

汎関数の計算

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2024 年 6 月 3 日

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, $F : (A \rightarrow B) \rightarrow C$ など. このとき, $\varphi : A \rightarrow B$ 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, 通常関数 $g : C \rightarrow D$ 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, 独自の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 $\varphi : [a, b] \rightarrow \mathbb{R}$ の汎関数 $F[\varphi(x)]$ を考える. I の分割 $a = x_0 < \dots < x_N = b$ 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 $f_N(\varphi_0, \dots, \varphi_N)$ 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 $F[\varphi(x)] = \int_a^b dx \varphi(x)$ では, 分割幅を $\Delta x_n := x_n - x_{n-1}$ として, Riemann 積分の考え方をいれれば^{*3},

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

^{*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 $\varepsilon : A \rightarrow A$ 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 $x_n := a + \frac{n(b-a)}{N}$, 分割幅 $\Delta x := \frac{b-a}{N}$ に対し, 例えば $\varphi(x) := x^2$ とすると,

$$f_N(x_0^2, \dots, x_N^2) = \sum_{n=1}^N \Delta x \times x_n^2$$

$$\xrightarrow{N \rightarrow \infty} F[x^2] = \int_a^b dx x^2.$$

このような汎関数の離散的な表現を考えることも, 汎関数の計算に役立つ.

0.1.1 汎関数の例

以下は汎関数である:

1. 積分

$$i_N(\varphi_0, \dots, \varphi_N) = \sum_{n=1}^N \Delta x \times g(\varphi_n)$$

$$\xrightarrow{N \rightarrow \infty} I[\varphi(x)] = \int dx g(\varphi(x)).$$

2. 代入

$$s(\varphi_0, \dots, \varphi_N; x_m = x') = \sum_{n=1}^N \Delta x \times \varphi_n \frac{\delta_{nm}}{\Delta x} = \varphi_m$$

$$\xrightarrow{N \rightarrow \infty} S[\varphi(x)](x') = \int dx \varphi(x) \delta(x - x') = \varphi(x').$$

汎関数中のデルタ関数 $\delta(x - x')$ は, 離散表現の $\frac{\delta_{nm}}{\Delta x}$ に対応している.

3. Fourier 変換

$$f_N(\varphi_0, \dots, \varphi_N; k_m) = \sum_{n=1}^N \frac{\Delta x}{\sqrt{2\pi}} \times \varphi_n e^{-ik_m x_n}$$

$$\xrightarrow{N \rightarrow \infty} \mathcal{F}[\varphi(x)](k) = \int \frac{dx}{\sqrt{2\pi}} \varphi(x) e^{-ikx}.$$

4. Fourier 逆変換

$$f_N^{\text{"-1"}}(\tilde{\varphi}_0, \dots, \tilde{\varphi}_N; x_n) = \sum_{m=1}^N \frac{\Delta k}{\sqrt{2\pi}} \times \tilde{\varphi}_m e^{ik_m x_n}$$

$$\xrightarrow{N \rightarrow \infty} \mathcal{F}^{-1}[\tilde{\varphi}(k)](x) = \int \frac{dk}{\sqrt{2\pi}} \tilde{\varphi}(k) e^{ikx};$$

実際, $\mathcal{F}^{-1}[\mathcal{F}[\varphi(x)](k)](x) = \varphi(x)$.

5. 汎関数のダミー変数を関数にしたもの

$$g_N(x_0, \dots, x_N) = f_N(\varphi_0, \dots, \varphi_N)$$

$$\xrightarrow{N \rightarrow \infty} G_t[x] := F_{x(t)}[\varphi].$$

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

$$g_N(x_0, \dots, x_N) = f_N(\varphi_0, \dots, \varphi_N) = \sum_{n=1}^N \Delta x \times \varphi_n = \sum_{n=1}^N \Delta t \times \frac{\Delta x}{\Delta t} \varphi(x_n)$$

$$\xrightarrow{N \rightarrow \infty} G_t[x] = F_{x(t)}[\varphi] = \int dx(t) \varphi(x(t)) = \int dt \frac{dx}{dt} \varphi(x(t)).$$

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:

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

物理では汎関数微分を変分とも呼び, 単に $\frac{\delta F[\varphi]}{\delta \varphi}$ 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

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

したがって, 汎関数微分演算子 $\frac{\delta}{\delta \varphi(y)}$ に対応する離散表現は $\frac{1}{\Delta x} \frac{\partial}{\partial \varphi_m}$ 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 $\frac{\delta F[\varphi(x)]}{\delta \varphi(y)}$ を計算する:

$$1. F[\varphi(x)] = \int dx g(x) \varphi(x):$$

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

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

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

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. $F[\varphi(x)] = \int dx g(\varphi(x))$:

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

離散表現では, $y = x_m$ として,

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

4. $F[\varphi(x)] = \int dx g(\varphi'(x))$:

$$\begin{aligned} & \frac{\delta}{\delta\varphi(y)} \int dx g(\varphi'(x)) \\ &= \lim_{h \rightarrow 0} \frac{1}{h} \left[\int dx g\left(\frac{d\{\varphi(x) + h\delta(x - y)\}}{dx}\right) - \int dx g\left(\frac{d\varphi(x)}{dx}\right) \right] \\ &= \lim_{h \rightarrow 0} \frac{1}{h} \left[\int dx g\left(\frac{d\varphi(x)}{dx} + h \frac{d\delta(x - y)}{dx}\right) - \int dx g\left(\frac{d\varphi(x)}{dx}\right) \right] \\ &= \lim_{h \rightarrow 0} \frac{1}{h} \left\{ \int dx \left[h \frac{dg(d\varphi(x)/dx)}{d(d\varphi(x)/dx)} \frac{d\delta(x - y)}{dx} + O(h^2) \right] \right\} \\ &= \lim_{h \rightarrow 0} \frac{1}{h} \left\{ \int dx \left[-h \frac{d}{dx} \frac{dg(d\varphi(x)/dx)}{d(d\varphi(x)/dx)} \delta(x - y) + h \frac{d}{dt} \left(\frac{dg(d\varphi(x)/dx)}{d(d\varphi(x)/dx)} \delta(x - y) \right) + O(h^2) \right] \right\} \\ & \quad (\because \text{部分積分}) \\ &= \lim_{h \rightarrow 0} \frac{1}{h} \left[-h \frac{d}{dy} \frac{dg(d\varphi(y)/dy)}{d(d\varphi(y)/dy)} + h \int d\left(\frac{dg(d\varphi(x)/dx)}{d(d\varphi(x)/dx)} \delta(x - y) \right) + O(h^2) \right] \\ &= - \frac{d}{dy} \frac{dg(d\varphi(y)/dy)}{d(d\varphi(y)/dy)} + \int d\left(\frac{dg(d\varphi(x)/dx)}{d(d\varphi(x)/dx)} \delta(x - y) \right) \\ &= - \frac{d}{dy} \frac{dg(\varphi'(y))}{d\varphi'(y)} + \int d\left(\frac{dg(\varphi'(x))}{d\varphi'(x)} \delta(x - y) \right). \end{aligned}$$

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,

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

離散表現では, $y = x_m$ として,

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

5. $F[\varphi(x)] = \int dx g(\varphi(x), \varphi'(x))$:

上の例を繰り返し使うことで,

$$\frac{\delta}{\delta\varphi(y)} \int dx g(\varphi(x), \varphi'(x)) = \frac{\partial g}{\partial\varphi(y)} - \frac{d}{dy} \frac{\partial g}{\partial\varphi'(y)} + \int d\left(\frac{\partial g}{\partial\varphi'(x)} \delta(x-y)\right),$$

あるいは, y が積分範囲の内部にあるとき,

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

0.3 汎関数冪級数

連続な汎関数は Taylor 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,

$$\begin{aligned} F[\varphi(x) + \eta(x)] &= F[\varphi(x)] + \int dy \frac{\delta F[\varphi(x)]}{\delta\varphi(y)} \eta(y) \\ &\quad + \frac{1}{2} \int dy_1 \int dy_2 \frac{\delta^2 F[\varphi(x)]}{\delta\varphi(y_1) \delta\varphi(y_2)} \eta(y_1) \eta(y_2) + \dots \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \int dy_1 \dots \int dy_n \frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1) \dots \delta\varphi(y_n)} \eta(y_1) \dots \eta(y_n). \end{aligned}$$

特に, $\varphi = 0$ まわりの冪展開は,

$$\begin{aligned} F[\varphi(x)] &= F[0] + \int dy \frac{\delta F[\varphi(x)]}{\delta\varphi(y)} \Big|_{\varphi=0} \varphi(y) + \frac{1}{2} \int dy_1 \int dy_2 \frac{\delta^2 F[\varphi(x)]}{\delta\varphi(y_1) \delta\varphi(y_2)} \Big|_{\varphi=0} \varphi(y_1) \varphi(y_2) + \dots \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \int dy_1 \dots \int dy_n \frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1) \dots \delta\varphi(y_n)} \Big|_{\varphi=0} \varphi(y_1) \dots \varphi(y_n). \end{aligned}$$

汎関数冪級数の離散表現は,

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

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 $\frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)}$ が y_1, \dots, y_n について対称であると仮定して, $\frac{\delta^n F}{\delta\varphi^n}$ と略記する。

また,

$$\frac{\delta^n F}{\delta\varphi^n} * \eta^n := \int dy_1 \cdots \int dy_n \frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)} \eta(y_1)\cdots\eta(y_n)$$

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

$$\begin{aligned} & \frac{\delta}{\delta\eta(y)} \left(\frac{\delta^n F}{\delta\varphi^n} * \eta^n \right) \\ &= \lim_{h \rightarrow 0} \frac{1}{h} \left[\int dy_1 \cdots \int dy_n \frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)} [\eta(y_1) + h\delta(y_1 - y)] \cdots [\eta(y_n) + h\delta(y_n - y)] \right. \\ & \quad \left. - \int dy_1 \cdots \int dy_n \frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)} \eta(y_1)\cdots\eta(y_n) \right] \\ &= \lim_{h \rightarrow 0} \frac{1}{h} \left[\sum_{i=0}^n \int dy_1 \cdots \int dy_n \frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)} \eta(y_1)\cdots\widehat{\eta(y_i)}\cdots\eta(y_n) h\delta(y_i - y) + O(h^2) \right] \\ &= \sum_{i=0}^n \int dy_1 \cdots \int dy_n \frac{\delta^n F[\varphi(x)]}{\delta\varphi(y_1)\cdots\delta\varphi(y_n)} \eta(y_1)\cdots\widehat{\eta(y_i)}\cdots\eta(y_n) \delta(y_i - y) \\ &= n \int dy_1 \cdots \int dy_{n-1} \frac{\delta^n F[\varphi(x)]}{\delta\varphi(y)\delta\varphi(y_1)\cdots\delta\varphi(y_{n-1})} \eta(y_1)\cdots\eta(y_{n-1}) \\ &= n \frac{\delta}{\delta\varphi(y)} \left(\frac{\delta^{n-1} F}{\delta\varphi^{n-1}} \right) * \eta^{n-1} \quad \left(=: n \frac{\delta^n F}{\delta\varphi^n} * \eta^{n-1} \text{とも書く} \right). \end{aligned}$$

2. $g(F[\varphi(x)])$ の汎関数微分:

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

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

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

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,

$$\begin{aligned}
& F_{x'(t)}[\varphi'] \\
&= F_{x(t)+\delta x(t)}[\varphi'] \\
&\quad \left(= G_t[x + \delta x] = G_t[x] + \int dx_0 \frac{\delta G_t[x]}{\delta x(t_0)} \delta x(t_0) \right) \\
&= F_{x(t)}[\varphi'] + \int dt_0 \frac{\delta F_{x(t)}[\varphi']}{\delta x(t_0)} \delta x(t_0) \\
&= F_{x(t)}[\varphi + \delta^L \varphi] + \int dt_0 \frac{\delta F_{x(t)}[\varphi + \delta^L \varphi]}{\delta x(t_0)} \delta x(t_0) \\
&= F_{x(t)}[\varphi + \delta^L \varphi] + \int dt_0 \frac{\delta F_{x(t)}[\varphi]}{\delta x(t_0)} \delta x(t_0).
\end{aligned}$$

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

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

次に $F_{x(t)}[\varphi']$ を 1 次で展開して,

$$\begin{aligned}
& F_{x(t)}[\varphi + \delta^L \varphi] \\
&= F_{x(t)}[\varphi] + \int dx(t_0) \frac{\delta F_{x(t)}[\varphi]}{\delta \varphi(x(t_0))} \delta^L \varphi(x(t_0)) \\
&= F_{x(t)}[\varphi] + \int dx(t_0) \frac{\delta F_{x(t)}[\varphi]}{\delta \varphi(x(t_0))} \delta \varphi(x(t_0)) - \int dx(t_0) \frac{\delta F_{x(t)}[\varphi]}{\delta \varphi(x(t_0))} \frac{d\varphi(x(t_0))}{dx(t_0)} \delta x(t_0) \\
&= F_{x(t)}[\varphi] + \int dx(t_0) \frac{\delta F_{x(t)}[\varphi]}{\delta \varphi(x(t_0))} \delta \varphi(x(t_0)) - \int dt_0 \frac{\delta F_{x(t)}[\varphi]}{\delta \varphi(x(t_0))} \frac{d\varphi(x(t_0))}{dt_0} \delta x(t_0).
\end{aligned}$$

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:

$$\begin{aligned} F_{x'(t)}[\varphi'] &= F_{x(t)}[\varphi] + \int dx(t_0) \frac{\delta F_{x(t)}[\varphi]}{\delta \varphi(x(t_0))} \delta^L \varphi(x(t_0)) + \int dt_0 \frac{\delta F_{x(t)}[\varphi]}{\delta x(t_0)} \delta x(t_0) \\ &= F_{x(t)}[\varphi] + \int dx(t_0) \frac{\delta F_{x(t)}[\varphi]}{\delta \varphi(x(t_0))} \delta \varphi(x(t_0)) \\ &\quad + \int dt_0 \left[\frac{\delta F_{x(t)}[\varphi]}{\delta x(t_0)} - \frac{\delta F_{x(t)}[\varphi]}{\delta \varphi(x(t_0))} \frac{d\varphi(x(t_0))}{dt_0} \right] \delta x(t_0). \end{aligned}$$

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:

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

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:

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

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. $F[\varphi(x)] = \exp \left[i \int_a^b dx \frac{A}{2} \{\varphi(x)\}^2 \right]$ の汎関数積分 $I(\varphi) = \int_{\varphi_0}^{\varphi} \mathcal{D}\varphi(x) F[\varphi(x)]$, ただし

$\int d\varphi I(\varphi) = 1$ 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,

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

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

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

正規化条件より定数 C を決定すると,

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

したがって,

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

2. $F[\varphi(x)] = \exp \left[i \int_a^b dx \frac{A}{2} \{\varphi'(x)\}^2 \right]$ の汎関数積分 $I(\varphi) = \int_{\varphi_0}^{\varphi} \mathcal{D}\varphi(x) F[\varphi(x)]$, ただし

$\int d\varphi I(\varphi) = 1$ として正規化:

$F[\varphi(x)]$ の離散表現は,

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

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,

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

ここで φ_{N-k} の積分について考えると,

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

より, $k = 1, \dots, N-1$ で順に積分することで,

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

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,

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

正規化条件より定数 C を決定すると,

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

したがって,

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

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,

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

実際,

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

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 $F_{x \in [a, b]}[\varphi] = \exp \left[\int_a^b dx \varphi(x) \right]$) に対しては,

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

実際,

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

0.5 参考文献

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