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One atom basis phonons in 2D

Let's tackle a problem like the 2D problem of the final exam, but first more generally. Instead of a square lattice consider the lattice with the geometry illustrated in fig. 1.1.

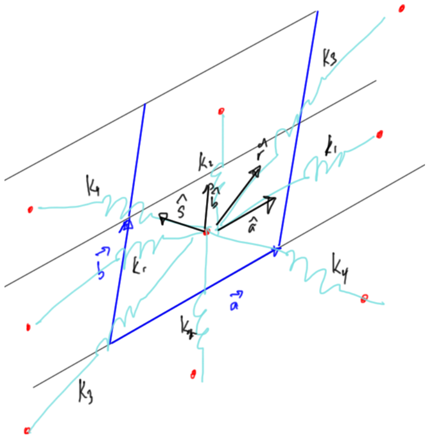

Figure 1.1: Oblique one atom basis

Here, $\mathbf{a}$ and $\mathbf{b}$ are the vector differences between the equilibrium positions separating the masses along the K_1 and K_2 interaction directions respectively. The equilibrium spacing for the cross coupling harmonic forces are

$$\begin{aligned}\mathbf{r} &= (\mathbf{b} + \mathbf{a})/2 \\ \mathbf{s} &= (\mathbf{b} - \mathbf{a})/2.\end{aligned} \tag{1.1}$$

Based on previous calculations, we can write the equations of motion by inspection

$$
\begin{aligned}
m\ddot{\mathbf{u}}_{\mathbf{n}} = &- K_1 \operatorname{Proj}_{\hat{\mathbf{a}}} \sum_{\pm} \left(\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}\pm(1,0)}\right)^2 \\
&- K_2 \operatorname{Proj}_{\hat{\mathbf{b}}} \sum_{\pm} \left(\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}\pm(0,1)}\right)^2 \\
&- K_3 \operatorname{Proj}_{\hat{\mathbf{r}}} \sum_{\pm} \left(\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}\pm(1,1)}\right)^2 \\
&- K_4 \operatorname{Proj}_{\hat{\mathbf{s}}} \sum_{\pm} \left(\mathbf{u}_{\mathbf{n}} - \mathbf{u}_{\mathbf{n}\pm(1,-1)}\right)^2 .
\end{aligned}
\tag{1.2}
$$

Inserting the trial solution

$$
\mathbf{u}_{\mathbf{n}} = \frac{1}{\sqrt{m}} \boldsymbol{\epsilon}(\mathbf{q}) e^{i(\mathbf{r}_{\mathbf{n}} \cdot \mathbf{q} - \omega t)},
\tag{1.3}
$$

and using the matrix form for the projection operators, we have

$$
\begin{aligned}
\omega^2 \boldsymbol{\epsilon} = &\frac{K_1}{m} \hat{\mathbf{a}}\hat{\mathbf{a}}^{\mathrm{T}} \boldsymbol{\epsilon} \sum_{\pm} \left(1 - e^{\pm i \mathbf{a} \cdot \mathbf{q}}\right) \\
&+ \frac{K_2}{m} \hat{\mathbf{b}}\hat{\mathbf{b}}^{\mathrm{T}} \boldsymbol{\epsilon} \sum_{\pm} \left(1 - e^{\pm i \mathbf{b} \cdot \mathbf{q}}\right) \\
&+ \frac{K_3}{m} \hat{\mathbf{b}}\hat{\mathbf{b}}^{\mathrm{T}} \boldsymbol{\epsilon} \sum_{\pm} \left(1 - e^{\pm i (\mathbf{b}+\mathbf{a}) \cdot \mathbf{q}}\right) \\
&+ \frac{K_3}{m} \hat{\mathbf{b}}\hat{\mathbf{b}}^{\mathrm{T}} \boldsymbol{\epsilon} \sum_{\pm} \left(1 - e^{\pm i (\mathbf{b}-\mathbf{a}) \cdot \mathbf{q}}\right) \\
&= \frac{4K_1}{m} \hat{\mathbf{a}}\hat{\mathbf{a}}^{\mathrm{T}} \boldsymbol{\epsilon} \sin^2\left(\mathbf{a} \cdot \mathbf{q}/2\right) + \frac{4K_2}{m} \hat{\mathbf{b}}\hat{\mathbf{b}}^{\mathrm{T}} \boldsymbol{\epsilon} \sin^2\left(\mathbf{b} \cdot \mathbf{q}/2\right) \\
&+ \frac{4K_3}{m} \hat{\mathbf{r}}\hat{\mathbf{r}}^{\mathrm{T}} \boldsymbol{\epsilon} \sin^2\left((\mathbf{b}+\mathbf{a}) \cdot \mathbf{q}/2\right) + \frac{4K_4}{m} \hat{\mathbf{s}}\hat{\mathbf{s}}^{\mathrm{T}} \boldsymbol{\epsilon} \sin^2\left((\mathbf{b}-\mathbf{a}) \cdot \mathbf{q}/2\right) .
\end{aligned}
\tag{1.4}
$$

This fully specifies our eigenvalue problem. Writing

$$
\begin{aligned}
S_1 &= \sin^2\left(\mathbf{a} \cdot \mathbf{q}/2\right) \\
S_2 &= \sin^2\left(\mathbf{b} \cdot \mathbf{q}/2\right) \\
S_3 &= \sin^2\left((\mathbf{b}+\mathbf{a}) \cdot \mathbf{q}/2\right) \\
S_4 &= \sin^2\left((\mathbf{b}-\mathbf{a}) \cdot \mathbf{q}/2\right)
\end{aligned}
\tag{1.5a}
$$

$$
\boxed{A = \frac{4}{m}\left(K_1 S_1 \hat{\mathbf{a}}\hat{\mathbf{a}}^{\mathrm{T}} + K_2 S_2 \hat{\mathbf{b}}\hat{\mathbf{b}}^{\mathrm{T}} + K_3 S_3 \hat{\mathbf{r}}\hat{\mathbf{r}}^{\mathrm{T}} + K_4 S_4 \hat{\mathbf{s}}\hat{\mathbf{s}}^{\mathrm{T}}\right),}
\tag{1.5b}
$$

we wish to solve

$$
A\boldsymbol{\epsilon} = \omega^2 \boldsymbol{\epsilon} = \lambda \boldsymbol{\epsilon}.
\tag{1.6}
$$

Neglecting the specifics of the matrix at hand, consider a generic two by two matrix

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \tag{1.7}$$

for which the characteristic equation is

$$\begin{aligned} 0 &= \begin{vmatrix} \lambda - a & -b \\ -c & \lambda - d \end{vmatrix} \\ &= (\lambda - a)(\lambda - d) - bc \\ &= \lambda^2 - (a + d)\lambda + ad - bc \\ &= \lambda^2 - (TrA)\lambda + |A| \\ &= \left(\lambda - \frac{TrA}{2}\right)^2 - \left(\frac{TrA}{2}\right)^2 + |A|. \end{aligned} \tag{1.8}$$

So our angular frequencies are given by

$$\omega^2 = \frac{1}{2}\left(TrA \pm \sqrt{(TrA)^2 - 4|A|}\right). \tag{1.9}$$

The square root can be simplified slightly

$$\begin{aligned} (TrA)^2 - 4|A| &= (a + d)^2 - 4(ad - bc) \\ &= a^2 + d^2 + 2ad - 4ad + 4bc \\ &= (a - d)^2 + 4bc, \end{aligned} \tag{1.10}$$

so that, finally, the dispersion relation is

$$\boxed{\omega^2 = \frac{1}{2}\left(d + a \pm \sqrt{(d - a)^2 + 4bc}\right),} \tag{1.11}$$

Our eigenvectors will be given by

$$0 = (\lambda - a)\epsilon_1 - b\epsilon_2, \tag{1.12}$$

or

$$\epsilon_1 \propto \frac{b}{\lambda - a}\epsilon_2. \tag{1.13}$$

So, our eigenvectors, the vectoral components of our atomic displacements, are

$$\epsilon \propto \begin{bmatrix} b \\ \omega^2 - a \end{bmatrix}, \tag{1.14}$$

or

$$\boxed{\epsilon \propto \begin{bmatrix} 2b \\ d - a \pm \sqrt{(d - a)^2 + 4bc} \end{bmatrix}.} \tag{1.15}$$

Square lattice There is not too much to gain by expanding out the projection operators explicitly in general. However, let's do this for the specific case of a square lattice (as on the exam problem). In that case, our projection operators are

$$\hat{\mathbf{a}}\hat{\mathbf{a}}^{\mathrm{T}} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \tag{1.16a}$$

$$\hat{\mathbf{b}}\hat{\mathbf{b}}^{\mathrm{T}} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \tag{1.16b}$$

$$\hat{\mathbf{r}}\hat{\mathbf{r}}^{\mathrm{T}} = \frac{1}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \tag{1.16c}$$

$$\hat{\mathbf{s}}\hat{\mathbf{s}}^{\mathrm{T}} = \frac{1}{2} \begin{bmatrix} -1 \\ 1 \end{bmatrix} \begin{bmatrix} -1 & 1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{1.16d}$$

$$\begin{aligned} S_1 &= \sin^2 (\mathbf{a} \cdot \mathbf{q}) \\ S_2 &= \sin^2 (\mathbf{b} \cdot \mathbf{q}) \\ S_3 &= \sin^2 ((\mathbf{b} + \mathbf{a}) \cdot \mathbf{q}) \\ S_4 &= \sin^2 ((\mathbf{b} - \mathbf{a}) \cdot \mathbf{q}) , \end{aligned} \tag{1.17}$$

Our matrix is

$$A = \frac{2}{m} \begin{bmatrix} 2K_1S_1 + K_3S_3 + K_4S_4 & K_3S_3 - K_4S_4 \\ K_3S_3 - K_4S_4 & 2K_2S_2 + K_3S_3 + K_4S_4 \end{bmatrix} , \tag{1.18}$$

where, specifically, the squared sines for this geometry are

$$S_1 = \sin^2 (\mathbf{a} \cdot \mathbf{q}/2) = \sin^2 (a q_x/2) \tag{1.19a}$$

$$S_2 = \sin^2 (\mathbf{b} \cdot \mathbf{q}/2) = \sin^2 (a q_y/2) \tag{1.19b}$$

$$S_3 = \sin^2 ((\mathbf{b} + \mathbf{a}) \cdot \mathbf{q}/2) = \sin^2 (a(q_x + q_y)/2) \tag{1.19c}$$

$$S_4 = \sin^2 ((\mathbf{b} - \mathbf{a}) \cdot \mathbf{q}/2) = \sin^2 (a(q_y - q_x)/2) . \tag{1.19d}$$

Using eq. (1.14), the dispersion relation and eigenvectors are

$$\omega^2 = \frac{2}{m} \left(\sum_i K_i S_i \pm \sqrt{(K_2S_2 - K_1S_1)^2 + (K_3S_3 - K_4S_4)^2} \right) \tag{1.20a}$$

$$\epsilon \propto \begin{bmatrix} K_3S_3 - K_4S_4 \\ K_2S_2 - K_1S_1 \pm \sqrt{(K_2S_2 - K_1S_1)^2 + (K_3S_3 - K_4S_4)^2} \end{bmatrix} . \tag{1.20b}$$

This calculation is confirmed in oneAtomBasisPhononSquareLatticeEigensystem.nb. Mathematica calculates an alternate form (equivalent to using a zero dot product for the second row), of

$$\epsilon \propto \begin{bmatrix} K_1S_1 - K_2S_2 \pm \sqrt{(K_2S_2 - K_1S_1)^2 + (K_3S_3 - K_4S_4)^2} \\ K_3S_3 - K_4S_4 \end{bmatrix} . \tag{1.21}$$

Either way, we see that $K_3S_3 - K_4S_4 = 0$ leads to only horizontal or vertical motion.

With the exam criteria In the specific case that we had on the exam where $K_1 = K_2$ and $K_3 = K_4$, these are

$$\omega^2 = \frac{2}{m}\left(K_1(S_1 + S_2) + K_3(S_3 + S_4) \pm \sqrt{K_1^2(S_2 - S_1)^2 + K_3^2(S_3 - S_4)^2}\right) \tag{1.22a}$$

$$\epsilon \propto \begin{bmatrix} K_3\,(S_3 - S_4) \\ K_1\left((S_1 - S_2) \pm \sqrt{(S_2 - S_1)^2 + \left(\frac{K_3}{K_1}\right)^2 (S_3 - S_4)^2}\right)\end{bmatrix}. \tag{1.22b}$$

For horizontal and vertical motion we need $S_3 = S_4$, or for a $2\pi \times$ integer difference in the absolute values of the sine arguments

$$\pm(a(q_x + q_y)/2) = a(q_y - q_y)/2 + 2\pi n. \tag{1.23}$$

That is, one of

$$\begin{aligned} q_x &= \frac{2\pi}{a} n \\ q_y &= \frac{2\pi}{a} n \end{aligned} \tag{1.24}$$

In the first BZ, that is one of $q_x = 0$ or $q_y = 0$.

System in rotated coordinates On the exam, where we were asked to solve for motion along the cross directions explicitly, there was a strong hint to consider a rotated (by $\pi/4$) coordinate system. The rotated the lattice basis vectors are $\mathbf{a} = a\mathbf{e}_1, \mathbf{b} = a\mathbf{e}_2$, and the projection matrices. Writing $\hat{\mathbf{r}} = \mathbf{f}_1$ and $\hat{\mathbf{s}} = \mathbf{f}_2$, where $\mathbf{f}_1 = (\mathbf{e}_1 + \mathbf{e}_2)/\sqrt{2}, \mathbf{f}_2 = (\mathbf{e}_2 - \mathbf{e}_1)/\sqrt{2}$, or $\mathbf{e}_1 = (\mathbf{f}_1 - \mathbf{f}_2)/\sqrt{2}, \mathbf{e}_2 = (\mathbf{f}_1 + \mathbf{f}_2)/\sqrt{2}$. In the $\{\mathbf{f}_1, \mathbf{f}_2\}$ basis the projection matrices are

$$\hat{\mathbf{a}}\hat{\mathbf{a}}^{\mathrm{T}} = \frac{1}{2}\begin{bmatrix} 1 \\ -1 \end{bmatrix}\begin{bmatrix} 1 & -1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{1.25a}$$

$$\hat{\mathbf{b}}\hat{\mathbf{b}}^{\mathrm{T}} = \frac{1}{2}\begin{bmatrix} 1 \\ 1 \end{bmatrix}\begin{bmatrix} 1 & 1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \tag{1.25b}$$

$$\hat{\mathbf{r}}\hat{\mathbf{r}}^{\mathrm{T}} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \tag{1.25c}$$

$$\hat{\mathbf{s}}\hat{\mathbf{s}}^{\mathrm{T}} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \tag{1.25d}$$

The dot products that show up in the squared sines are

$$\mathbf{a} \cdot \mathbf{q} = a\frac{1}{\sqrt{2}}(\mathbf{f}_1 - \mathbf{f}_2) \cdot (\mathbf{f}_1 k_u + \mathbf{f}_2 k_v) = \frac{a}{\sqrt{2}}(k_u - k_v) \tag{1.26a}$$

$$\mathbf{b} \cdot \mathbf{q} = a\frac{1}{\sqrt{2}}(\mathbf{f}_1 + \mathbf{f}_2) \cdot (\mathbf{f}_1 k_u + \mathbf{f}_2 k_v) = \frac{a}{\sqrt{2}}(k_u + k_v) \tag{1.26b}$$

$$(\mathbf{a}+\mathbf{b})\cdot\mathbf{q} = \sqrt{2}ak_u \tag{1.26c}$$

$$(\mathbf{b}-\mathbf{a})\cdot\mathbf{q} = \sqrt{2}ak_v \tag{1.26d}$$

So that in this basis

$$\begin{aligned}
S_1 &= \sin^2\left(\frac{a}{\sqrt{2}}(k_u - k_v)\right) \\
S_2 &= \sin^2\left(\frac{a}{\sqrt{2}}(k_u + k_v)\right) \\
S_3 &= \sin^2\left(\sqrt{2}ak_u\right) \\
S_4 &= \sin^2\left(\sqrt{2}ak_v\right)
\end{aligned} \tag{1.27}$$

With the rotated projection operators eq. (1.5b) takes the form

$$A = \frac{2}{m}\begin{bmatrix} K_1S_1 + K_2S_2 + 2K_3S_3 & K_2S_2 - K_1S_1 \\ K_2S_2 - K_1S_1 & K_1S_1 + K_2S_2 + 2K_4S_4 \end{bmatrix}. \tag{1.28}$$

This clearly differs from eq. (1.18), and results in a different expression for the eigenvectors, but the same as eq. (1.20a) for the angular frequencies.

$$\epsilon \propto \begin{bmatrix} K_2S_2 - K_1S_1 \\ K_4S_4 - K_3S_3 \mp \sqrt{(K_2S_2 - K_1S_1)^2 + (K_3S_3 - K_4S_4)^2} \end{bmatrix}, \tag{1.29}$$

or, equivalently

$$\epsilon \propto \begin{bmatrix} K_4S_4 - K_3S_3 \mp \sqrt{(K_2S_2 - K_1S_1)^2 + (K_3S_3 - K_4S_4)^2} \\ K_1S_1 - K_2S_2 \end{bmatrix}, \tag{1.30}$$

For the $K_1 = K_2$ and $K_3 = K_4$ case of the exam, this is

$$\epsilon \propto \begin{bmatrix} K_1(S_2 - S_1) \\ K_3\left(S_4 - S_3 \mp \sqrt{\left(\frac{K_1}{K_3}\right)^2 (S_2 - S_1)^2 + (S_3 - S_4)^2}\right) \end{bmatrix}. \tag{1.31}$$

Similar to the horizontal coordinate system, we see that we have motion along the diagonals when

$$\pm\frac{a}{\sqrt{2}}(k_u - k_v) = \frac{a}{\sqrt{2}}(k_u + k_v) + 2\pi n, \tag{1.32}$$

or one of

$$\begin{aligned}
k_u &= \sqrt{2}\frac{\pi}{a}n \\
k_v &= \sqrt{2}\frac{\pi}{a}n
\end{aligned} \tag{1.33}$$

Stability? The exam asked why the cross coupling is required for stability. Clearly we have more complex interaction. The constant ω surfaces will also be more complex. However, I still don't have a good intuition what exactly was sought after for that part of the question.

Numerical computations A Manipulate allowing for choice of the spring constants and lattice orientation, as shown in fig. 1.2, is available in phy487/oneAtomBasisPhonon.nb. This interface also provides a numerical calculation of the distribution relation as shown in fig. 1.3, and provides an animation of the normal modes for any given selection of $\mathbf{q}$ and $\omega(\mathbf{q})$ (not shown).

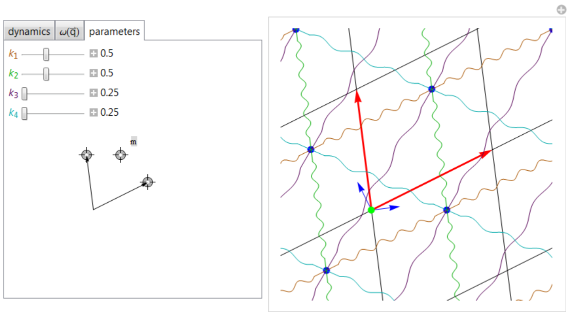

Figure 1.2: 2D Single atom basis Manipulate interface

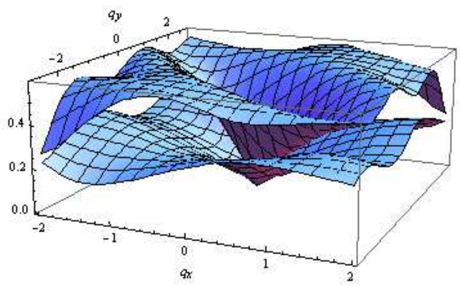

Figure 1.3: Sample distribution relation for 2D single atom basis.