3.1 From particles to fields

3.1.1 Continuum limit

A particular realization of the model of N blocks connected by springs is a set of beads glued at equidistant separations a along a stretched rubber band. In the case of the masses connected to fixed walls, an open rubber band would be stretched to a length $L = (N + 1)a$ between two nails; in the periodic case, a closed rubber band could tighten around a circle of perimeter $2\pi R = Na$. If each bead, labelled by n, is now displaced by u_n from its equilibrium position, the additional elastic energy stored in the rubber band is in the harmonic (quadratic) approximation (valid for small displacements) given by

$$V(u_1, \cdots, u_N) = \frac{\tilde{K}}{2}\left[(u_2 - u_1)^2 + \cdots + (u_N - u_{N-1})^2\right] + V_{\rm BC}(u_1, u_N)\,, \tag{3.1.1}$$

where

$$V_{\rm BC}(u_1, u_N) = \begin{cases} \dfrac{\tilde{K}}{2}(u_1^2 + u_N^2) & \text{for a pinned chain,} \\ \dfrac{\tilde{K}}{2}(u_1 - u_N)^2 & \text{for a periodic chain.} \end{cases} \tag{3.1.2}$$

(Any interactions of the particles with a supporting surface/ring are ignored.) Rather than actual beads glued to the rubber band, we could just indicate their positions by tick marks along the band, and Eq. (3.1.1) describes the potential energy cost of expanding and contracting different discrete segments of the rubber band. A finer description of the local strains and stretches of the rubber band can be obtained by doubling the number of tick marks to $2N$ at equilibrium separation of $a/2$. This effective spring constant for the finely spaced marks would be different from $\tilde{K}$, and to emphasize this dependence on the chosen spacing will be denoted by K_a.

The *continuum limit* is obtained as $N \to \infty$ and $a \to 0$, while maintaining a fixed $L = Na$. In this limit, we shall replace the discrete displacements $\{u_n\}$ with the continuous function $u(x)$ which we shall refer to as *field* defined the interval $0 \le x \le L$. The local elastic cost $K_a(u_{n+1} - u_n)^2/2$ is replaced with $K_a a^2 (du/dx)^2$, and the sum over these local costs with an integral, $\sum_{n=1}^{N} \to \int_0^L dx/a$, to arrive at

$$V[u(x)] = \frac{K}{2}\int_0^L dx \left(\frac{du}{dx}\right)^2 . \tag{3.1.3}$$

In making the transition from the discrete variables $\{u_n\}$ in Eq. (3.1.1) to the continuum limit of Eq. (3.1.3), we should note the following points:

- The potential energy is now a function of the function $u(x)$. This *functional* dependance is usually indicated by the square brackets, as $V[u(x)]$. However, the final result does not depend on x, in the same sense that the discrete version is a scalar variable without an index.

- The integration variable x, introduces a factor of length, which is removed through division by a, hence $\sum_n \to \int dx/a$.

- There can in principle be higher order derivatives in the expansion of the local energy, since (since with $x = na$)

$$u_{n+1} - u_n = u(x+a) - u(x) = a\frac{du}{dx} + \frac{a^2}{2}\frac{d^2u}{dx^2} + \cdots . \tag{3.1.4}$$

  To see if ignoring higher order derivatives is justified, let us consider a deformation over a characteristic distance λ. For simplicity we choose a form $u_n \propto \exp(an/\lambda)$ where each additional derivative is equivalent to multiplication by a factor of a/λ. This also holds for other deformation profiles, with the neglect of higher order derivatives justified for $\lambda \gg a$. The "gradient expansion" is thus valid for deformations that are much larger than any underlying microscopic scale (e.g. atomic size).

- Following these changes, the coefficient of the squared gradient is aK_a. The continuum elastic modulus K is then obtained as $K = \lim_{a\to 0}(aK_a)$.

- The pinned and periodic chains are now distinguished by *boundary conditions*: $u(L) = u(0) = 0$ for the former, while $u(L) = u(0)$ for the latter.