3.1.2 Functional derivatives

From the potential in Eq. (3.1.1), woth $\tilde{K} = K_a$, we obtain a force acting on the nth bead via gradient descent as

$$F_n = -\frac{dV}{du_n} = K_a[(u_{n+1} - u_n) - (u_n - u_{n-1})] = K_a(u_{n+1} + u_{n-1} - 2u_n)\,. \qquad (3.1.5)$$

In the continuum limit, using $K_a = K/a$, the above expression goes over to a second derivative, resulting in a *force density*

$$\mathcal{F}(x) = -\frac{\delta V}{\delta u(x)} = K\frac{d^2u}{dx^2} \equiv Ku''\,. \qquad (3.1.6)$$

(To simplify equations, spacial derivatives will sometimes be denoted by primes; not to be confused with time derivatives indicated by dots.) $\mathcal{F}(x)$ is a *density* at x, as it is a force acting on an infinitesimal element of size dx around the point $x = na$. The symbol $\delta V/\delta u(x)$ indicates a *functional derivative*, charting the change in the value of the functional if its argument– the function $u(x)$– is changed by an infinitesimal amount at position x. As in the case of the elastic band, we shall mostly deal with functionals that can be expressed as an integral of a density, such as

$$V[f(x)] = \int dx\, U\left(f, f', f'', \cdots\right)\,. \qquad (3.1.7)$$

The integrand, $U(x) = U(f(x), f'(x).f''(x), \cdots)$, depends on the function and its derivatives at point x. The functional derivative is then obtained as

$$\frac{\delta V}{\delta f(x)} = \frac{dU}{df} - \frac{d}{dx}\frac{dU}{df'} + \frac{d^2}{dx^2}\frac{dU}{df''} + \cdots\,, \qquad (3.1.8)$$

and does depend on x, much as in the dependence of the force F_n in Eq. (3.1.5) on n. Only the second term is present in taking the functional derivative of Eq. (3.1.3), as in this case $U = \frac{K}{2}(u')^2$, such that $\frac{dU}{du} = 0$ $\frac{dU}{du'} = Ku'$, $\frac{dU}{du''} = 0$, and so on. The integration of Eq. (3.1.7) shows that U has different units than V, so that U is a *potential density*, and its derivative $\mathcal{F}$ in Eq. (3.1.6) is a *force density*.