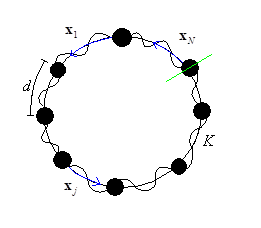
**Coupled Harmonic Oscillators**

Wanted to get a little experience calculating some K’s, and L’s. So here we go:

**Example: Applying this formalism to 1D crystal**

Let’s apply this formalism to our 1D crystal, just to verify that everything checks out.



We have:



We’ll expand to 2nd order in the displacements. Note,



So we can say,



Now we can discard irrelevant constants, and note the linear terms drop out of the sum since j = 2 cancels out the j = 1 term, and j = 4 cancels out j = 3 term, etc. So we have:



And now recognize/define KT = K(1-ℓ/d), which implies Kℓ/d = K – KT. So we can write:



Finally, in the 3rd line, **x**j2 + **x**j+12 = 2**x**j2 because the j = 1 term will add with the j = 2 term, etc. And we want to write our 1D crystal Lagrangian in the following form,



So here we go…



(the second line isn’t the most straightforward translation to δ’s, but using it because it’ll match previous results better) So we have:



And we saw in previous file that the solution is:



where the **ε**(kλ) and ωkλ are the eigenvectors and frequencies of the Fourier transformed K-matrix (again, there are just N distinct ΔRj’s),



Therefore the eigenvectors and eigenvalues of the system are determined by the equation:



which gives us identical results to what was found earlier. As so it follows that the eigenvectors and eigenvalues are:



and then that the general solution is:



where the **ε**(λ) are just the Cartesian unit vectors **e**λ. Just as we’d found before.

**Example: Van der Waals attraction**

Consider the Van der Waals attraction.



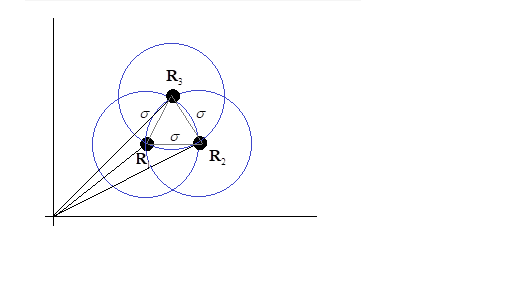
We can do a harmonic approximation. The minimum is at:



and the concavity there is:



Say we have three atoms. These would be locked in a triangle, as this configuration would have the minimum energy.



Let’s put the origin at **R**1. And the x-axis along **R**2-**R**1. Then equilibrium coordinates would be:



Then refering to previous file, we found:



For us, M simplifies to:



and the different **M**’s are:



And so for **K** we got:



So the potential energy is:



Taking account of the symmetry of **K**, we can write:



**Example: Coulomb Potential**

If we specialize to the Coulomb potential we get:



and so,



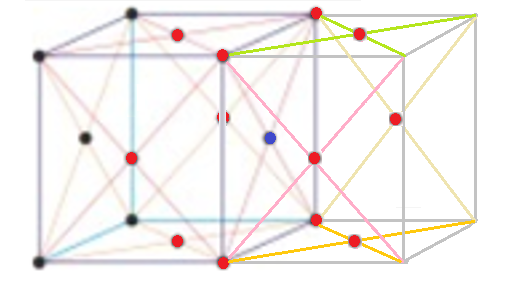
and so,



**Example. FCC crystal nearest-neighbors interaction**

Let’s consider a face-centered cubic crystal,

Chart, radar chart

Description automatically generated 

And consider that a typical ion has interactions only with its nearest neighbors. In this case, there’s 12 of them. I drew a blue guy, and its 12 n.n. in red. What is the **K** matrix for this guy? Let the blue guy above be the origin of our coordinate system, for these purposes. And say that each of the red n.n. interacts with the blue guy via a potential energy φ(ΔR) which is only dependent on the magnitude of ΔR = d. A Coulomb interaction would be one such example. All twelve Δ**R**’s are (points to right, points into page, and points up):



and we can work out K in different ways. But let’s go with our general pair-wise potential formula,



and restricting the sum over k, for a given i, to the nearest neighbors, we get:



where z = 12 is the number of nearest neighbors. Now we have to work out that tensor sum over all these guys.



Well, here’s all 12…



The sum of the squares:



So now we have:



Now let’s work out the Fourier transform. From previous file, recall we found,



The same colored Δ**R**ij’s above result in the same summand, so just doing unique terms, we have:



I don’t feel like we can simplify further. Say **q** = q. Then this does simplifies to:



which simplifies to:



The eigenvalue/vector equation,



tells us the polarizations and frequencies of the oscillatory modes of the given wavevector. So for us, we clearly have:



So one mode (longitudinal) is parallel to **q**, and the other two (transverse) are perpendicular. Plus the two transverse ones are degenerate in frequency. I imagine that if we chose a different **q**, less symmetrically oriented, we’d find the ωλ(**q**) to be completely non-degenerate and the **ε**λ(**q**) to be not necessarily longitudinal and transverse w/r to **q**.

**Example. simple cubic crystal nearest-neighbors interaction**

Let’s consider a simple cubic crystal,

A picture containing text, worktable

Description automatically generated

And consider that a typical ion has interactions only with its nearest neighbors. In this case, there’s 6 of them. And say that each of the n.n. interacts with via a potential energy φ(ΔR) which is only dependent on the magnitude of ΔR = d. A Coulomb interaction would be one such example. All six Δ**R**’s are (points to right, points into page, and points up):



and we’ll recall K is given by:



and restricting the sum over k, for a given i, to the nearest neighbors, we get:



where z = 6 is the number of nearest neighbors. Now we have to work out that tensor sum over all these guys. Well, clearly,



which happens to be what we got last time too. So,



Now let’s work out the Fourier transform. From previous file, recall we found,



and finally,



So this is clearly a diagonal matrix. But for general **q**, the eigenvalues are non-degenerate. But the eigenvectors will be, interestingly, always , , . So only if **q** is along one of these directions will one of the waves be longitudinal and the others transverse.