

Supporting Information

Part I

Transverse vibrations of a linear infinite chain under stress - single force constant

1 Springs chain

the distance between atom n and atoms $n+1$ is

$$d_{n,n+1} = (\Delta x^2 + (y_{n+1} - y_n)^2)^{1/2} \quad (1)$$

where Δx is the separation in the x-direction and y_n is the y coordinate of the n atom. The leading order in $1/d_{n,n+1}$ is

$$\frac{1}{d_{n,n+1}} \approx \frac{1}{\Delta x} \left(1 - \frac{1}{2} \left(\frac{y_n - y_{n+1}}{\Delta x} \right)^2 \right) \quad (2)$$

the force in the y direction

$$F_{n,n+1}^y = -c(d_{n,n+1} - L_0) \cdot \sin(\alpha_{n,n+1}) \quad (3)$$

$$= -c(d_{n,n+1} - L_0) \cdot \frac{y_n - y_{n+1}}{d_{n,n+1}} \quad (4)$$

$$= -c \left[y_n - y_{n+1} - L_0 \cdot \frac{y_n - y_{n+1}}{d_{n,n+1}} \right] \quad (5)$$

$$= -c \left[y_n - y_{n+1} - L_0 \cdot (y_n - y_{n+1}) \frac{1}{\Delta x} \left(1 - \frac{1}{2} \left(\frac{y_n - y_{n+1}}{\Delta x} \right)^2 \right) \right] \quad (6)$$

To the leading order

$$F_{n,n+1}^y \approx -c \cdot (y_n - y_{n+1}) \left(1 - \frac{L_0}{\Delta x} \right) \quad (7)$$

and

$$F_{n,n-1}^y = -c \cdot (y_n - y_{n-1}) \left(1 - \frac{L_0}{\Delta x} \right) \quad (8)$$

The next order (unharmonic)

$$F_{n,n+1}^y \approx -\frac{1}{2} c L_0 \cdot \frac{(y_n - y_{n+1})^3}{\Delta x^3} \quad (9)$$

$$F_{n,n-1}^y \approx -\frac{1}{2} c L_0 \cdot \frac{(y_n - y_{n-1})^3}{\Delta x^3} \quad (10)$$

The total first order (harmonic term) force on mass n is

$$F_{total}^y = F_{n,n+1}^y + F_{n,n-1}^y = -c \left(1 - \frac{L_0}{\Delta x} \right) (2y_n - y_{n-1} - y_{n+1}) \quad (11)$$

therefore, this chain is not stable under pressing, as the effective spring constant for transverse motion, $\beta = c \left(1 - \frac{L_0}{\Delta x} \right)$, is negative.

2 Chain with springs and bending term

$$F_y^{springs} = -c\left(1 - \frac{L_0}{\Delta x}\right)(2y_n - y_{n-1} - y_{n+1}) \quad (12)$$

the three body term is

$$E_{bending} \approx \frac{1}{2}\xi \sum_n (2y_n - y_{n-1} - y_{n+1})^2 \quad (13)$$

$$F_{bending} = -\frac{\partial E_{bending}}{\partial y_n} = \quad (14)$$

$$\approx -\xi \cdot [2(2y_n - y_{n-1} - y_{n+1}) - (2y_{n-1} - y_{n-2} - y_n) - (2y_{n+1} - y_n - y_{n+2})] \quad (15)$$

$$= -\xi \cdot [6y_n - 4y_{n-1} - 4y_{n+1} + y_{n-2} + y_{n+2}] \quad (16)$$

Here we neglect the difference between Δx and L_0 . The total force is

$$F_y^{total} = -c\left(1 - \frac{L_0}{\Delta x}\right)(2y_n - y_{n-1} - y_{n+1}) - \xi \cdot [6y_n - 4y_{n-1} - 4y_{n+1} + y_{n-2} + y_{n+2}] \quad (17)$$

$$= -y_n\left(2c\left(1 - \frac{L_0}{\Delta x}\right) + 6 \cdot \xi\right) + y_{n-1}\left(c\left(1 - \frac{L_0}{\Delta x}\right) + 4\xi\right) + y_{n+1}\left(c\left(1 - \frac{L_0}{\Delta x}\right) + 4\xi\right) - \xi y_{n-2} - \xi y_{n+2} \quad (18)$$

solution in the form

$$y_n = B \cdot e^{i(-\omega t + k \Delta x n)} \quad (19)$$

substitution

$$-\omega^2 m = -\left(2c\left(1 - \frac{L_0}{\Delta x}\right) + 6 \cdot \xi\right) + \left(c\left(1 - \frac{L_0}{\Delta x}\right) + 4\xi\right)e^{-ik\Delta x} + \left(c\left(1 - \frac{L_0}{\Delta x}\right) + 4\xi\right)e^{ik\Delta x} - \xi(e^{-2ik\Delta x} + e^{2ik\Delta x}) \quad (20)$$

and the dispersion relation is:

$$\omega^2 m = 2c\left(1 - \frac{L_0}{\Delta x}\right) + 6 \cdot \xi - 2 \left(c\left(1 - \frac{L_0}{\Delta x}\right) + 4\xi\right) \cos(\Delta x \cdot k) + 2\xi \cos(2\Delta x \cdot k) \quad (21)$$

$$\omega^2 m = 2\beta + 6 \cdot \xi - 2(\beta + 4\xi) \cos(\Delta x \cdot k) + 2\xi \cos(2\Delta x \cdot k) \quad (22)$$

at $k = 0$

$$\omega^2 m = 2\beta + 6 \cdot \xi - 2\beta - 8\xi + 2\xi = 0 \quad (23)$$

at $k = \pi/\Delta x$

$$\omega^2 m = 4\beta + 16 \cdot \xi \quad (24)$$

3 Long wave-length limit

at $ka \ll 1$

$$\omega^2 m = 2\beta + 6 \cdot \xi - 2(\beta + 4\xi) \left(1 - \frac{1}{2}(\Delta x \cdot k)^2\right) + 2\xi \left(1 - \frac{1}{2}(2\Delta x \cdot k)^2\right) \quad (25)$$

$$\omega^2 m = 2\beta + 6 \cdot \xi + (-2\beta - 8\xi) \left(1 - \frac{1}{2}(\Delta x \cdot k)^2\right) + 2\xi \left(1 - \frac{1}{2}(2\Delta x \cdot k)^2\right) \quad (26)$$

$$\omega^2 m = 2\beta + 6 \cdot \xi - 2\beta - 8\xi - (-2\beta - 8\xi) \frac{1}{2}(\Delta x \cdot k)^2 + 2\xi - 4\xi(\Delta x \cdot k)^2 \quad (27)$$

$$\omega^2 m = -(-2\beta - 8\xi) \frac{1}{2}(\Delta x \cdot k)^2 - 4\xi(\Delta x \cdot k)^2 \quad (28)$$

$$\omega^2 m = \beta(\Delta x \cdot k)^2 \quad (29)$$

$$\omega = \left(\sqrt{\frac{\beta}{m}} \Delta x\right) \cdot k \quad (30)$$

Here, the interesting results is that the long wave-length limit do not influence by the bending term (ω do not depend on ξ). At zero strain, the first order vanish, and the dispersion relation is parabolic, $\omega \sim k^2$. This is a non-Debye dependence where the sound velocity is zero. However, at pressing the chain is not stable and at tension the chain return to the Debye limit, $\omega \sim k$.

4 Higher order expansion of dispersion relation

$$\omega^2 m = \beta(\Delta x \cdot k)^2 - 2(\beta + 4\xi) \frac{1}{4!}(\Delta x \cdot k)^4 + 2\xi \frac{1}{4!}(2\Delta x \cdot k)^4 \quad (31)$$

$$\omega^2 m = \beta(\Delta x \cdot k)^2 - 2\beta \frac{1}{4!}(\Delta x \cdot k)^4 - 8\xi \frac{1}{4!}(\Delta x \cdot k)^4 + 2\xi \frac{1}{4!}(2\Delta x \cdot k)^4 \quad (32)$$

$$\omega^2 m = \beta(\Delta x \cdot k)^2 - \frac{1}{12}\beta(\Delta x \cdot k)^4 + \xi(\Delta x \cdot k)^4 \quad (33)$$

the condition for stability is $\omega^2 > 0$

$$\beta(\Delta x \cdot k)^2 - \frac{1}{12}\beta(\Delta x \cdot k)^4 + \xi(\Delta x \cdot k)^4 > 0 \quad (34)$$

$$\beta - \frac{1}{12}\beta(\Delta x \cdot k)^2 + \xi(\Delta x \cdot k)^2 > 0 \quad (35)$$

$$\beta(1 - \frac{1}{12}(\Delta x \cdot k)^2) + \xi(\Delta x \cdot k)^2 > 0 \quad (36)$$

$$\frac{L_0}{\Delta x} - 1 < \frac{\xi}{c} \frac{(\Delta x \cdot k)^2}{(1 - \frac{1}{12}(\Delta x \cdot k)^2)} \quad (37)$$

This stability condition can be reformulated using the definition

$$\alpha \equiv \frac{\xi}{c} \frac{(\Delta x \cdot k)^2}{(1 - \frac{1}{12}(\Delta x \cdot k)^2)} \quad (38)$$

to be

$$\epsilon > -\frac{\alpha}{\alpha + 1} \quad (39)$$

where ϵ is the strain defined as

$$\epsilon \equiv \frac{\Delta x - L_0}{L_0} \quad (40)$$

Part II

Chain with two force constants and bending term

There are two equations of motion:

$$F_y^{spring} = F_{y_n^1} = -c_1(1 - \frac{L_0^1}{\Delta x^1})(y_n^1 - y_{n-1}^2) - c_2(1 - \frac{L_0^2}{\Delta x^2})(y_n^1 - y_n^2) \quad (41)$$

$$F_{y_n^2} = -c_2(1 - \frac{L_0^2}{\Delta x^2})(y_n^2 - y_n^1) - c_1(1 - \frac{L_0^1}{\Delta x^1})(y_n^2 - y_{n+1}^1) \quad (42)$$

the force of the three body term is

$$F_{bending} = F_{y_n^1} \approx -\xi \cdot [6y_n^1 - 4y_{n-1}^2 - 4y_n^2 + y_{n-1}^1 + y_{n+1}^1] \quad (43)$$

$$F_{bending} = F_{y_n^2} \approx -\xi \cdot [6y_n^2 - 4y_{n+1}^1 - 4y_n^1 + y_{n-1}^2 + y_{n+1}^2] \quad (44)$$

total force

$$F_{y_n^1} = -c_1(1 - \frac{L_0^1}{\Delta x^1})(y_n^1 - y_{n-1}^2) - c_2(1 - \frac{L_0^2}{\Delta x^2})(y_n^1 - y_n^2) - \xi \cdot [6y_n^1 - 4y_{n-1}^2 - 4y_n^2 + y_{n-1}^1 + y_{n+1}^1] \quad (45)$$

$$F_{y_n^2} = -c_2(1 - \frac{L_0^2}{\Delta x^2})(y_n^2 - y_n^1) - c_1(1 - \frac{L_0^1}{\Delta x^1})(y_n^2 - y_{n+1}^1) - \xi \cdot [6y_n^2 - 4y_{n+1}^1 - 4y_n^1 + y_{n-1}^2 + y_{n+1}^2] \quad (46)$$

Lets define the lattice parameter $\Delta x = \frac{1}{2}(\Delta x^1 + \Delta x^2)$ now we try solutions

$$y_n^1 = A_1 e^{i(-\omega t + 2k\Delta x n)} \quad (47)$$

$$y_n^2 = A_2 e^{i(-\omega t + 2k\Delta x n)} \quad (48)$$

substitution

$$m\omega^2 A_1 = c_1 \left(1 - \frac{L_0^1}{\Delta x^1}\right) (A_1 - A_2 e^{-2ik\Delta x}) + c_2 \left(1 - \frac{L_0^2}{\Delta x^2}\right) (A_1 - A_2) \quad (49)$$

$$+ \xi \cdot [6A_1 - 4A_2 e^{-2ik\Delta x} - 4A_2 + A_1 e^{-2ik\Delta x} + A_1 e^{2ik\Delta x}] \quad (50)$$

$$m\omega^2 A_2 = c_2 \left(1 - \frac{L_0^2}{\Delta x^2}\right) (A_2 - A_1) + c_1 \left(1 - \frac{L_0^1}{\Delta x^1}\right) (A_2 - A_1 e^{2ik\Delta x}) \quad (51)$$

$$+ \xi \cdot [6A_2 - 4A_1 e^{2ik\Delta x} - 4A_1 + A_2 e^{-2ik\Delta x} + A_2 e^{2ik\Delta x}] \quad (52)$$

lets define two effective spring constants for transverse motion $\beta_1 = c_1 \left(1 - \frac{L_0^1}{\Delta x^1}\right)$ and $\beta_2 = c_2 \left(1 - \frac{L_0^2}{\Delta x^2}\right)$ and, in matrix form

$$m\omega^2 \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = \begin{pmatrix} \beta_1 + \beta_2 + 6\xi + 2\xi \cos(2k\Delta x) & -\beta_1 e^{-2ik\Delta x} - \beta_2 - 4\xi e^{-2ik\Delta x} - 4\xi \\ -\beta_2 - \beta_1 e^{2ik\Delta x} - 4\xi e^{2ik\Delta x} - 4\xi & \beta_1 + \beta_2 + 6\xi + 2\xi \cos(2k\Delta x) \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} \quad (53)$$

thus

$$\det \begin{pmatrix} \beta_1 + c_2 \left(1 - \frac{L_0^2}{\Delta x^2}\right) + 6\xi + 2\xi \cos(2k\Delta x) - m\omega^2 & -\beta_1 e^{-2ik\Delta x} - \beta_2 - 4\xi e^{-2ik\Delta x} - 4\xi \\ -\beta_2 - \beta_1 e^{2ik\Delta x} - 4\xi e^{2ik\Delta x} - 4\xi & \beta_1 + \beta_2 + 6\xi + 2\xi \cos(2k\Delta x) - m\omega^2 \end{pmatrix} = 0 \quad (54)$$

this equation is in the form

$$\det \begin{pmatrix} a & b + ic \\ b - ic & a \end{pmatrix} = 0 \quad (55)$$

where

$$a \equiv \beta_1 + \beta_2 + 6\xi + 2\xi \cos(2k\Delta x) - m\omega^2 \quad (56)$$

$$b \equiv -\beta_2 - \beta_1 \cos(2k\Delta x) - 4\xi \cos(2k\Delta x) - 4\xi \quad (57)$$

$$c \equiv -\beta_1 \sin(2k\Delta x) - 4\xi \sin(2k\Delta x) \quad (58)$$

the dispersion relation is

$$a^2 - (b^2 + c^2) = 0 \quad (59)$$

substitution gives

$$(\beta_1 + \beta_2 + 6\xi + 2\xi \cos(2k\Delta x) - m\omega^2)^2 \quad (60)$$

$$- \left((\beta_2 + \beta_1 \cos(2k\Delta x) + 4\xi \cos(2k\Delta x) + 4\xi)^2 + (\beta_1 \sin(2k\Delta x) + 4\xi \sin(2k\Delta x))^2 \right) = 0 \quad (61)$$

$$m\omega^2 = \beta_1 + \beta_2 + 6\xi + 2\xi \cos(2k\Delta x) \quad (62)$$

$$\pm \sqrt{(\beta_2 + \beta_1 \cos(2k\Delta x) + 4\xi \cos(2k\Delta x) + 4\xi)^2 + (\beta_1 \sin(2k\Delta x) + 4\xi \sin(2k\Delta x))^2} \quad (63)$$

5 Stability condition using high order expansion for the long wavelength limit

The high-order long wave-length limit is

$$m\omega^2 = \beta_1 + \beta_2 + 6\xi + 2\xi \left(1 - \frac{1}{2}(2k\Delta x)^2 + \frac{1}{4!}(2k\Delta x)^4\right) \quad (64)$$

$$- (\beta_2 + \beta_1 + 8\xi) \left[1 + \frac{1}{2} \left\{ \left(-\beta_1 \frac{1}{2}(2k\Delta x)^2 - 4\xi \frac{1}{2}(2k\Delta x)^2\right)^2 + \beta_1 \frac{1}{2}(2k\Delta x)^2 4\xi \frac{1}{2}(2k\Delta x)^2 \right\} \right] \quad (65)$$

$$+ 2(\beta_2 + \beta_1 + 8\xi)^2 \cdot \left(-\beta_1 \frac{1}{2}(2k\Delta x)^2 + \beta_1 \frac{1}{4!}(2k\Delta x)^4 - 4\xi \frac{1}{2}(2k\Delta x)^2 + 4\xi \frac{1}{4!}(2k\Delta x)^4 \right) \quad (66)$$

$$+ (\beta_1 2k\Delta x)^2 + (4\xi 2k\Delta x)^2 + (4\xi 2k\Delta x + \beta_1 2k\Delta x)^2 \quad (67)$$

$$+ 2(4\xi 2k\Delta x + \beta_1 2k\Delta x) \left(-\beta_1 \frac{1}{3!}(2k\Delta x)^3 + 4\xi \frac{1}{3!}(2k\Delta x)^3 \right) / (\beta_2 + \beta_1 + 8\xi)^2 \quad (68)$$

which have the form

$$m\omega^2 = \eta_1 (k\Delta x)^2 + \eta_2 (k\Delta x)^4 \quad (69)$$

similar to the one-spring case.

Part III

Continuum model - wave equation

6 Derivation of the wave equation in two dimensions

In the continuum limit, one can think on the chain as a string with the bending term. In this approach, two forces acting on an infinitesimal unit of the chain: 1. the springs term and 2. the forces caused by the bending (change in bond angles). The forces caused by the springs is the same as the forces acting in string (like a guitar string) and it is

$$F_{springs} = -T_0 \Delta x \frac{d^2 y}{dx^2} \quad (70)$$

where T_0 is the tension in the chain, equal to the springs force

$$T_0 = c \Delta L \quad (71)$$

where ΔL is the change in the spring distance from its relaxed position, L_0 . The force from the bending term (see above)

$$F_{bending} = -\frac{\partial E_{bending}}{\partial y_n} = \quad (72)$$

$$\approx -\xi \cdot [2(2y_n - y_{n-1} - y_{n+1}) - (2y_{n-1} - y_{n-2} - y_n) - (2y_{n+1} - y_n - y_{n+2})] \quad (73)$$

$$= -\Delta x^2 \cdot \xi \cdot \left[2 \frac{(2y_n - y_{n-1} - y_{n+1})}{\Delta x^2} - \frac{(2y_{n-1} - y_{n-2} - y_n)}{\Delta x^2} - \frac{(2y_{n+1} - y_n - y_{n+2})}{\Delta x^2} \right] \quad (74)$$

$$= \Delta x^2 \cdot \xi \cdot \left[2 \frac{d^2 y}{dx^2}(x) - \frac{d^2 y}{dx^2}(x - \Delta x) - \frac{d^2 y}{dx^2}(x + \Delta x) \right] \quad (75)$$

$$= -\Delta x^4 \cdot \xi \cdot \frac{d^4 y}{dx^4} \quad (76)$$

The total forces is

$$F_{total} = -T_0 \Delta x \frac{d^2 y}{dx^2} - \Delta x^4 \cdot \xi \cdot \frac{d^4 y}{dx^4} \quad (77)$$

The force is zero at a stationary state, thus the wave equation is

$$-T_0 \Delta x \frac{d^2 y}{dx^2} = \Delta x^4 \cdot \xi \cdot \frac{d^4 y}{dx^4} \quad (78)$$

lets define $\psi(x) = \Delta x \cdot d^2 y/dx^2$, which is the bond angles in the chain in the continuum limit ($\psi = 0$ is a straight line with no curvature, thus, no bending). Using this definition, the wave equation becomes

$$-T_0 \psi(x) = \Delta x^3 \cdot \xi \cdot \frac{d^2 \psi}{dx^2} \quad (79)$$

and

$$-\Delta x^3 \frac{\xi}{c} \cdot \frac{d^2 \psi}{dx^2} = \Delta L \psi(x) \quad (80)$$

Here, c/ξ and Δx are constants. This is a wave equation in the form of the Schrodinger equation for free particles. The eigenvalues and eigenfunctions are determine the geometry of the chain. The eigenvalues, ΔL , is the spring geometry parameter and the eigenfunctions, ψ , is the bond angles, the bending geometry parameter. The assumption is that the spring distance is the same for all springs, however the angles are not the same.

7 Derivation of the wave equation in three-dimensions

The bond angle angle is given by

$$\cos(\alpha) = \frac{\vec{v}_1 \cdot \vec{v}_2}{|\vec{v}_1| \cdot |\vec{v}_2|} \quad (81)$$

where

$$\vec{v}_1 = (x_n - x_{n-1}, y_n - y_{n-1}, z_n - z_{n-1}) \quad (82)$$

$$\vec{v}_2 = (x_{n+1} - x_n, y_{n+1} - y_n, z_{n+1} - z_n) \quad (83)$$

where r_n is the r coordinate of the n 'th atom. Under the assumption of small angles

$$\alpha_n^2 = \frac{(2y_n - y_{n-1} - y_{n+1})^2}{\Delta x^2} + \frac{(2z_n - z_{n-1} - z_{n+1})^2}{\Delta x^2} \quad (84)$$

Thus, the bending energy is

$$E_{bending} = \frac{1}{2} \cdot L_0^2 \cdot \xi \cdot \sum_n \alpha_n^2 = \frac{1}{2} \cdot L_0^2 \cdot \xi \sum_n ((2y_n - y_{n-1} - y_{n+1})^2 + (2z_n - z_{n-1} - z_{n+1})^2) \quad (85)$$

and thus the force in z will have the same form as in y , and y and z are not conjugate.

The springs force are also the same, because ΔL is the same and thus the equations in three-dimensional are

$$-\Delta x^3 \cdot \frac{\xi}{c} \cdot \frac{d^2 \psi_y}{dx^2} = \Delta L \psi_y \quad (86)$$

$$-\Delta x^3 \cdot \frac{\xi}{c} \cdot \frac{d^2 \psi_z}{dx^2} = \Delta L \psi_z \quad (87)$$

where $\psi_y = \Delta x \partial^2 y / \partial x^2$ and $\psi_z = \Delta x \partial^2 z / \partial x^2$. These equations do not have the same mathematical form as the the Schrodinger equation for free particles.

These equations are valid just if ψ_y and ψ_z have the same period and thus, ΔL will be the same. In the cases where ψ_y and ψ_z do not have the same period, the wave equations are not valid and Δx is not constant

8 Solution of the wave equation

The solutions are

$$\psi(x) = A' \cdot \sin(kx) \quad (88)$$

substitution to the wave equation gives

$$\Delta x^3 \cdot \xi \cdot k^2 = c \Delta L \quad (89)$$

periodic boundary conditions gives

$$k = \frac{2\pi n}{L} \quad (90)$$

where n is an integer and

$$a_x^3 \cdot \xi \cdot \left(\frac{2\pi n}{L}\right)^2 = c \Delta L \quad (91)$$

$$\Delta L = \frac{\xi}{c} \Delta x^3 \cdot \left(\frac{2\pi n}{L}\right)^2 \quad (92)$$

9 The energy of the chain - two dimensions

Under the assumption that all the springs have the same length (same ΔL), the total springs energy (for unit-cell with N atoms) is

$$E_{springs} = \frac{8\Delta x^2 c \left(\frac{\xi}{c}\right)^2 \pi^4}{N^3} n^4 = E_1^{springs} n^4 \quad (93)$$

The bending energy can be calculated using

$$E_{bending} = \frac{1}{2} \Delta x^3 \xi \sum_n \left(\frac{2y_n - y_{n-1} - y_{n+1}}{\Delta x^2}\right)^2 \Delta x = \frac{1}{2} \Delta x^3 \xi \int_0^L \left(\frac{d^2 y}{dx^2}\right)^2 dx \quad (94)$$

to be

$$E_{bending} = \frac{4\pi^4 \xi A^2}{N^3} n^4 \quad (95)$$

where the amplitude A can be found using that the total length of the chain is $l = N \cdot (L_0 - \Delta L)$. This leads to the following equation

$$N \cdot \left(L_0 - \frac{\xi}{c} \Delta x^3 \cdot (2 \cdot \pi n / (\Delta x \cdot N))^2 \right) - \int_0^{2\pi} \sqrt{\left(\frac{\Delta x \cdot N}{2\pi} \right)^2 + (n \cdot A \cdot \cos(t))^2} dt = 0 \quad (96)$$

This integral is not easy to solve. If we assume $L_0 \gg \xi/c \cdot \Delta x^3 \cdot (2 \cdot \pi n / (\Delta x \cdot N))^2$, which is reasonable in long chains, then

$$A = b/n \quad (97)$$

and thus

$$E_{bending} = E_1^{bending} \cdot n^2 \quad (98)$$

The total energy is the sum of both contributions

$$E_{total} = E_1^{bending} \cdot n^2 + E_1^{springs} \cdot n^4 \quad (99)$$

10 The energy of the chain - three dimensions

From the same considerations, the energy of the chain in three dimensions

$$E_{bending} = E_1^{springs} n^4 \quad (100)$$

$$E_{bending} = E_1^{bending} \cdot n^2 \quad (101)$$

$$E_{total} = E_1^{bending} \cdot n^2 + E_1^{springs} \cdot n^4 \quad (102)$$