_m).
$$

2. $F[\varphi(x)] = \varphi(x')$:

$$\frac{\delta\varphi(x')}{\delta\varphi(y)} = \frac{\delta}{\delta\varphi(y)}\int \mathrm{d}z\,\varphi(z)\delta(x'-z) = \delta(x'-y).$$

離散表現では, $y = x_m, x' = x_k$ として,

$$\frac{1}{\Delta x}\frac{\partial}{\partial\varphi_m}\sum_{n=1}^{N}\Delta x\times\varphi_n\frac{\delta_{nk}}{\Delta x} = \frac{\delta_{mk}}{\Delta x}.$$

3. $F[\varphi(x)] = \displaystyle\int \mathrm{d}x\,\mathrm{g}(\varphi(x))$:

$$\begin{aligned}
&\frac{\delta}{\delta\varphi(y)}\int \mathrm{d}x\,\mathrm{g}(\varphi(x)) \\
&= \lim_{h\to 0}\frac{1}{h}\left[\int \mathrm{d}x\,\mathrm{g}(\varphi(x)+h\delta(x-y)) - \int \mathrm{d}x\,\mathrm{g}(\varphi(x))\right] \\
&= \lim_{h\to 0}\frac{1}{h}\left\{\int \mathrm{d}x\left[h\frac{\mathrm{dg}(\varphi(x))}{\mathrm{d}\varphi(x)}\delta(x-y)+O(h^2)\right]\right\} \\
&= \lim_{h\to 0}\frac{1}{h}\left[h\frac{\mathrm{dg}(\varphi(y))}{\mathrm{d}\varphi(y)}+O(h^2)\right] \\
&= \frac{\mathrm{dg}(\varphi(y))}{\mathrm{d}\varphi(y)}.
\end{aligned}$$

離散表現では, $y = x_m$ として,

$$\frac{1}{\Delta x}\frac{\partial}{\partial\varphi_m}\sum_{n=1}^{N}\Delta x\times\mathrm{g}(\varphi_n) = \frac{\mathrm{dg}(\varphi_m)}{\mathrm{d}\varphi_m}.$$

4. $F[\varphi(x)] = \displaystyle\int \mathrm{d}x\,\mathrm{g}(\varphi'(x))$:

$$\begin{aligned}
&\frac{\delta}{\delta\varphi(y)}\int \mathrm{d}x\,\mathrm{g}(\varphi'(x)) \\
&= \lim_{h\to 0}\frac{1}{h}\left[\int \mathrm{d}x\,\mathrm{g}\left(\frac{\mathrm{d}\{\varphi(x)+h\delta(x-y)\}}{\mathrm{d}x}\right) - \int \mathrm{d}x\,\mathrm{g}\left(\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}\right)\right] \\
&= \lim_{h\to 0}\frac{1}{h}\left[\int \mathrm{d}x\,\mathrm{g}\left(\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}+h\frac{\mathrm{d}\delta(x-y)}{\mathrm{d}x}\right) - \int \mathrm{d}x\,\mathrm{g}\left(\frac{\mathrm{d}\varphi(x)}{\mathrm{d}x}\right)\right] \\
&= \lim_{h\to 0}\frac{1}{h}\left\{\int \mathrm{d}x\left[h\frac{\mathrm{dg}(\mathrm{d}\varphi(x)\,/\,\mathrm{d}x)}{\mathrm{d}(\mathrm{d}\varphi(x)\,/\,\mathrm{d}x)}\frac{\mathrm{d}\delta(x-y)}{\mathrm{d}x}+O(h^2)\right]\right\} \\
&= \lim_{h\to 0}\frac{1}{h}\left\{\int \mathrm{d}x\left[-h\frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{dg}(\mathrm{d}\varphi(x)\,/\,\mathrm{d}x)}{\mathrm{d}(\mathrm{d}\varphi(x)\,/\,\mathrm{d}x)}\delta(x-y)+h\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathrm{dg}(\mathrm{d}\varphi(x)\,/\,\mathrm{d}x)}{\mathrm{d}(\mathrm{d}\varphi(x)\,/\,\mathrm{d}x)}\delta(x-y)\right)+O(h^2)\right]\right\} \\
&\quad (\because \text{部分積分}) \\
&= \lim_{h\to 0}\frac{1}{h}\left[-h\frac{\mathrm{d}}{\mathrm{d}y}\frac{\mathrm{dg}(\mathrm{d}\varphi(y)\,/\,\mathrm{d}y)}{\mathrm{d}(\mathrm{d}\varphi(y)\,/\,\mathrm{d}y)}+h\int \mathrm{d}\left(\frac{\mathrm{dg}(\mathrm{d}\varphi(x)\,/\,\mathrm{d}x)}{\mathrm{d}(\mathrm{d}\varphi(x)\,/\,\mathrm{d}x)}\delta(x-y)\right)+O(h^2)\right] \\
&= -\frac{\mathrm{d}}{\mathrm{d}y}\frac{\mathrm{dg}(\mathrm{d}\varphi(y)\,/\,\mathrm{d}y)}{\mathrm{d}(\mathrm{d}\varphi(y)\,/\,\mathrm{d}y)}+\int \mathrm{d}\left(\frac{\mathrm{dg}(\mathrm{d}\varphi(x)\,/\,\mathrm{d}x)}{\mathrm{d}(\mathrm{d}\varphi(x)\,/\,\mathrm{d}x)}\delta(x-y)\right) \\
&= -\frac{\mathrm{d}}{\mathrm{d}y}\frac{\mathrm{dg}(\varphi'(y))}{\mathrm{d}\varphi'(y)}+\int \mathrm{d}\left(\frac{\mathrm{dg}(\varphi'(x))}{\mathrm{d}\varphi'(x)}\delta(x-y)\right).
\end{aligned}$$

特に y が積分範囲の内部にあるとき, 発散項を消すことができて,

$$\frac{\delta}{\delta\varphi(y)}\int \mathrm{d}x\, \mathrm{g}(\varphi'(x)) = -\frac{\mathrm{d}}{\mathrm{d}y}\frac{\mathrm{dg}(\varphi'(y))}{\mathrm{d}\varphi'(y)}.$$

離散表現では, $y = x_m$ として,

$$\frac{1}{\Delta x}\frac{\partial}{\partial\varphi_m}\sum_{n=1}^{N}\Delta x \times \mathrm{g}\Big(\frac{\varphi_n - \varphi_{n-1}}{\Delta x}\Big) = -\frac{\mathrm{g}'\Big(\frac{\varphi_{m+1}-\varphi_m}{\Delta x}\Big) - \mathrm{g}'\Big(\frac{\varphi_m - \varphi_{m-1}}{\Delta x}\Big)}{\Delta x}.$$

5. $F[\varphi(x)] = \int \mathrm{d}x\, \mathrm{g}(\varphi(x), \varphi'(x))$:
上の例を繰り返し使うことで,

$$\frac{\delta}{\delta\varphi(y)}\int \mathrm{d}x\, \mathrm{g}(\varphi(x), \varphi'(x)) = \frac{\partial \mathrm{g}}{\partial\varphi(y)} - \frac{\mathrm{d}}{\mathrm{d}y}\frac{\partial \mathrm{g}}{\partial\varphi'(y)} + \int \mathrm{d}\Big(\frac{\partial \mathrm{g}}{\partial\varphi'(x)}\delta(x-y)\Big),$$

あるいは, y が積分範囲の内部にあるとき,

$$\frac{\delta}{\delta\varphi(y)}\int \mathrm{d}x\, \mathrm{g}(\varphi(x), \varphi'(x)) = \frac{\partial \mathrm{g}}{\partial\varphi(y)} - \frac{\mathrm{d}}{\mathrm{d}y}\frac{\partial \mathrm{g}}{\partial\varphi'(y)}.$$

0.3 汎関数冪級数

連続な汎関数は Tayler 級数に相当する以下の冪級数に展開することができる. これを **Volterra 級数** Volterra series という: 微小な関数 $\eta(x)$ を用いて,

$$\begin{aligned}F[\varphi(x)+\eta(x)] = F[\varphi(x)] &+ \int \mathrm{d}y\, \frac{\delta F[\varphi(x)]}{\delta\varphi(y)}\eta(y) \\ &+ \frac{1}{2}\int \mathrm{d}y_1 \int \mathrm{d}y_2\, \frac{\delta^2 F[\varphi(x)]}{\delta\varphi(y_1)\delta\varphi(y_2)}\eta(y_1)\eta(y_2) + \cdots \\ = \sum_{n=0}^{\infty}\frac{1}{n!}\int \mathrm{d}y_1 \cdots \int \mathrm{d}y_n\, &\frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)}\eta(y_1)\cdots\eta(y_n).\end{aligned}$$

特に, $\varphi = 0$ まわりの冪展開は,

$$\begin{aligned}F[\varphi(x)] &= F[0] + \int \mathrm{d}y\, \frac{\delta F[\varphi(x)]}{\delta\varphi(y)}\Big|_{\varphi=0}\varphi(y) + \frac{1}{2}\int \mathrm{d}y_1\int \mathrm{d}y_2\, \frac{\delta^2 F[\varphi(x)]}{\delta\varphi(y_1)\delta\varphi(y_2)}\Big|_{\varphi=0}\varphi(y_1)\varphi(y_2) + \cdots \\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\int \mathrm{d}y_1\cdots\int \mathrm{d}y_n\, \frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)}\Big|_{\varphi=0}\varphi(y_1)\cdots\varphi(y_n).\end{aligned}$$

汎関数冪級数の離散表現は,

$$\begin{aligned}&f_N(\varphi_0+\eta_0, \dots, \varphi_N+\eta_N) \\ &= f_N(\varphi_0, \dots, \varphi_N) + \sum_{m=0}^{N}\Delta x\frac{1}{\Delta x}\frac{\partial f_N}{\partial\varphi_m}\eta_m + \frac{1}{2}\sum_{m_1=0}^{N}\Delta x\sum_{m_2=0}^{N}\Delta x\frac{1}{(\Delta x)^2}\frac{\partial^2 f_N}{\partial\varphi_{m_1}\partial\varphi_{m_2}}\eta_{m_1}\eta_{m_2} + \cdots \\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\sum_{m_1=0}^{N}\Delta x\cdots\sum_{m_n=0}^{N}\Delta x\frac{1}{(\Delta x)^n}\frac{\partial^n f_N(\varphi_0, \dots, \varphi_N)}{\partial\varphi_{m_1}\cdots\partial\varphi_{m_n}}\eta_{m_1}\cdots\eta_{m_n}.\end{aligned}$$

この表現は関数 $f_N(\varphi_0+\eta_0,\dots,\varphi_N+\eta_N)$ の $(\varphi_0,\dots,\varphi_N)$ まわりでの Taylor 展開になっている.

n 階汎関数微分 $\dfrac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)}$ が $y_1,\dots,y_n$ について対称であると仮定して, $\dfrac{\delta^n F}{\delta\varphi^n}$ と略記する. また,

$$\frac{\delta^n F}{\delta\varphi^n}*\eta^n := \int \mathrm{d}y_1\cdots\int \mathrm{d}y_n\,\frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)}\eta(y_1)\cdots\eta(y_n)$$

とすると, Volterra 級数は以下のように書き直せる:

$$F[\varphi(x)+\eta(x)] = \sum_{n=0}^{\infty}\frac{1}{n!}\frac{\delta^n F}{\delta\varphi^n}*\eta^n.$$

0.3.1 冪級数を用いた計算例

1. $\dfrac{\delta^n F}{\delta\varphi^n}*\eta^n$ の $\eta(y)$ による汎関数微分:

$$\begin{aligned}
&\frac{\delta}{\delta\eta(y)}\left(\frac{\delta^n F}{\delta\varphi^n}*\eta^n\right)\\
&= \lim_{h\to 0}\frac{1}{h}\Bigg[\int \mathrm{d}y_1\cdots\int \mathrm{d}y_n\,\frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)}[\eta(y_1)+h\delta(y_1-y)]\cdots[\eta(y_n)+h\delta(y_n-y)]\\
&\qquad\qquad -\int \mathrm{d}y_1\cdots\int \mathrm{d}y_n\,\frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)}\eta(y_1)\cdots\eta(y_n)\Bigg]\\
&= \lim_{h\to 0}\frac{1}{h}\left[\sum_{i=0}^{n}\int \mathrm{d}y_1\cdots\int \mathrm{d}y_n\,\frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)}\eta(y_1)\cdots\widehat{\eta(y_i)}\cdots\eta(y_n)h\delta(y_i-y)+O(h^2)\right]\\
&= \sum_{i=0}^{n}\int \mathrm{d}y_1\cdots\int \mathrm{d}y_n\,\frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)}\eta(y_1)\cdots\widehat{\eta(y_i)}\cdots\eta(y_n)\delta(y_i-y)\\
&= n\int \mathrm{d}y_1\cdots\int \mathrm{d}y_{n-1}\,\frac{\delta^n F[\varphi(x)]}{\delta\varphi(y)\delta\varphi(y_1)\cdots\delta\varphi(y_{n-1})}\eta(y_1)\cdots\eta(y_{n-1})\\
&= n\frac{\delta}{\delta\varphi(y)}\left(\frac{\delta^{n-1}F}{\delta\varphi^{n-1}}\right)*\eta^{n-1}\quad\left(=:\ n\frac{\delta^n F}{\delta\varphi^n}*\eta^{n-1}\ \text{とも書く}\right).
\end{aligned}$$

2. $g(F[\varphi(x)])$ の汎関数微分:

$$\begin{aligned}
&\frac{\delta g(F[\varphi(x)])}{\delta\varphi(y)}\\
&= \lim_{h\to 0}\frac{1}{h}[g(F[\varphi(x)+h\delta(x-y)])-g(F[\varphi(x)])]\\
&= \lim_{h\to 0}\frac{1}{h}\left[g\left(F[\varphi(x)]+\int \mathrm{d}z\,\frac{\delta F[\varphi(x)]}{\delta\varphi(z)}h\delta(z-y)+O(h^2)\right)-g(F[\varphi(x)])\right]\\
&= \lim_{h\to 0}\frac{1}{h}\left[g\left(F[\varphi(x)]+h\frac{\delta F[\varphi(x)]}{\delta\varphi(y)}+O(h^2)\right)-g(F[\varphi(x)])\right]\\
&= \lim_{h\to 0}\frac{1}{h}\left[h\frac{\mathrm{d}g(F[\varphi(x)])}{\mathrm{d}F[\varphi(x)]}\frac{\delta F[\varphi(x)]}{\delta\varphi(y)}+O(h^2)\right]\\
&= \frac{\mathrm{d}g(F[\varphi(x)])}{\mathrm{d}F[\varphi(x)]}\frac{\delta F[\varphi(x)]}{\delta\varphi(y)}.
\end{aligned}$$

3. x の積分で定義される汎関数 $F[\varphi(x,t)]$ に対し, 微分 $\dfrac{\mathrm{d}}{\mathrm{d}t}F[\varphi(x,t)]$:

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}F[\varphi(x,t)] \\
&= \lim_{h\to 0}\frac{F[\varphi(x,t+h)]-F[\varphi(x,t)]}{h} \\
&= \lim_{h\to 0}\frac{1}{h}\left\{F\left[\varphi(x,t)+h\frac{\partial\varphi(x,t)}{\partial t}+O(h^2)\right]-F[\varphi(x,t)]\right\} \\
&= \lim_{h\to 0}\frac{1}{h}\left\{F[\varphi(x,t)]+h\int \mathrm{d}y\,\frac{\delta F[\varphi(x)]}{\delta\varphi(y)}\frac{\partial\varphi(y,t)}{\partial t}+O(h^2)-F[\varphi(x,t)]\right\} \\
&= \int \mathrm{d}y\,\frac{\delta F[\varphi(x,t)]}{\delta\varphi(y,t)}\frac{\partial\varphi(y,t)}{\partial t}.
\end{aligned}
$$

4. 微小変換 $x(t)\mapsto x'(t)=x(t)+\delta x(t)$ に対し $\varphi(x(t))\mapsto\varphi'(x'(t))=\varphi(x(t))+\delta\varphi(x(t))$ と変換されるとき, 汎関数 $F_{x'(t)}[\varphi']$ を 1 次まで展開することを考える. 汎関数 $F_{x(t)}[\varphi']$ をパラメータ $x(t)$ に関する汎関数 $G_t[x]:=F_{x(t)}[\varphi']$ と見れば $\delta x(t)$ の 1 次で展開することができ,

$$
\begin{aligned}
&F_{x'(t)}[\varphi'] \\
&= F_{x(t)+\delta x(t)}[\varphi'] \\
&\left(= G_t[x+\delta x] = G_t[x]+\int \mathrm{d}x_0\,\frac{\delta G_t[x]}{\delta x(t_0)}\delta x(t_0)\right) \\
&= F_{x(t)}[\varphi']+\int \mathrm{d}t_0\,\frac{\delta F_{x(t)}[\varphi']}{\delta x(t_0)}\delta x(t_0) \\
&= F_{x(t)}\big[\varphi+\delta^L\varphi\big]+\int \mathrm{d}t_0\,\frac{\delta F_{x(t)}\big[\varphi+\delta^L\varphi\big]}{\delta x(t_0)}\delta x(t_0) \\
&= F_{x(t)}\big[\varphi+\delta^L\varphi\big]+\int \mathrm{d}t_0\,\frac{\delta F_{x(t)}[\varphi]}{\delta x(t_0)}\delta x(t_0).
\end{aligned}
$$

ただし, $\delta^L\varphi(x(t))$ は Lie 微分である:

$$
\delta^L\varphi(x(t)) := \varphi'(x(t))-\varphi(x(t)) = \delta\varphi(x(t))-\frac{\mathrm{d}\varphi(x(t))}{\mathrm{d}x(t)}\delta x(t).
$$

次に $F_{x(t)}[\varphi']$ を 1 次で展開して,

$$
\begin{aligned}
&F_{x(t)}[\varphi+\delta^L\varphi] \\
&= F_{x(t)}[\varphi]+\int \mathrm{d}x(t_0)\,\frac{\delta F_{x(t)}[\varphi]}{\delta\varphi(x(t_0))}\delta^L\varphi(x(t_0)) \\
&= F_{x(t)}[\varphi]+\int \mathrm{d}x(t_0)\,\frac{\delta F_{x(t)}[\varphi]}{\delta\varphi(x(t_0))}\delta\varphi(x(t_0))-\int \mathrm{d}x(t_0)\,\frac{\delta F_{x(t)}[\varphi]}{\delta\varphi(x(t_0))}\frac{\mathrm{d}\varphi(x(t_0))}{\mathrm{d}x(t_0)}\delta x(t_0) \\
&= F_{x(t)}[\varphi]+\int \mathrm{d}x(t_0)\,\frac{\delta F_{x(t)}[\varphi]}{\delta\varphi(x(t_0))}\delta\varphi(x(t_0))-\int \mathrm{d}t_0\,\frac{\delta F_{x(t)}[\varphi]}{\delta\varphi(x(t_0))}\frac{\mathrm{d}\varphi(x(t_0))}{\mathrm{d}t_0}\delta x(t_0).
\end{aligned}
$$

これを前の式に代入すれば, $F_{x'(t)}[\varphi']$ の 1 次の展開が得られる:

$$
\begin{aligned}
F_{x'(t)}[\varphi'] &= F_{x(t)}[\varphi] + \int \mathrm{d}x(t_0)\, \frac{\delta F_{x(t)}[\varphi]}{\delta\varphi(x(t_0))}\delta^L\varphi(x(t_0)) + \int \mathrm{d}t_0\, \frac{\delta F_{x(t)}[\varphi]}{\delta x(t_0)}\delta x(t_0) \\
&= F_{x(t)}[\varphi] + \int \mathrm{d}x(t_0)\, \frac{\delta F_{x(t)}[\varphi]}{\delta\varphi(x(t_0))}\delta\varphi(x(t_0)) \\
&\qquad + \int \mathrm{d}t_0 \left[\frac{\delta F_{x(t)}[\varphi]}{\delta x(t_0)} - \frac{\delta F_{x(t)}[\varphi]}{\delta\varphi(x(t_0))}\frac{\mathrm{d}\varphi(x(t_0))}{\mathrm{d}t_0} \right]\delta x(t_0).
\end{aligned}
$$

0.4 汎関数積分

$x \in [a, b]$ の関数上で定義される $F[\varphi(x)]$ の**汎関数積分** functional integration は, 以下で定義される:

$$
\begin{aligned}
\int \mathcal{D}\varphi(x) F[\varphi(x)] &:= \frac{1}{\theta}\left(\prod_{x\in[a,b]} \int \mathrm{d}\varphi(x) \right) F[\varphi(x)] \\
&:= \lim_{N\to\infty} \frac{1}{\theta(N)} \int \mathrm{d}\varphi_0 \cdots \int \mathrm{d}\varphi_N\, f_N(\varphi_0, \dots, \varphi_N).
\end{aligned}
$$

ただし, θ は有限値に収束させるための正規化因子, $f_N(\varphi_0, \dots, \varphi_N)$ は $F[\varphi(x)]$ の離散表現である. 単に $\int \mathcal{D}\varphi F[\varphi]$ とも略記される.

$\varphi(x)$ の端を固定した汎関数積分も重要である:

$$
\begin{aligned}
\int_{\varphi_0}^{\varphi} \mathcal{D}\varphi(x) F[\varphi(x)] &:= \frac{1}{\theta}\left(\prod_{x\in(a,b)} \int \mathrm{d}\varphi(x) \right) F[\varphi(x)] \Big|_{\varphi(a)=\varphi_0}^{\varphi(b)=\varphi} \\
&:= \lim_{N\to\infty} \frac{1}{\theta(N)} \int \mathrm{d}\varphi_1 \cdots \int \mathrm{d}\varphi_{N-1}\, f_N(\varphi_0, \varphi_1, \dots, \varphi_{N-1}, \varphi).
\end{aligned}
$$

これは, 端点を固定した経路の経路上各点について積分した積になっていることから, **経路積分**とも呼ばれる.

0.4.1 汎関数積分の計算例

1. $F[\varphi(x)] = \exp\left[i \int_a^b \mathrm{d}x\, \frac{A}{2}\{\varphi(x)\}^2 \right]$ の汎関数積分 $I(\varphi) = \int_{\varphi_0}^{\varphi} \mathcal{D}\varphi(x) F[\varphi(x)]$, ただし $\int \mathrm{d}\varphi\, I(\varphi) = 1$ として正規化:
   $F[\varphi(x)]$ の離散表現は,

$$
f_N(\varphi_0, \varphi_1, \dots, \varphi_{N-1}, \varphi) = \exp\left[i \sum_{n=1}^{N} \Delta x \times \frac{A}{2}\varphi_n^2 \right]_{\varphi_0=\varphi_0}^{\varphi_N=\varphi}.
$$

ただし, 分割幅を $\Delta x := (b-a)/N$ とした. したがって $F[\varphi(x)]$ の汎関数積分は,

$$\begin{aligned}
I(\varphi) &= \int_{\varphi(a)=\varphi_0}^{\varphi(b)=\varphi} \mathcal{D}\varphi(x) \exp\left[i\int_a^b \mathrm{d}x \frac{A}{2}\{\varphi(x)\}^2\right] \\
&= \lim_{N\to\infty} \frac{1}{\theta(N)} \int \mathrm{d}\varphi_1 \cdots \int \mathrm{d}\varphi_{N-1} \exp\left[i\sum_{n=1}^{N} \Delta x \times \frac{A}{2}\varphi_n^2\right]_{\varphi_0=\varphi_0}^{\varphi_N=\varphi} \\
&= \lim_{N\to\infty} \frac{1}{\theta(N)} \exp\left[i\Delta x \times \frac{A}{2}\varphi^2\right] \prod_{n=1}^{N-1} \int \mathrm{d}\varphi_n \exp\left[i\frac{A\Delta x}{2}\varphi_n^2\right] \\
&\quad \left(\int \mathrm{d}x \exp\left(-iax^2\right) = \sqrt{\frac{\pi}{ia}}\right) \\
&= \lim_{N\to\infty} \frac{1}{\theta(N)} \left(\frac{2\pi i}{A\Delta x}\right)^{(N-1)/2} \exp\left[i\frac{A\Delta x}{2}\varphi^2\right].
\end{aligned}$$

ここで, 定数 C を用いて $\theta(N) = \dfrac{1}{C}\left(\dfrac{2\pi i}{A\Delta x}\right)^{N/2}$ とすれば,

$$\begin{aligned}
I(\varphi) &= \lim_{N\to\infty} C\left(\frac{A\Delta x}{2\pi i}\right)^{N/2} \left(\frac{2\pi i}{A\Delta x}\right)^{(N-1)/2} \exp\left[i\frac{A\Delta x}{2}\varphi^2\right] \\
&= \lim_{N\to\infty} C\sqrt{\frac{A\Delta x}{2\pi i}} \exp\left[i\frac{A\Delta x}{2}\varphi^2\right].
\end{aligned}$$

正規化条件より定数 C を決定すると,

$$1 = \int \mathrm{d}\varphi\, I(\varphi) = \lim_{N\to\infty} C \int \mathrm{d}\varphi \sqrt{\frac{A\Delta x}{2\pi i}} \exp\left[i\frac{A\Delta x}{2}\varphi^2\right] = C.$$

したがって,

$$I(\varphi) = \lim_{N\to\infty} \sqrt{\frac{A\Delta x}{2\pi i}} \exp\left[i\frac{A\Delta x}{2}\varphi^2\right] = \lim_{N\to\infty} \sqrt{\frac{A(b-a)}{2\pi i N}} \exp\left[i\frac{A(b-a)}{2N}\varphi^2\right].$$

2. $F[\varphi(x)] = \exp\left[i\int_a^b \mathrm{d}x \dfrac{A}{2}\{\varphi'(x)\}^2\right]$ の汎関数積分 $I(\varphi) = \displaystyle\int_{\varphi_0}^{\varphi} \mathcal{D}\varphi(x) F[\varphi(x)]$, ただし $\displaystyle\int \mathrm{d}\varphi\, I(\varphi) = 1$ として正規化:
$F[\varphi(x)]$ の離散表現は,

$$f_N(\varphi_0, \varphi_1, \ldots, \varphi_{N-1}, \varphi) = \exp\left[i\sum_{n=1}^{N} \Delta x \times \frac{A}{2}\left(\frac{\varphi_n - \varphi_{n-1}}{\Delta x}\right)^2\right]_{\varphi_0=\varphi_0}^{\varphi_N=\varphi}.$$

ただし, 分割幅を $\Delta x := (b-a)/N$ とした. したがって $F[\varphi(x)]$ の汎関数積分は,

$$
\begin{aligned}
I(\varphi) &= \int_{\varphi(a)=\varphi_0}^{\varphi(b)=\varphi} \mathcal{D}\varphi(x) \exp\left[i \int_a^b \mathrm{d}x \, \frac{A}{2} \{\varphi'(x)\}^2 \right] \\
&= \lim_{N\to\infty} \frac{1}{\theta(N)} \int \mathrm{d}\varphi_1 \cdots \int \mathrm{d}\varphi_{N-1} \exp\left[i \sum_{n=1}^{N} \Delta x \times \frac{A}{2} \left(\frac{\varphi_n - \varphi_{n-1}}{\Delta x} \right)^2 \right]_{\varphi_0=\varphi_0}^{\varphi_N=\varphi} \\
&= \lim_{N\to\infty} \frac{1}{\theta(N)} \int \mathrm{d}\varphi_1 \cdots \int \mathrm{d}\varphi_{N-1} \exp\left[\frac{iA}{2\Delta x} \sum_{n=1}^{N} (\varphi_n - \varphi_{n-1})^2 \right]_{\varphi_0=\varphi_0}^{\varphi_N=\varphi} \\
&= \lim_{N\to\infty} \frac{1}{\theta(N)} \int \mathrm{d}\varphi_1 \cdots \int \mathrm{d}\varphi_{N-1} \exp\left\{ \frac{iA}{2\Delta x} \left[(\varphi - \varphi_{N-1})^2 + \sum_{k=1}^{N-1} (\varphi_{N-k} - \varphi_{N-(k+1)})^2 \right] \right\}_{\varphi_0=\varphi_0} .
\end{aligned}
$$

ここで φ_{N-k} の積分について考えると,

$$
\begin{aligned}
&\int \mathrm{d}\varphi_{N-k} \exp\left\{ \frac{iA}{2\Delta x} \left[\frac{1}{k} (\varphi - \varphi_{N-k})^2 + (\varphi_{N-k} - \varphi_{N-(k+1)})^2 \right] \right\} \\
=& \int \mathrm{d}\varphi_{N-k} \exp\left\{ \frac{iA}{2\Delta x} \left[\frac{k+1}{k} \varphi_{N-k}^2 - 2\left(\frac{1}{k}\varphi + \varphi_{N-(k+1)} \right) \varphi_{N-k} + \left(\frac{1}{k}\varphi^2 + \varphi_{N-(k+1)}^2 \right) \right] \right\} \\
=& \int \mathrm{d}\varphi_{N-k} \exp\left[\frac{iA}{2\Delta x} \frac{k+1}{k} \varphi_{N-k}^2 - \frac{iA}{2\Delta x} 2\left(\frac{1}{k}\varphi + \varphi_{N-(k+1)} \right) \varphi_{N-k} + \frac{iA}{2\Delta x} \left(\frac{1}{k}\varphi^2 + \varphi_{N-(k+1)}^2 \right) \right] \\
& \left(\int \mathrm{d}x \exp\left(-iax^2 + ibx \right) = \sqrt{\frac{\pi}{ia}} \exp\left(\frac{ib^2}{4a} \right) \right) \\
=& \sqrt{\frac{k}{k+1}} \sqrt{\frac{2\pi i \Delta x}{A}} \exp\left[-\frac{iA}{2\Delta x} \frac{k}{k+1} (\varphi + \varphi_{N-(k+1)})^2 + \frac{iA}{2\Delta x} \left(\frac{1}{k}\varphi^2 + \varphi_{N-(k+1)}^2 \right) \right] \\
=& \sqrt{\frac{k}{k+1}} \sqrt{\frac{2\pi i \Delta x}{A}} \exp\left[\frac{iA}{2\Delta x} \frac{1}{k+1} \left(\varphi - \varphi_{N-(k+1)} \right)^2 \right]
\end{aligned}
$$

より, $k = 1, \ldots, N-1$ で順に積分することで,

$$
\begin{aligned}
I(\varphi) &= \lim_{N\to\infty} \frac{1}{\theta(N)} \sqrt{\frac{1}{2}} \sqrt{\frac{2}{3}} \cdots \sqrt{\frac{N-1}{N}} \left(\sqrt{\frac{2\pi i \Delta x}{A}} \right)^{N-1} \exp\left[\frac{iA}{2N\Delta x} (\varphi - \varphi_0)^2 \right] \\
&= \lim_{N\to\infty} \frac{1}{\theta(N)} \frac{1}{\sqrt{N}} \left(\frac{2\pi i \Delta x}{A} \right)^{(N-1)/2} \exp\left[\frac{iA}{2N\Delta x} (\varphi - \varphi_0)^2 \right].
\end{aligned}
$$

ここで, 定数 C を用いて $\theta(N) = \frac{1}{C} \left(\frac{2\pi i \Delta x}{A} \right)^{N/2}$ とすれば,

$$
\begin{aligned}
I(\varphi) &= \lim_{N\to\infty} C \left(\frac{A}{2\pi i \Delta x} \right)^{N/2} \frac{1}{\sqrt{N}} \left(\frac{2\pi i \Delta x}{A} \right)^{(N-1)/2} \exp\left[\frac{iA}{2N\Delta x} (\varphi - \varphi_0)^2 \right] \\
&= \lim_{N\to\infty} C \sqrt{\frac{a}{2\pi i N \Delta x}} \exp\left[\frac{iA}{2N\Delta x} (\varphi - \varphi_0)^2 \right] \\
&= C \sqrt{\frac{A}{2\pi i (b-a)}} \exp\left[i \frac{A}{2} \frac{(\varphi - \varphi_0)^2}{b-a} \right].
\end{aligned}
$$

正規化条件より定数 C を決定すると,

$$1=\int \mathrm{d}\varphi\, I(\varphi)=C\int \mathrm{d}\varphi \sqrt{\frac{A}{2\pi i(b-a)}}\exp\left[i\frac{A}{2}\frac{(\varphi-\varphi_0)^2}{b-a}\right]=C.$$

したがって,

$$I(\varphi)=\int_{\varphi(a)=\varphi_0}^{\varphi(b)=\varphi}\mathcal{D}\varphi(x)\exp\left[i\int_a^b \mathrm{d}x\,\frac{A}{2}\{\varphi'(x)\}^2\right]=\sqrt{\frac{A}{2\pi i(b-a)}}\exp\left[i\frac{A}{2}\frac{(\varphi-\varphi_0)^2}{b-a}\right].$$

3. 汎関数積分の連結:

$x_3>x_2>x_1$ に対し, $x\in[x_3,x_1]$ の関数上で定義される汎関数 $F[\varphi(x)]$ について,

$$\int_{\varphi_1}^{\varphi_2}\mathcal{D}\varphi(x)\int \mathrm{d}\varphi_2\int_{\varphi_2}^{\varphi_3}\mathcal{D}\varphi(x)F[\varphi(x)]=\int_{\varphi_1}^{\varphi_3}\mathcal{D}\varphi(x)F[\varphi(x)].$$

実際,

$$\begin{aligned}&\int_{\varphi_1}^{\varphi_2}\mathcal{D}\varphi(x)\int \mathrm{d}\varphi_2\int_{\varphi_2}^{\varphi_3}\mathcal{D}\varphi(x)\mathrm{g}(\varphi_2)F[\varphi(x)]\\&=\frac{1}{\theta}\left(\prod_{x\in(t_1,t_2)}\int \mathrm{d}\varphi(x)\right)\int \mathrm{d}\varphi(x_2)\left(\prod_{x\in(t_2,t_3)}\int \mathrm{d}\varphi(x)\right)F[\varphi(x)]\\&=\frac{1}{\theta}\left(\prod_{x\in(t_1,t_3)}\int \mathrm{d}\varphi(x)\right)F[\varphi(x)]\quad(\because(t_1,t_2)\cup\{t_2\}\cup(t_2,t_3)=(t_1,t_3))\\&=\int_{\varphi_1}^{\varphi_3}\mathcal{D}\varphi(x)F[\varphi(x)].\end{aligned}$$

特に, 指数法則 $F_{x\in A}[\varphi]F_{x\in B}[\varphi]=F_{x\in A\cup B}[\varphi]$ を満たす汎関数 (例えば $F_{x\in[a,b]}[\varphi]=\exp\left[\int_a^b \mathrm{d}x\,\varphi(x)\right]$) に対しては,

$$\begin{aligned}&\int \mathrm{d}\varphi_2\,\mathrm{g}(\varphi_2)\left(\int_{\varphi_1}^{\varphi_2}\mathcal{D}\varphi(x)F_{x\in[x_1,x_2]}[\varphi]\right)\left(\int_{\varphi_2}^{\varphi_3}\mathcal{D}\varphi(x)F_{x\in[x_2,x_3]}[\varphi]\right)\\&=\int_{\varphi_1}^{\varphi_3}\mathcal{D}\varphi(x)F_{x\in[x_1,x_3]}[\varphi]\mathrm{g}(\varphi(x_2)).\end{aligned}$$

実際,

$$\begin{aligned}&\int \mathrm{d}\varphi_2\,\mathrm{g}(\varphi_2)\left(\int_{\varphi_1}^{\varphi_2}\mathcal{D}\varphi(x)F_{x\in[x_1,x_2]}[\varphi]\right)\left(\int_{\varphi_2}^{\varphi_3}\mathcal{D}\varphi(x)F_{x\in[x_2,x_3]}[\varphi]\right)\\&=\int_{\varphi_1}^{\varphi_2}\mathcal{D}\varphi(x)\int \mathrm{d}\varphi_2\int_{\varphi_2}^{\varphi_3}\mathcal{D}\varphi'(x)\mathrm{g}(\varphi_2)F_{x\in[x_1,x_2]}[\varphi]F_{x\in[x_2,x_3]}[\varphi']\\&=\int_{\varphi_1}^{\varphi_3}\mathcal{D}\varphi(x)\mathrm{g}(\varphi(x_2))F_{x\in[x_1,x_3]}[\varphi].\end{aligned}$$

0.5 参考文献

- Stevens, C. F. The Six Core Theories of Modern Physics (United Kingdom, MIT Press, 1995)