Physics 106a 5 December, 2013

Lecture 19: Modes in a crystal and continuum

The vibrational modes of the periodic array of a very large number of atoms in crystals provide another good example of the use of normal modes. For mode wavelengths large compared with the atomic spacing a continuum limit may be taken. Alternatively the continuum theory can be derived directly by setting up a continuum Lagrangian, and using a generalization of the usual Euler-Lagrange equations, leading to continuum equations of motion. Since space-time is uniform in many problems, conservation laws play an important role in continuum equations.

Linear chain of balls and springs

Consider a linear chain of identical masses m and springs with spacing a. For displacements u_j of the jth mass the kinetic and potential energies are

$$T = \tfrac{1}{2}\sum_j m\dot{u}_j^2, \quad V = \tfrac{1}{2}\sum_j K(u_{j+1}-u_j)^2, \tag{1}$$

so that the Lagrangian is

$$L = \tfrac{1}{2}\sum_j m\dot{u}_j^2 - \tfrac{1}{2}\sum_j K(u_{j+1}-u_j)^2. \tag{2}$$

We could be considering longitudinal displacements and then K is the spring constant, or transverse displacements when $K = T/a$ with T the tension in the springs. Equation (2) models a simple one dimensional crystal, with the spring constant modeling the quadratic behavior of the interatomic potential near the equilibrium positions. The Euler-Lagrange equations of motion are[1]

$$m\ddot{u}_j = K(u_{j-1} - 2u_j + u_{j-1}). \tag{3}$$

To solve for the normal modes we introduce the kinetic energy matrix $\boldsymbol{T}$ which is diagonal with elements m, and the potential energy matrix $\boldsymbol{V}$ which is *tridiagonal* with elements $2K$ on the diagonal, $-K$ adjacent to the diagonal, and 0 elsewhere. We could alternatively solve the equations of motion directly. Setting $u_j(t) = \Upsilon_j e^{i\omega t}$ for the normal modes the eigenvalue problem is

$$\boldsymbol{V}\cdot\boldsymbol{\Upsilon} - \omega^2\boldsymbol{T}\cdot\boldsymbol{\Upsilon} = 0\,. \tag{4}$$

This is easiest to solve in component form: the jth row is

$$K(2\Upsilon_j - \Upsilon_{j-1} - \Upsilon_{j+1}) - m\omega^2\Upsilon_j = 0\,. \tag{5}$$

We can solve this by noticing that $\Upsilon_j \propto e^{i\gamma j}$ is a solution (or sin or cos, linear combinations, etc.) if γ satisfies

$$\omega^2 = \frac{4K}{m}\sin^2\left(\frac{\gamma}{2}\right). \tag{6}$$

[1] Hand and Finch §9.7 studies transverse oscillations of masses on a string and find the same Lagrangian, with the effective spring constant given by the tension divided by the separation.

If you are unhappy about solving by guesswork, you can be comforted that there are deeper reasons for this choice: the equation has discrete translational symmetry, and the functions $e^{i\gamma j}$ are representations of this symmetry group.

For a finite chain we can enforce boundary conditions by including fixed masses at $j = 0$, $j = N + 1$ giving N dynamic masses. The boundary conditions are then $u_0 = u_{N+1} = 0$. The first of these is satisfied if we use the sin version of the solution $\Upsilon_j \propto \sin \gamma j$, and then the second is satisfied only if γ takes on one of the values γ_n with

$$\gamma_n = \frac{n\pi}{N+1}, \tag{7}$$

with n an integer. This then gives the eigenmodes and their frequencies

$$\Upsilon_j^{(n)} = \sqrt{\frac{1}{m}}\sqrt{\frac{2}{N+1}} \sin\left(\frac{n\pi j}{N+1}\right), \qquad \omega_n = 2\sqrt{\frac{K}{m}} \sin\left(\frac{n\pi}{2(N+1)}\right). \tag{8}$$

The range of n giving different solutions is $n = 1$ to N, so that there are as many normal modes as degrees of freedom[2]. The constant prefactor in the $\Upsilon_j^{(n)}$ is chosen so that the vectors are orthonormal with respect to the matrix $\boldsymbol{T}$, which is proportional to the unit matrix in this case[3]

$$\tilde{\boldsymbol{\Upsilon}}^{(n)} \cdot \boldsymbol{T} \cdot \boldsymbol{\Upsilon}^{(n')} = m\tilde{\boldsymbol{\Upsilon}}^{(n)} \cdot \boldsymbol{\Upsilon}^{(n')} = \delta_{nn'} \tag{9}$$

as you can check by evaluating the component sums[4]. The spectrum and modes are plotted in the accompanying Mathematica notebook.

In treating very large systems where we think the details of the boundaries are not important, for example in calculating the specific heat of a solid by adding up all the energy in the modes of vibration, we often replace realistic boundary conditions by *periodic boundary conditions*, where we imagine a chain wrapping around so that particle $N+1$ is identified with particle 1, and particle 0 with particle N. This has the advantage that the modes can be taken to be the exponentials $\Upsilon_j^{(n)} \propto e^{i\gamma_n j}$ with now $\gamma_n = 2n\pi/N$ with $-N/2 < n \leq N/2$. The range of n or wave vectors n/a is known as the *first Brillouin zone*.

Continuum limit

For mode wave lengths large compared with the spacing a the discrete nature of the system should be unimportant and we can make a continuum approximation. I will use the language for a longitudinal mode, although similar results apply for the transverse modes.

The continuum limit is given by letting $a \to 0, N \to \infty$ with $(N+1)a = L =$ constant, $u_j \to u(x = ja)$, and defining constants to keep the energy, Lagrangian, etc., finite. Write the Lagrangian in the form

$$L = \frac{1}{2}\sum_j a\left[\frac{m}{a}\dot{u}_j^2 - Ka\left(\frac{u_{j+1}-u_j}{a}\right)^2\right]. \tag{10}$$

[2]To see this note that increasing n by a multiple of $2(N+1)$ gives the same values of Υ_j. Also $n = 0$ or $n = N+1$ gives $\Upsilon_j = 0$, which is not a mode. Finally, the values of n given by $(N+1) \pm m$ do not give independent modes (one gives displacements that are just the negative of the displacements for the other) and so the range from $N+2$ to $2N+1$ does not give independent solutions.

[3]Note that a more conventional normalization choice might be to leave out the factor involving m so that the $\Upsilon^{(n)}$ orthogonality would be $\tilde{\boldsymbol{\Upsilon}}^{(n)} \cdot \boldsymbol{\Upsilon}^{(n')} = \delta_{nn'}$.

[4]Writing the sin functions in exponential form gives a number of geometric series to sum.

As $a \to 0$ we take $m/a \to \rho$ the mass per unit length, and $Ka \to E$ Young's modulus, and the Lagrangian becomes

$$L = \frac{1}{2}\int \left[\rho \dot{u}^2 - E u'^2\right] dx \tag{11}$$

with $u' = \partial u/\partial x$.

The normal mode Eq. (8) becomes

$$\Upsilon^{(n)}(x) \propto \sin\left(\frac{n\pi x}{L}\right) = \sin(k_n x) \tag{12}$$

with k_n the wave number $n\pi/L$, and the frequency given by (expand the sin in the small argument in the limit $N \to \infty$)

$$\omega_n = c k_n \quad \text{with} \quad c = \sqrt{E/\rho}. \tag{13}$$

This is a linear spectrum $\omega(k)$ characteristic of waves in a continuous medium, with the coefficient $c = \sqrt{E/\rho}$ giving the speed of propagation of the waves. The linear approximation for the spectrum is good for $k \ll 1/a$. A physical example is sound waves in a solid, where the wavelength at frequencies we hear is of order a meter compared with the atomic spacing 0.1nm.

The continuum limit can also be performed directly on the equations of motion. Equation (3) becomes

$$\frac{m}{a}\ddot{u}_j = (Ka)\frac{(u_{j-1} - 2u_j + u_{j-1})}{a^2} \quad \to \quad \rho\ddot{u} = E u''. \tag{14}$$

This is the one dimensional wave equation, with wave speed $c = \sqrt{E/\rho}$ as before.

Classical field theory

Stretched string

The stretched string is a nice example illustrating the general application of the calculus of variations, here to a case with more than one independent variable (t and x, the coordinate along the string). It is Hand and Finch Problem 2-13.

The problem is to find the equation of motion of small transverse displacements $y(x,t)$ of a string stretched between points $x = 0$ and $x = d$ (e.g. a guitar string). This is a continuum *field theory* rather than a problem of discrete particles, so we can't just plug into the formulas that we have developed. Instead, we need to redo the mathematical manipulations based on the same physics ideas as we go along. (Note: for obvious reasons I am calling the length of the string d rather than L as Hand and Finch use.)

First derive expressions for the kinetic and potential energy. I will use the notation $\dot{y} = \partial y/\partial t$ and $y' = \partial y/\partial x$.

Potential energy: For a small displacement $y(x,t)$ an element δx of string is stretched to a length $\delta x\sqrt{1+y'^2}$. Expanding to lowest order in y' gives the amount of stretch $\frac{1}{2}y'^2\delta x$. If the string is under tension T the amount of work done is $\frac{1}{2}Ty'^2\delta x$, and the potential energy is the integral of this over the length.

Kinetic energy: For a mass per unit length ρ the kinetic energy of the element δx is $\frac{1}{2}\rho\dot{y}^2\delta x$.

The Lagrangian is $L = \int_0^d \mathcal{L}\,dx$ with the Lagrangian density $\mathcal{L}(y, y', \dot{y})$ given by

$$\mathcal{L} = \tfrac{1}{2}\rho\dot{y}^2 - \tfrac{1}{2}Ty'^2 \,. \tag{15}$$

In general $\mathcal{L}$ might also depend on x, t, but does not do so in the present case. Can you see when $\mathcal{L}$ might depend on these variables?

The action for starting time 0 and ending time t_f is

$$S = \int_0^{t_f} dt \int_0^d dx\, \mathcal{L}(y, y', \dot{y}). \tag{16}$$

The variation of S under a small change $\delta y(x,t)$ with $y(0,t) = y(d,t) = 0$ (ends fixed) and $y(x,0)$, $y(x,t_f)$ fixed (variational principle) is

$$\delta S = \int_0^{t_f} dt \int_0^d dx \left[\frac{\partial\mathcal{L}}{\partial y}\delta y + \frac{\partial\mathcal{L}}{\partial\dot{y}}\delta\dot{y} + \frac{\partial\mathcal{L}}{\partial y'}\delta y'\right] . \tag{17}$$

Now integrate by parts the $\delta\dot{y}$ with respect to t and the $\delta y'$ term with respect to x using $\delta\dot{y} = \partial\delta y/\partial t$ etc., and $\delta y = 0$ at $t = 0, t = t_f, x = 0, x = d$ which eliminates the endpoint terms, to find

$$\delta S = \int_0^{t_f} dt \int_0^d dx \left[\frac{\partial\mathcal{L}}{\partial y} - \frac{\partial}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{y}} - \frac{\partial}{\partial x}\frac{\partial\mathcal{L}}{\partial y'}\right]\delta y(x,t) \,. \tag{18}$$

Since $\delta y(x,t)$ is arbitrary, the stationary principle $\delta S = 0$ gives

$$\frac{\partial\mathcal{L}}{\partial y} - \frac{\partial}{\partial t}\frac{\partial\mathcal{L}}{\partial\dot{y}} - \frac{\partial}{\partial x}\frac{\partial\mathcal{L}}{\partial y'} = 0 \,. \tag{19}$$

Substituting in the string Lagrangian density Eq. (15) gives the equation of motion

$$\rho \frac{\partial^2 y}{\partial t^2} - T \frac{\partial^2 y}{\partial x^2} = 0 \,. \tag{20}$$

This is the wave equation. By direct substitution you can show that the equation is satisfied by any solution of the form $y = f(x \mp ct)$ as long as $c = \sqrt{T/\rho}$ — this is an arbitrarily shaped pulse traveling in the plus or minus x-direction with speed c. To match the end conditions however we need a standing wave solution, such as $y = A \sin kx \sin ckt$ with $k = n\pi/d$ and n an integer —check that this satisfies Eq. (20) too.

General formalism

Generalizing the discussion of the one dimensional continuum to the dynamics of a scalar degree of freedom in three dimensions, we seek to make stationary the action

$$S = \int \mathcal{L}\, dxdydzdt, \tag{21}$$

where $\mathcal{L}$ is the Lagrangian density. For a simple scalar wave system we would have

$$\mathcal{L} = \tfrac{1}{2}[\rho \dot{u}^2 - K(\vec{\nabla} u)^2], \tag{22}$$

leading to the Euler-Lagrange equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u, \tag{23}$$

the three dimensional wave equation with $c = \sqrt{K/\rho}$ the wave speed.

Displacement (sound) waves in a solid are more complicated, since they have a direction or polarization. In a solid we define the *strain tensor*

$$e_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \tag{24}$$

and then the potential energy of distortions is

$$V = \tfrac{1}{2}\boldsymbol{e} \cdot \boldsymbol{\lambda} \cdot \boldsymbol{e}, \tag{25}$$

with $\boldsymbol{\lambda}$ the fourth rank *elasticity tensor* with components λ_{ijkl}. (The combination of derivatives as in Eq. (24) but with a minus sign corresponds to a rotation, and does not contribute to the potential energy.) A 4th rank tensor has $3^4 = 81$ components, but not all are independent. As you can imagine, it is important to use the symmetries of the solid to find out how many independent constants we need to specify. First of all, the stress tensor is symmetric under the separate exchanges $i \leftrightarrow j$, $k \leftrightarrow l$, and $ij \leftrightarrow kl$ (the antisymmetric combinations would drop out in forming the potential energy sum). There are three isotropic 4th rank tensors: $\delta_{ij}\delta_{kl}$, $\delta_{ik}\delta_{jl}$, and $\delta_{il}\delta_{jk}$. Restricting to combinations with the right index symmetry yields the elastic tensor for an isotropic material such as a glass

$$\lambda_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \quad \Rightarrow \quad V = \tfrac{1}{2}\lambda e_{ii}^2 + \mu e_{ij}^2, \tag{26}$$

so that there are two independent elastic coefficients λ, μ called the *Lamé coefficients*. (In Eq. (26) I am using the repeated index convention so $e_{ij}^2 \equiv e_{ij}e_{ij} = \sum_{ij} e_{ij}e_{ij}$, etc.) It is often convenient to write the deformation as the sum of a volume deformation and a pure shear that does not change the volume

$$e_{ij} = \tfrac{1}{3}\delta_{ij}e_{kk} + (e_{ij} - \tfrac{1}{3}\delta_{ij}e_{kk}). \tag{27}$$

In terms of these combinations the potential energy becomes

$$V = \tfrac{1}{2}Ke_{ii}^2 + \mu(e_{ij} - \tfrac{1}{3}\delta_{ij}e_{kk})^2, \tag{28}$$

with $K = \lambda + \frac{2}{3}\mu$ the bulk modulus, and μ is now called the shear modulus. Sometimes, the Young's modulus E and the Poisson ratio σ given by

$$E = \frac{9K\mu}{3K + \mu}, \quad \sigma = \frac{3K - 2\mu}{2(3K + \mu)}, \tag{29}$$

are used as the two independent coefficients. (Young's modulus gives the ratio of the tension/area to the extension of a rod under tension, and the Poisson ratio gives the ratio of the transverse compression to the longitudinal extension of the rod.) The kinetic energy term in the Lagrangian is the same as in Eq. (22), and working through the Euler-Lagrange equations finally (exercise for the student!) leads to the result of two types of propagating waves: transverse waves with $\vec{\nabla}\cdot\vec{u}=0$ propagating with the speed $\sqrt{\mu/\rho}$, and longitudinal waves with $\vec{\nabla}\times\vec{u}=0$ propagating with speed $\sqrt{(\lambda+2\mu)/\rho}$. (A good references on elasticity theory is volume 7 of the Landau and Lifshitz series, e.g. chapter I for the basic physics and chapter III for the waves.)

All this complication was for an isotropic material! For a material with cubic symmetry it turns out there are three independent elastic constants (three fold rotations about the cube diagonal tell us $\lambda_{xyxy}=\lambda_{xzxz}$, for example), and for crystals of lower symmetry even more – up to 21 in a crystal with triclinic symmetry or a material with no symmetry. Group theory is useful in understanding these systems.

Conservation laws

As we saw in the one dimensional example, the space and time variable play a rather symmetric role in deriving the Euler-Lagrange equations, since t, x, y, z, are independent variables in the path variation. For formal manipulations it is useful to introduce the 4-component notation x^ν where x^ν for $\nu=0,1,2,3$ means t, x, y, and z. I will proceed using the simple scalar example Eq. (22), but with a notation that is sufficiently general to be extended to more complicated cases such as Eq. (25). The Euler-Lagrange equation can be written

$$\frac{d}{dx^\nu}\left(\frac{\partial\mathcal{L}}{\partial u_{,\nu}}\right)-\frac{\partial\mathcal{L}}{\partial u}=0 \tag{30}$$

(repeated indices to be summed over as usual). The notion $u_{,\nu}$ stands for $\partial u/\partial x^\nu$, so $u_{,0}\equiv\dot{u}$ for example.[5] The comma here allows for including fields with a number of components u_α, such as the vector displacement $\vec{u}$ for sound waves in a liquid or solid: in this case $u_1\equiv u_x$, and then $u_{\alpha,\nu}$ gives the derivatives, e.g. $u_{1,2}\equiv\partial u_x/\partial y$. For the Lagrangian (22) the Euler-Lagrange equation is the 3-d wave equation Eq. (23).

For a time independent particle Lagrangian we found a conserved quantity – the Hamiltonian. For the continuum Lagrangian density we can ask what happens if $\mathcal{L}$ is independent of both time and space $\partial\mathcal{L}/\partial x^\nu=0$. Following the lines of the calculation in Lecture 3 we calculate the total derivative of $\mathcal{L}$ with respect to x^μ

$$\frac{d\mathcal{L}}{dx^\mu}=\frac{\partial\mathcal{L}}{\partial u}u_{,\mu}+\frac{\partial\mathcal{L}}{\partial u_{,\nu}}u_{,\mu\nu}+\frac{\partial\mathcal{L}}{\partial x^\mu}. \tag{31}$$

Using the Euler-Lagrange equation (30) this can be changed to

$$\frac{d\mathcal{L}}{dx^\mu}=\frac{d}{dx^\nu}\left(\frac{\partial\mathcal{L}}{\partial u_{,\nu}}u_{,\mu}\right)+\frac{\partial\mathcal{L}}{\partial x^\mu}. \tag{32}$$

For $\partial\mathcal{L}/\partial x^\nu=0$ this gives

$$\frac{d}{dx^\nu}\left[\frac{\partial\mathcal{L}}{\partial u_{,\nu}}u_{,\mu}-\mathcal{L}\delta_{\mu\nu}\right]=0. \tag{33}$$

[5]The "up-down" placement of the indices is unimportant here, but will be important when we look at relativity next term. I am following the notation of Goldstein et al., §13.3, and you can fill in more details from there if you are interested.

These are a set of *conservation laws*

$$\frac{dT_\mu{}^0}{dt} + \vec{\nabla} \cdot \vec{T}_\mu = 0 \tag{34}$$

where T^0_μ and $\vec{T}_\mu$ can be read off from the [ ]. For example, for the Lagrangian (22) the $\mu = 0$ components are

$$T_0{}^0 = \tfrac{1}{2}\rho[\dot{u}^2 + c^2(\vec{\nabla}u)^2] \qquad \text{energy density,} \tag{35}$$

$$\vec{T}_0 = -\rho c^2 \vec{\nabla} u\, \dot{u} \qquad \text{energy current.} \tag{36}$$

The second equation makes sense thinking about the ball and spring model since $\rho c^2 \vec{\nabla} u$ corresponds to the force from compressing the springs, and $\dot{u}$ is the velocity of the masses, so the product is the rate of work done. The $\mu = 1, 2, 3$ components give the change in the momentum density in terms of a momentum current or stress tensor. Integrating Eq. (34) over some volume and using Gauss's theorem shows that the change of $T_\mu{}^0$ integrated over the volume is the integral of the current $\vec{T}_\mu$ into the volume.

Michael Cross, December 5, 2013