

Cranking the AFD mode in STO: displaced spring model

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This is a simple spring model for the AFD mode in STO. The main idea is to forcefully crank one particular unit cell by some amount and allow the rest of the unit cells to relax and see how the perturbation decays away from the constraint. The model is the simplest possible one of a 1D chain (could be 3D but with planar periodic displacements so we describe the behavior in the orthogonal direction).

Let u_j be the (scalar) displacement of the j th unit cell. This could be the angle of the AFD mode in that cell away from its equilibrium value. A “cell” could be a primitive unit cell or a larger cell with coherent rotation or twisting. A harmonic model gives us the energy

$$E = \frac{1}{2} \sum_{j,k} u_j K_{j,k} u_k.$$

In a nearest neighbor model, let the diagonals be $K_{j,j} = a > 0$ and the off-diagonal be $K_{j,j+1} = K_{j,j-1} = b$. This particular model has Bloch waves $u_j = \text{Real}\{\text{Constant} \times e^{ij\theta}\}$ for some real θ as eigenmodes with eigen spring constants $K_\theta = a + 2b \cos \theta$. The values of θ depend on the boundary conditions but there will be N of them.

The big assumption is that these AFD modes are some type of generalized “optic” mode: they have positive restoring force no matter what type of displacement pattern is made (they are not acoustic for $\theta \rightarrow 0$.) So $K_\theta > 0$ and thus $a > 2|b|$.

The main question is how a perturbation at some site, say $j = 0$, decays away. There are two ways to do this.

(1) The elementary method is to constrain $u_0 = 1$ to be a fixed value. Then we’re interested in how u_j behaves at equilibrium for $j > 1$. We’ll assume the chain ends at site N . Equilibrium means zero net force or $\partial E / \partial u_j = 0$ so we have the conditions

$$u_0 = 1 \quad , \quad bu_{j-1} + au_j + bu_{j+1} = 0 \text{ for } 0 < j < N \quad , \quad bu_{N-1} + au_N = 0.$$

Let's start at the end $j = N$ and work inwards towards $j = 1$. The end conditions solves to $u_{N-1} = -(a/b)u_N$ which is one unknown u_N . The remaining conditions can be written as 2×2 matrix iteration

$$\begin{pmatrix} u_{j-1} \\ u_j \end{pmatrix} = \begin{pmatrix} -a/b & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u_j \\ u_{j+1} \end{pmatrix}.$$

The eigenvalues of the matrix are $\lambda_{\pm} = \frac{-a/b \pm \sqrt{(a/b)^2 - 4}}{2}$. These are approximately $-b/a$ and $-a/b$ for $|a/b| \gg 1$. Both are real since $|a/b| > 2$ as per our main assumption above. Furthermore, $\lambda_+ \lambda_- = 1$ so $|\lambda_-| > 1$ and $|\lambda_+| < 1$. Upon iteration inwards from the boundary, the λ_- will be exponentiated by N and completely swamp λ_+ (unless $|a/b|$ is extremely close to 2 which means a soft mode which we exclude). So then working back to match $u_0 = 1$ gives us basically an exponentially damped envelope $u_j \approx u_0(\lambda_+)^j$ going forwards.

As a sanity check consider $|a/b| \gg 1$ which gives $\lambda_+ \approx -b/a$ which means the on-site spring is much stronger than the springs linking the neighboring sites. Then if we fix site $u_0 = 1$, this creates a force $-b$ on the $j = 1$ site and it displaces by an amount mainly given by its on-site spring constant stretching to accommodate and this gives $u_j \approx -b/a$. The pattern then continues with a further factor of $-b/a$ to the next site and so on.

(2) A more fancy variant is not to fix the displacement but instead to put an external force f_j on each site. The energy is instead

$$E = \frac{1}{2} \sum_{j,k} u_j K_{j,k} u_k - \sum_j f_j u_j.$$

Equilibrium means $Ku = f$ or $u = K^{-1}f$ in vector-matrix notation. Say we put a fixed force on the $j = 0$ site so $f_j = \delta_{j,0}$. Then we can use the eigenmode description to invert K and get

$$u_j = \frac{1}{N} \sum_{\theta} \frac{e^{ij\theta}}{a + 2b \cos \theta}.$$

For very large N , we can turn the sum into an integral over θ and then do contour methods by realizing the θ integral is a contour integral over the unit circle $z = e^{i\theta}$:

$$u_j = \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{e^{ij\theta}}{a + 2b \cos \theta} = \frac{1}{2\pi i} \oint_{|z|=1} \frac{dz}{z} \frac{z^j}{a + bz + b/z}.$$

The denominator has a pole when $\cos \hat{\theta} = -a/(2b)$. This means complex θ since $|a/b| > 2$. Set $\hat{\theta} = \pi + i\gamma$ which gives then $\cosh \gamma = a/(2b)$ and we know $\cosh^{-1} z = \ln(z + \sqrt{z^2 - 1})$. So the key factor in the residue of the pole determining the j dependence is just the exponential evaluated at $\hat{\theta}$ which is

$$e^{ij\hat{\theta}} = (-1)^j e^{-j\gamma} = (-1)^j \cdot \left(a/(2b) + \sqrt{(a/2b)^2 - 1} \right)^{-j} = (\lambda_+)^j$$

as expected. Again, we get exponential decay away from the perturbation site with each site dropping by a factor of λ_+ compared to the previous when N is very large.