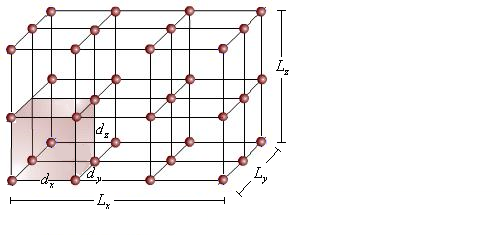
**3D Elastic Solid**

Let’s do this again, in 3D. Consider a solid, like pictured below, though not necessarily a simple cubic crystal.



In the harmonic approximation, we can write the Lagrangian as:



where **x** is the position vector, with components xα = (x, y, z). Let’s do some work on the potential energy part. So going to write it a little differentily, taking advantage of the fact that ΣiKαβ(Ri-Rj) = ΣjKαβ(Ri-Rj) = 0, and that Kαβ is symmetric w/r to its indices.



Now let’s go to the continuum limit. In this limit, we’ll let the oscillator spacing go to zero, or equivalently, the unit cell volume go to 0. And so in this limit Rk, where k runs from 1 to N will become a continuous variable, as N → ∞. Also in this limit, we suppose the crystal displacements vary only slowly, so that the vector field xδ(**R**k) (where k runs from 1 to N, and δ over x, y, z), can be considered a continuous and differentiable field xδ(**R**). In that case, supposing only neari-ish neighbors interact, then over the span of |**R**i – **R**j|, xα(**R**i) and xβ(**R**j) vary only a tiny amount, and continuously, it would be appropriate to expand these in a Taylor series. Well, I’m going to change notation now. I’m going to replace the **x**’s with **φ**’s. So assuming small variation, we have:



Filling into our V,



where δ = x, y, z and γ = x, y, z denote the components of positions **R**i, and **R**j. And ∇(i)δ = ∂/∂Ri(δ), etc. So now we can write:



And we define (note this doesn’t depend on j, thanks to the crystal’s periodic translation symmetry):



With this definition, we now have:



I guess we can go to the continuum limit. Can facilitate this by inserting 1 in the form of,



where we now let R become a continuous variable that is denoted R­j when it is within the jth cell. And so we come to:



and now we can say, where integral runs over entire crystal, and dropping the superfluous j subscript,



**Symmetries of the Elastic Tensor αβ;δγ**

Problem is our elastic constant thingy Eαβ;δγ apparently has 3×3×3×3 = 81 d.o.f. Well we can see that it’s symmetric w/r to transposition of (α,β) and also w/r to (δ,γ). So that reduces it to [# distinct (αβ)’s] × [# distinct (δγ)’s] = [3×2][3×2] = 36 d.o.f. There is a further reduction in the number of d.o.f. The energy of our elastic solid should be invariant w/r to translations and rotations, just as we said it was before in the context of the discrete crystal lattice a few files ago. Let’s say we have some initial displacement field **φ**(**R**) = **φ**0(**R**). And then we displace the crystal by a uniform amount δ**φ** = **a**, independent of **R** (***a*** will have to be small, since we have made a Harmonic approximation to the potential which is only valid for displacements of ions in a small neighborhood about their equilibrium points – note we’re displacing the atoms, but not their equilibrium positions; the equilibrium positions remain fixed). Then the relative displacement of the oscillators w/r to their equilibrium points will be **φ**(**R**) = **φ**0(**R**) + **a**. And when we plug this into V, we will get some V = V0 + δV. And we would expect that δV is zero, if we have translational symmetry. Well, since **φ** only enters into V via the gradient, δV will be zero, so we do already have translational symmetry. Apropos rotational symmetry, if we start every oscillator off in **φ0**(**R**) again and then rotate the crystal by a small angle **θ**, then the relative displacement of every element of the crystal, from its equilibrium point, will be **φ**(**R**) = **φ**0(**R**) + (**R**+**φ0**(**R**))×**θ**. This equation is only good for small **θ**’s. Further, since **φ**(**R**) is ’first order in smallness’, it only makes sense to keep terms to first order in smallness (note we’re rotating the atoms, not their equilibrium positions). But **φ**0(**R**)×**θ** would be second order in smallness. So we’ll just say **φ**(**R**) ≈ **φ**0(**R**) + **R**×**θ**. In terms of components, this means φi(**R**) = φ0i(**R**) + ΣjkεijkRjδθk, where i, j, k are the Cartesian components of **φ**, **R**, and δ**θ**. Since this rotation shouldn’t change the energy of our crystal, if we plug this into V, we should get δV = 0 again. Well,



δV is the term first order in δ**θ** (the 2nd order term is ignored, because our formula for the rotation δ**φ** = **R**×δ**θ** is only good to first order in δθ anyway.



Since this expression must be zero for every δθk=1,2,3, we need,



Now this should be zero for arbitrary initial displacements and derivatives too. So,



So we need, Eαβ;δγ to be symmetric in αδ indices. Since it is symmetric in αβ and δγ indices as well, this means its symmetric w/r to its βγ indices too. So to summarize, we have Eαβ;δγ and the sets of pairs {(α,β)} = {(δ,γ)} = {(1,1), (1,2), (1,3), (2,2), (2,3), (3,3)}. This makes 36 independent coefficients. This is illustrated below.



But thanks to the rotation symmetry Eαβ;δγ = Eδγ;αβ, so that E is symmetric w/r to exchange of pairs, that leaves us with 21 independent coefficients, say the blue ones.

**Final form for Lagrangian**

So noting all that, still, we have:



And all total we could write L as:



But I see people writing it like this, emphasizing the fact that the derivatives come in symmetric pairs, thanks to the symmetry of E,



**Simplification: Isotropy**

How would this simplify for isotropic crystals? I think with isotropic symmetry, we’re not rotating the atoms as a whole per se´, and thereby angularly displacing every oscillator by the same amount. Rather, we’re replacing the displacement of oscilator φα(**R**) with the displacement of oscilator φα(**R** + **R**×**θ**). So we’re making the mapping φα(**R**) → φα(**R** + **R**×**θ**). And we’re saying that this leaves the energy invariant. Similarly, homogeneity would mean replacing the displacement of oscillator φα(**R**) with the displacement of oscilator φα(**R** + **a**), i.e., φα(**R**) → φα(**R** + **a**). Anyway, expanding to first order, φα(**R**) → φα(**R**) + ∇iφα(**R**) ΣjkεijkRjδθk­ (implicit summation over repeated incides). And filling in,



Now expanding out to first order in δθ,



The second term in the KE goes to zero since can say,



We crossed out this term because εiik = 0. But then we have LHS = RHS = -LHS. So LHS = 0 too. So then we have now,



And the bottom term must be zero.



Well the term in brackets is symmetric w/r to interchange of (α,β) and interchange of (δ,γ). That means αβ;δγ must be antisymmetric w/r to interchange of these variables. But αβ;δγ is symmetric w/r to interchange of these variables. So that means that αβ;δγ must be zero. Except when α = β, and δ = γ. As then our expression is already zero,



And I think this last term is zero because IBP will give us negative the same thing. Maybe should look into this a little more closely. But moving on….quickly….we then see our tensor is diagonal in (α,β) and diagonal in (δ,γ). So it would look like,



And our Lagrangian would simplify to:



**Example: constructing L for cubic crystal**

Let’s refer back to an earlier file, where we found K for a simple cubic crystal. And let’s see what L would be in the continuum limit. So,



and,



We’ll observe that it’s symmetric w/r to transposition of (α,β), and (δ,γ), and w/r to the transposition of (α,β) with (δ,γ), like it’s supposed to be. And now let’s get L:



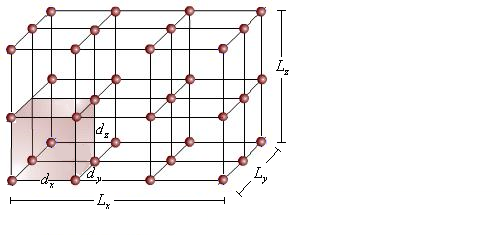
So we end up with:



and α, β of course run over the Cartesian components of the field. Note this congrues with our general result for an isotropic crystal.

**Example: constructing L for cubic crystal**

Let’s ignore all this, and work out an expression for the Lagrangian of a cubic crystal from scratch. We’ll use the simplest model we can to describe our elastic solid. I’m going to switch out notation. Let **R** → **x**, and let’s consider our particles on a grid:



And let’s say consider a particle at the corner of one of those cubes, say at coordinate (x,y,z). Let’s its displacement from this coordinate be **φ**(x,y,z;t) = φx(x,y,z;t)**i** + φy(x,y,z;t)**j** + φz(x,y,z;t)**k**. The kinetic energy of our solid will be the sum of the kinetic energies of each particle. The velocity of our particle at coordinate (x,y,z) is (x,y,z;t). So,



where ρ is the mass density, and i runs through the components x, y, z. Now it shares potential energy with its neighbors at coordinates (x+dx,y,z), (x,y+dy,z), and (x,y,z+dz) [it also has potential energy with those at (x-dx,y,z), (x,y-dy,z), (x,y,z-dz), but we’re not considering those because we would end up overcounting the PE by factor of 2 when we sum over all particles]. In the simplest scenario, the PE between a particle and its neighbors is directly proportional to their distance squared. And so we can say (changing notation from dx → dx, dy → dy, dz → dz):



where for short we denote xi as x,y,z for i = 1,2,3. And same for j. If we sum/integrate over all coordinates then we’ll have the total potential energy of our solid:



Let the constant of proportionality be B, the bulk modulus. Then we’ll have:



So then our Lagrangian can be written as:



where we explicitly indicate the time dependence of the deviations φ. This corresponds to the simplest example of our more general cubic model above, where φ´(d)/d = φ´´(d) = B. And this also congrues with our general result for an isotropic crystal.

**Example: Solving L for cubic crystal**

Now we want to solve for the **φ**(**x**,t) by getting its equation of motion. So we form the action and take the functional derivative…



and,



Now integrate by parts to get the derivatives off of the δ’s,



Should recognize the entity operating on φα, on the right, as the Laplacian. So we have, dividing by ρ,



Or, in terms of the vector **φ**,



This is the wave equation in 3D. Now we want to solve this equation. So analogous to before, we will assume a solution of the form,



and we will also impose periodic boundary conditions for simplicity. So plugging this into the equation we get:



We’ll assume a trial solution u(**x**) = ei**q**·**x**. Then we get:



So this is the frequency of wave oscillations. And then imposing the periodic boundary conditions, we see that:

Then defining,



we can write the eigenvalues (frequencies) and eigenvectors (normal modes) as:



where **n** is just a reference to the tuplet of values (nx, ny, nz). **ε** has been undetermined so far, and that’s because any orthonormal set of basis vectors will do for a homogeneous isotropic medium. Still, it is common to use a particular basis.



(**k** and **k**n are synonymous) So basically, we’re using a different basis with every wave. But this basis is convenient when we add interactions with other things within our solid, like with electrons, or light, etc., because these interactions most naturally couple to **k**, and not the Cartesian basis vectors. So having said that, our general solution is:



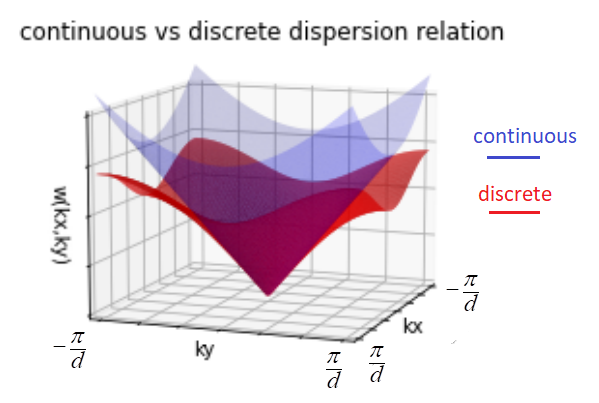
where we redefined Anλ as the modulus of its former self, and the caveat about the n = 0 term applies here, as it did in all the other previous files. So we have:



If we want the Cartesian components of our wave, then we can just dot both sides by **e**α (where **e**α = , , ),



where εα(kλ) would clearly be the αth Cartesian component of **ε**(kλ)­. The plot of 2D ωn vs. kn is shown below, in comparison with the discrete version.



As you can see, the continuum model approximates the discrete one well only for small wave numbers (large wavelengths). Often this suffices. Now let’s consider the speed of the waves. The speed is just:



This is a well known result for the speed of longitudinal waves through a medium.