Chapter 3

Continuous fields

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

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

where

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

(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 $0 \leq x \leq L$. 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 $x = na$)

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

  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.

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

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

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

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

(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*.

3.1.3 The gradient expansion

In considering a single degree of freedom, u, we noted that simple reasonings based on continuity, small amplitudes, and slow variations, lead to typical force of the form

$$F(u) = f_0 + f_1 u + f_2\frac{u^2}{2} + \cdots \approx -Ju. \qquad (3.1.9)$$

For deformations around a stable equilibrium we must have $f_0 = 0$, and $f_1 < 0$, and can ignore higher order terms and small amplitudes, as implemented in the second part of the equation ($J > 0$).

We anticipate that the time evolution of the field at each position is governed by a force density F that depends on its value at that position, as well as values at nearby locations as in Eq. (3.1.5). Assuming smooth variations over scales larger than any underlying "microscopic" scale then suggests that the force density can be expanded in terms of derivatives of the field

at that location, as in Eq. (3.1.5). Indeed, the generalized Taylor expansion for the force density at position x takes the form

$$\mathcal{F}(u(x), u'(x), u''(x), \cdots) = f_0 + f_1 u + g_1 u' + h_1 u'' + \cdots + f_2 \frac{u^2}{2} + k u u' + g_2 \frac{u'^2}{2} + \cdots , \quad (3.1.10)$$

where primes indicate derivatives with respect to x. The various terms in this series expansion can be ordered according to powers of u and powers of the gradient.

Once more, we can rely on various arguments to focus on important terms in the series:

- If expanding around an equilibrium conditions, $u^*(x) = 0$, $f_0 = 0$, and $f_1 < 0$.

- The term g_1 is absent in Eq. (3.1.6). This is because of an implicit inversion symmetry $x \to -x$ for the rubber band. Indeed most of the examples we shall encounter have this symmetry.

- For deformations proportional to $\sin(qx)$, representing a sinusoidal distortion, the second derivative term generates a restoring force proportional to $-q^2 h_1$. For the field to be stable against such sinusoidally modulated deformations we need $h_1 > 0$.[1]

- For a deformation of characteristic range λ, the contribution of a term involving m factors of u and n derivatives scales as u^m / λ^n. The leading terms for small amplitude, long wavelength deformations around a steady state of a system with reflection symmetry thus take the generic form

$$\mathcal{F}(x) = -Ju + K \frac{d^2 u}{dx^2} . \quad (3.1.11)$$

- With the expansion terminated with the two terms in Eq. (3.1.11), the force density can be obtained from gradient descent in a functional

$$V[u(x)] = \int dx \left[\frac{J}{2} u^2 + \frac{K}{2} \left(\frac{du}{dx} \right)^2 \right] . \quad (3.1.12)$$

  While higher order terms in powers of u can also be represented by corresponding terms in the above functional, this is no necessarily the case for higher order terms involving derivatives. For example, you can check that the term $g_2 u'^2$ in Eq. (3.1.10) cannot be generated as a simple functional derivative.

The force density in Eq. (3.1.6) is even simpler than Eq. (3.1.11) in that the coefficient J of the linear term in u is also absent. Indeed, $J = 0$ is required for the rubber band by yet another symmetry: The energy density stored in the rubber band is not modified under the transformation $u(x) \to u(x) + c$ for any uniform displacement c. This is most obvious in

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[1] Strictly speaking, this constraint applies to the highest order derivative term included in the equation. In general, to ensure stability we must check that the restoring force is negative for any wavelength.

the ring geometry, as addition of c corresponds to rotating a distorted ring without changing any of the local distortions. From another perspective, the equilibrium condition requires the beads on the chain to be equidistant, but (barring pinning at the boundaries) does not specify an actual location. Adding a constant c corresponds to a shift of the chosen equilibrium state. The symmetry $u(x) \to u(x) + c$ thus forbids the term proportional to J in Eq. (3.1.12).

3.1.4 Partial Differential Equations

For the single coordinate u, the force $F(u)$ governs time evolution according to

$$\gamma \dot{u} + m\ddot{u} + \cdots = F(u) \approx -Ju + \cdots. \tag{3.1.13}$$

For small deformations around a stable equilibrium point, this equation has exponential solutions describing decay to equilibrium, or oscillations around it. We can ask if there are natural generalizations of Eq. (3.1.13), and corresponding forms of time evolution, for a continuous field $u(x)$. The natural extension of Eq. (3.1.13) takes the form

$$\eta \frac{\partial u}{\partial t} + \rho \frac{\partial^2 u}{\partial t^2} = \mathcal{F}(u) \approx -Ju + K \frac{\partial^2 u}{\partial x^2} + \cdots. \tag{3.1.14}$$

- We have used ∂u, rather than du to emphasize that Eq. (3.1.14) is a *partial differential equation* (PDE). The function $u(x, t)$ depends on two arguments; partial derivatives are taken with respect to one argument with the other treated as a constant.

- For $\eta = 0$, the PDE has time reversal symmetry. As in the single particle case of Eq. (1.1.6), the time invariant equation conserves an energy functional

$$E[u(x, t)] = \int dx \left[\frac{\rho}{2} \left(\frac{\partial u}{\partial t} \right)^2 + \frac{J}{2} u^2 + \frac{K}{2} \left(\frac{\partial u}{\partial x} \right)^2 \right]. \tag{3.1.15}$$

  Note that the application of chain rule gives

$$\frac{dE}{dt} = \int dx \left[\rho \frac{\partial^2 u}{\partial t^2} + Ju - K \frac{\partial^2 u}{\partial x^2} \right] \frac{\partial u}{\partial t}, \tag{3.1.16}$$

  where the difference in sign between the first and third terms is because only the third term involves derivatives with respect to the argument of the integration, and using integration by parts yields $\int (\partial_x u)(\partial_x \partial_t u) = -\int (\partial_x \partial_x u)(\partial_t u)$. For $\eta = 0$ in Eq. (3.1.14) the square brackets is zero and hence $dE/dt = 0$.

- For $\eta \neq 0$, substituting from Eq. (3.1.14) into Eq. (3.1.16) gives

$$\frac{dE}{dt} = -\eta \int dx \left(\frac{\partial u}{\partial t} \right)^2, \tag{3.1.17}$$

  quantifying the loss of energy due to friction.

The term proportional to J in Eq. (3.1.14) is absent in many physical systems due to symmetry or other constraints, leading to two of the most commonly encountered PDEs:

- **The diffusion equation** corresponds to the case of $\rho = 0$ (with symmetries appropriate to $J = 0$), and is generally written as

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}\,, \tag{3.1.18}$$

  where D is the *diffusion coefficient*.

  - If we integrate both sides of the equation with respect to x over an interval from a to b, we find

$$\frac{d}{dt}\int_a^b dx\,u(x,t) = D\int_a^b dx\frac{\partial^2 u}{\partial x^2} = D\left[\left.\frac{\partial u}{\partial x}\right|_b - \left.\frac{\partial u}{\partial x}\right|_a\right]\,, \tag{3.1.19}$$

    i.e. the change in the total amount of u in the interval comes only from the *flux* of u into and out of the interval at its edges.

  - The diffusion equation can thus be regarded as describing the dynamics of a *conserved* quantity, through a continuity equation

$$\frac{\partial u}{\partial t} = -\frac{\partial J}{\partial x}\,, \quad \text{with a flux (current)} \quad J = -D\frac{\partial u}{\partial x}\,. \tag{3.1.20}$$

- **The wave equation** describes the opposite limit of $\eta = 0$ in a system constrained by time reversal symmetry, and usually written as

$$\frac{\partial^2 u}{\partial t^2} = v^2\,\frac{\partial^2 u}{\partial x^2}\,, \tag{3.1.21}$$

  where v is the *wave velocity*. The wave equation admits solutions of the form $u(x,t) = u_\pm(x \pm vt)$ (i.e. a function only of either $x \pm vt$, rather than x and t separately) in which a deformation is simply translated forward or backward along space with speed v.

3.1.5   Initial conditions, Boundary conditions

In solving ODEs we had to supply initial values, one for the case of a first order equation and two for a second order equation. Solving for the full time evolution of PDEs also requires initial conditions in the form of functions, for example $u(x, t = 0)$ for a first order PDE, and additionally $\dot{u}(x, t = 0)$ for the second order one.

The **initial conditions** are related to, but distinct from **boundary conditions**. The latter arise because one typically needs to solve the problem over an interval of given extent in the space dimension, whose edges have to be treated carefully. Usually the complete description of a problem requires knowledge of what goes on at the boundaries. The most common boundary conditions are:

- **Dirichlet (closed):** The function is constrained to always be zero at an edge, such that
$$u(x = 0, t) = 0 \quad \text{for all times } t, \tag{3.1.22}$$
as in the case of the rubber band pinned to a wall at its edge.

- **Neumann (open):** The derivative is set to zero at an edge, i.e.
$$\frac{\partial u}{\partial x}(x = 0, t) = 0 \quad \text{for all times } t. \tag{3.1.23}$$
An open end that moves freely, and does not support a force is an example; no flux at edges of an interval in case of the diffusion equation is another.

- **Periodic:** When the two ends are joined together, forming a ring, like a snake biting its tail, we have
$$u(x = 0, t) = u(x = L, t) = 0.$$

There can also be mixed boundary conditions, e.g. a rope that is closed at one end, and open at the other, or **forced** at the edge to satisfy a particular motion, as in $u(x = 0, t) = a\cos(\omega t)$.

Recap

- The time evolution of a *continuous field $u(x)$* can be described by a partial differential equation (PDE).

- The diffusion equation $\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$ and the wave equation $\frac{\partial^2 u}{\partial t^2} = v^2\frac{\partial^2 u}{\partial x^2}$ are two commonly encountered PDEs.

- The full description of a PDE on an interval requires specification of *boundary conditions* at edges of the interval.