

Dynamical Matrix

Babak Nivi Richard Chang John Kymissis
Kent Lundberg

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This section describes our calculation of the dynamic matrix.

1 Basis

Our lattice vectors are $\mathbf{a}_1 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{y}})$, $\mathbf{a}_2 = \frac{a}{2}(\hat{\mathbf{x}} + \hat{\mathbf{z}})$, and $\mathbf{a}_3 = \frac{a}{2}(\hat{\mathbf{y}} + \hat{\mathbf{z}})$ where a is the cubic lattice spacing.

The basis consists of a Ga atom located at $\mathbf{0}$ and an As atom at $\mathbf{b}_1 = \frac{a}{4}(\hat{\mathbf{x}} + \hat{\mathbf{y}} + \hat{\mathbf{z}})$.

The Ga atom's nearest neighbours are at \mathbf{b}_1 , $\mathbf{b}_2 = \frac{a}{4}(-\hat{\mathbf{x}} - \hat{\mathbf{y}} + \hat{\mathbf{z}})$, $\mathbf{b}_3 = \frac{a}{4}(-\hat{\mathbf{x}} + \hat{\mathbf{y}} - \hat{\mathbf{z}})$, and $\mathbf{b}_4 = \frac{a}{4}(-\hat{\mathbf{x}} - \hat{\mathbf{y}} - \hat{\mathbf{z}})$. The As atom's nearest neighbours are at $\mathbf{0}$, \mathbf{a}_1 , \mathbf{a}_2 , and \mathbf{a}_3 .

2 Potential Energy

Let \mathbf{R} be an arbitrary GaAs fcc lattice vector. Let $u_i[\mathbf{R}]$ describe the displacement of atom i at lattice site \mathbf{R} . Then the terms of the crystal potential V that involve \mathbf{R} are

$$\begin{aligned} V = & \dots + \frac{1}{2}(\alpha_s - \alpha_\phi) \left[(\mathbf{b}_1 \cdot (u_1[\mathbf{R}] - u_2[\mathbf{R}]))^2 + \right. \\ & (\mathbf{b}_2 \cdot (u_1[\mathbf{R}] - u_2[\mathbf{R} + \mathbf{a}_1]))^2 + \\ & (\mathbf{b}_3 \cdot (u_1[\mathbf{R}] - u_2[\mathbf{R} + \mathbf{a}_2]))^2 + \\ & (\mathbf{b}_4 \cdot (u_1[\mathbf{R}] - u_2[\mathbf{R} + \mathbf{a}_3]))^2 + \\ & (\mathbf{b}_2 \cdot (u_1[\mathbf{R} - \mathbf{a}_1] - u_2[\mathbf{R}]))^2 + \\ & (\mathbf{b}_3 \cdot (u_1[\mathbf{R} - \mathbf{a}_2] - u_2[\mathbf{R}]))^2 + \\ & \left. (\mathbf{b}_4 \cdot (u_1[\mathbf{R} - \mathbf{a}_3] - u_2[\mathbf{R}]))^2 \right] \\ & + \frac{1}{2}\alpha_\phi \left[|u_1[\mathbf{R}] - u_2[\mathbf{R}]|^2 + \right. \\ & |u_1[\mathbf{R}] - u_2[\mathbf{R} + \mathbf{a}_1]|^2 + \\ & |u_1[\mathbf{R}] - u_2[\mathbf{R} + \mathbf{a}_2]|^2 + \\ & \left. |u_1[\mathbf{R}] - u_2[\mathbf{R} + \mathbf{a}_3]|^2 + \right] \end{aligned}$$

$$\begin{aligned}
& |u_1[\mathbf{R} - \mathbf{a}_1] - u_2[\mathbf{R}]|^2 + \\
& |u_1[\mathbf{R} - \mathbf{a}_2] - u_2[\mathbf{R}]|^2 + \\
& |u_1[\mathbf{R} - \mathbf{a}_3] - u_2[\mathbf{R}]|^2 \\
& + \dots
\end{aligned}$$

3 Force on a Single Atom

The force F on atom/direction i at position \mathbf{R} is given by

$$F = M_i \frac{\partial^2 u_i[\mathbf{R}]}{\partial t^2} = -\frac{\partial V}{\partial u_i[\mathbf{R}]}$$

Again, we used Mathematica to perform this tedious calculation (see Appendix A). For example, the force on in the x direction on atom 1 at position \mathbf{R} is given by

$$\begin{aligned}
M_i \frac{\partial^2 u_{1x}[\mathbf{R}]}{\partial t^2} = \frac{1}{3} (& \alpha_\phi \quad (-8u_{1x}[\mathbf{R}] + 2u_{2x}[\mathbf{R}] + 2u_{2x}[\mathbf{R} + \mathbf{a}_1] + 2u_{2x}[\mathbf{R} + \mathbf{a}_2] + 2u_{2x}[\mathbf{R} + \mathbf{a}_3] \\
& -u_{2y}[\mathbf{R}] - u_{2y}[\mathbf{R} + \mathbf{a}_1] + u_{2y}[\mathbf{R} + \mathbf{a}_2] + u_{2y}[\mathbf{R} + \mathbf{a}_3] \\
& -u_{2z}[\mathbf{R}] + u_{2z}[\mathbf{R} + \mathbf{a}_1] + u_{2z}[\mathbf{R} + \mathbf{a}_2] - u_{2z}[\mathbf{R} + \mathbf{a}_3]) \\
& + \alpha_s \quad (-4u_{1x}[\mathbf{R}] + u_{2x}[\mathbf{R}] + u_{2x}[\mathbf{R} + \mathbf{a}_1] + u_{2x}[\mathbf{R} + \mathbf{a}_2] + u_{2x}[\mathbf{R} + \mathbf{a}_3] \\
& + u_{2y}[\mathbf{R}] + u_{2y}[\mathbf{R} + \mathbf{a}_1] - u_{2y}[\mathbf{R} + \mathbf{a}_2] + u_{2y}[\mathbf{R} + \mathbf{a}_3] \\
& + u_{2z}[\mathbf{R}] - u_{2z}[\mathbf{R} + \mathbf{a}_1] + u_{2z}[\mathbf{R} + \mathbf{a}_2] + u_{2z}[\mathbf{R} + \mathbf{a}_3])
\end{aligned}$$

4 Dynamical Matrix

The elements of the dynamical matrix \mathbf{D} can be calculated by

$$\mathbf{D}_{ij}(\mathbf{k}) = \sum_{\mathbf{R}_p} \left(\frac{\partial^2 V}{\partial u_i[\mathbf{R} + \mathbf{R}_p] \partial u_j[\mathbf{R}]} \right)_{eq} e^{-i\mathbf{k}\mathbf{R}_p}$$

where i, j range over the ordered set $(1x, 2x, 1y, 2y, 1z, 2z)$ and the sum is over all lattice vectors.

The dispersion relation can then be determined through

$$\mathbf{M}^{-1} \mathbf{D}(\mathbf{k}) \vec{\epsilon} = \omega^2 \vec{\epsilon}$$

where \mathbf{M} is a diagonal matrix with the elements $(M_1, M_2, M_1, M_2, M_1, M_2)$ down the diagonal. M_1 is the mass of Ga and M_2 is the mass of As.

Rather than calculate the \mathbf{D}_{ij} by hand, we wrote a Mathematica program to calculate the \mathbf{D}_{ij} symbolically. The code is included in Appendix A. Our Mathematica and Matlab code orders \mathbf{D} according to the ordered set $A = (1x, 2x, 1y, 2y, 1z, 2z)$. All other discussions in this report assume this ordering. However \mathbf{D} has much more symmetry if we order it according to $B = (1x, 1y, 1z, 2x, 2y, 2z)$. If we order \mathbf{D} according to B ,

$$\mathbf{D} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^* & \mathbf{A} \end{pmatrix}$$

where

$$\mathbf{A} = \begin{pmatrix} \frac{4}{3}\alpha_s & 0 & 0 \\ 0 & \frac{4}{3}\alpha_s & 0 \\ 0 & 0 & \frac{4}{3}\alpha_s \end{pmatrix}$$

$$\mathbf{B} = \begin{pmatrix} \beta(1 + e^{i\mathbf{k}\cdot\mathbf{r}_1} + e^{i\mathbf{k}\cdot\mathbf{r}_2} + e^{i\mathbf{k}\cdot\mathbf{r}_3}) & \gamma(1 + e^{i\mathbf{k}\cdot\mathbf{r}_1} - e^{i\mathbf{k}\cdot\mathbf{r}_2} - e^{i\mathbf{k}\cdot\mathbf{r}_3}) & \gamma(1 - e^{i\mathbf{k}\cdot\mathbf{r}_1} + e^{i\mathbf{k}\cdot\mathbf{r}_2} - e^{i\mathbf{k}\cdot\mathbf{r}_3}) \\ \gamma(1 + e^{i\mathbf{k}\cdot\mathbf{r}_1} - e^{i\mathbf{k}\cdot\mathbf{r}_2} - e^{i\mathbf{k}\cdot\mathbf{r}_3}) & \beta(1 + e^{i\mathbf{k}\cdot\mathbf{r}_1} + e^{i\mathbf{k}\cdot\mathbf{r}_2} + e^{i\mathbf{k}\cdot\mathbf{r}_3}) & \gamma(1 - e^{i\mathbf{k}\cdot\mathbf{r}_1} - e^{i\mathbf{k}\cdot\mathbf{r}_2} + e^{i\mathbf{k}\cdot\mathbf{r}_3}) \\ \gamma(1 - e^{i\mathbf{k}\cdot\mathbf{r}_1} + e^{i\mathbf{k}\cdot\mathbf{r}_2} - e^{i\mathbf{k}\cdot\mathbf{r}_3}) & \gamma(1 - e^{i\mathbf{k}\cdot\mathbf{r}_1} - e^{i\mathbf{k}\cdot\mathbf{r}_2} + e^{i\mathbf{k}\cdot\mathbf{r}_3}) & \beta(1 + e^{i\mathbf{k}\cdot\mathbf{r}_1} + e^{i\mathbf{k}\cdot\mathbf{r}_2} + e^{i\mathbf{k}\cdot\mathbf{r}_3}) \end{pmatrix}$$

$$\beta = -\left(\frac{2}{3}\alpha_\phi + \frac{1}{3}\alpha_s\right)$$

$$\gamma = \left(\frac{1}{3}\alpha_\phi - \frac{1}{3}\alpha_s\right)$$

and $*$ denotes the conjugate transpose of a matrix.

The matrix is Hermitian.

5 Phonon Spectra

Figure 1 shows the phonon dispersion relation along the $L-\Gamma-X-L$ symmetry lines of the fcc lattice for $\alpha_s = 1$, $\alpha_\phi = 1/4$, and $M_1 = M_2 = 1$. The Matlab code that performed these calculations is included in Appendix B.

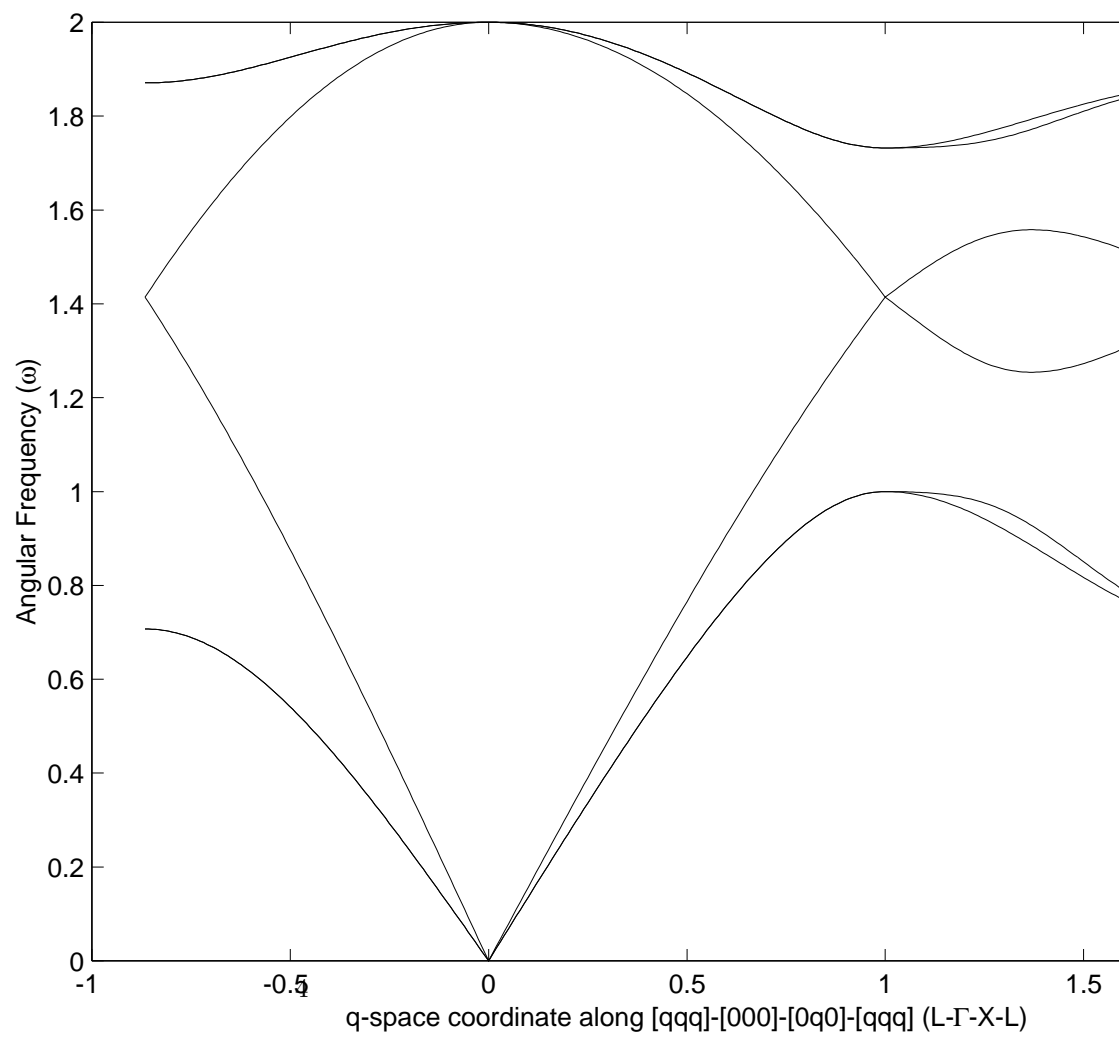
6 Atomic Motion

At Γ , for $\omega = 0$ the eigenvectors are

$$\begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}$$

and for $\omega = 2$, the eigenvectors ϵ are

$$\begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ -1 \end{pmatrix}$$



There are two modes at Γ .

The lowest modes at X have $\omega = 1$ and eigenvectors

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

The highest modes at X have $\omega = \sqrt{3}$ and eigenvectors

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ -1 \\ 0 \end{pmatrix}$$

At Γ and L , the acoustic modes have Ga and As moving perfectly in phase with each other and the optical modes have the Ga and As moving π radians out of phase with each other.

The lowest modes at L have $\omega = \frac{1}{\sqrt{2}}$ and eigenvectors

$$\begin{pmatrix} 2 \\ -2 \\ -1 \\ 1 \\ -1 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \\ -1 \\ 1 \end{pmatrix}$$

The highest modes at L have $\omega = \sqrt{\frac{7}{2}}$ and eigenvectors

$$\begin{pmatrix} 2 \\ 2 \\ -1 \\ -1 \\ -1 \\ -1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}$$

Strangely, at L , the highest mode is in phase and the lowest mode is out of phase.

A Symbolic Computation of the Dynamical Matrix

We use mathematica to calculate the dynamical matrix symbolically. The code follows.

In[25]:=

(* Calculate the dynamical matrix. *)
d[k] // FullSimplify

$$\begin{aligned}
 \text{Out}[25]= & \left\{ \left\{ 0, \frac{1}{3} \left(E^{-I k \cdot (-a_1)} + E^{-I k \cdot (-a_2)} + E^{-I k \cdot (-a_3)} \right) (-\alpha_s - 2 \alpha_\phi), \right. \right. \\
 & 0, \frac{1}{3} \left(-E^{-I k \cdot (-a_1)} + E^{-I k \cdot (-a_2)} + E^{-I k \cdot (-a_3)} \right) (\alpha_s - \alpha_\phi), \\
 & 0, \frac{1}{3} \left(E^{-I k \cdot (-a_1)} - E^{-I k \cdot (-a_2)} + E^{-I k \cdot (-a_3)} \right) (\alpha_s - \alpha_\phi) \left. \right\}, \\
 & \left\{ \frac{1}{3} \left(E^{-I k \cdot a_1} + E^{-I k \cdot a_2} + E^{-I k \cdot a_3} \right) (-\alpha_s - 2 \alpha_\phi), 0, \right. \\
 & \left. \frac{1}{3} \left(-E^{-I k \cdot a_1} + E^{-I k \cdot a_2} + E^{-I k \cdot a_3} \right) (\alpha_s - \alpha_\phi), 0, \frac{1}{3} \left(E^{-I k \cdot a_1} - E^{-I k \cdot a_2} + E^{-I k \cdot a_3} \right) \right\} \\
 & \left\{ 0, \frac{1}{3} \left(-E^{-I k \cdot (-a_1)} + E^{-I k \cdot (-a_2)} + E^{-I k \cdot (-a_3)} \right) (\alpha_s - \alpha_\phi), \right. \\
 & 0, \frac{1}{3} \left(E^{-I k \cdot (-a_1)} + E^{-I k \cdot (-a_2)} + E^{-I k \cdot (-a_3)} \right) (-\alpha_s - 2 \alpha_\phi), \\
 & 0, \frac{1}{3} \left(E^{-I k \cdot (-a_1)} + E^{-I k \cdot (-a_2)} - E^{-I k \cdot (-a_3)} \right) (\alpha_s - \alpha_\phi) \left. \right\}, \\
 & \left\{ \frac{1}{3} \left(-E^{-I k \cdot a_1} + E^{-I k \cdot a_2} + E^{-I k \cdot a_3} \right) (\alpha_s - \alpha_\phi), 0, \frac{1}{3} \left(E^{-I k \cdot a_1} + E^{-I k \cdot a_2} + E^{-I k \cdot a_3} \right) \right. \\
 & 0, \frac{1}{3} \left(E^{-I k \cdot a_1} + E^{-I k \cdot a_2} - E^{-I k \cdot a_3} \right) (\alpha_s - \alpha_\phi), 0 \left. \right\}, \\
 & \left\{ 0, \frac{1}{3} \left(E^{-I k \cdot (-a_1)} - E^{-I k \cdot (-a_2)} + E^{-I k \cdot (-a_3)} \right) (\alpha_s - \alpha_\phi), \right. \\
 & 0, \frac{1}{3} \left(E^{-I k \cdot (-a_1)} + E^{-I k \cdot (-a_2)} - E^{-I k \cdot (-a_3)} \right) (\alpha_s - \alpha_\phi), \\
 & 0, \frac{1}{3} \left(E^{-I k \cdot (-a_1)} + E^{-I k \cdot (-a_2)} + E^{-I k \cdot (-a_3)} \right) (-\alpha_s - 2 \alpha_\phi) \left. \right\}, \\
 & \left\{ \frac{1}{3} \left(E^{-I k \cdot a_1} - E^{-I k \cdot a_2} + E^{-I k \cdot a_3} \right) (\alpha_s - \alpha_\phi), 0, \frac{1}{3} \left(E^{-I k \cdot a_1} + E^{-I k \cdot a_2} - E^{-I k \cdot a_3} \right) \right. \\
 & \left. 0, \frac{1}{3} \left(E^{-I k \cdot a_1} + E^{-I k \cdot a_2} + E^{-I k \cdot a_3} \right) (-\alpha_s - 2 \alpha_\phi), 0 \right\}
 \end{aligned}$$

B Calculation of the Phonon Spectra

B.1 gaas_kent

```
function gaas_kent

%pick an odd number, please
points = 101;

a = 1; %length of side of unit cube in cm.

GammaX = linspace(0,1,points);
XL = linspace(1,1+sqrt(3)/2,points);
counter = [linspace(-sqrt(3)/2,0,points) GammaX(2:points) XL(2:points)] ;

% Direction L to Gamma to X to L
z = zeros(1,points);
X = linspace(0,2*pi/a,points);
Lx = linspace(0, pi/a,points);
Ly = linspace(2*pi/a, pi/a,points);
Lz = linspace(0,pi/a,points);
kx = [linspace(pi/a,0,points) z(2:points) Lx(2:points)];
ky = [linspace(pi/a,0,points) X(2:points) Ly(2:points)];
kz = [linspace(pi/a,0,points) z(2:points) Lz(2:points)];

for loop=1:(3*points-2)
    omega(:,loop) = sort(eig(dyngaas_kent(kx(loop),ky(loop),kz(loop))));
end

w1=abs(sqrt(omega(1,:)));
w2=abs(sqrt(omega(2,:)));
w3=abs(sqrt(omega(3,:)));
w4=abs(sqrt(omega(4,:)));
w5=abs(sqrt(omega(5,:)));
w6=abs(sqrt(omega(6,:)));

% Modes at Gamma, X and L
[V,D]=eig(dyngaas_kent(0,0,0))
[V,D]=eig(dyngaas_kent(0,2*pi/a,0))
[V,D]=eig(dyngaas_kent(pi/a,pi/a,pi/a))

hold off;
plot(counter,w1, ...
      counter,w2, ...
      counter,w3, ...
      counter,w4, ...
```

```

        counter,w5, ...
        counter,w6,'MarkerSize',3)

xlabel('q-space coordinate along [qqq]-[000]-[0q0]-[qqq] (L-\Gamma-X-L)');
ylabel('Angular Frequency (\omega)');
hold on;

```

B.2 dyngaas_kent

```

function MD = dyngaas_kent(kx,ky,kz);

% Fundamental constants, lattice spacing, masses, springs

a = 1; %length of side of unit cube in cm.
m1 = 1; %Gallium mass in grams
m2 = 1; %Arsenic mass in grams
alpha_s = 1;
alpha_phi = 0.25;

% Lattice vectors, k vector, mass matrix

a1 = a*[1 1 0]'/2;
a2 = a*[1 0 1]'/2;
a3 = a*[0 1 1]'/2;
k = [kx ky kz];
mass = [ m1 0 0 0 0 0 ;
         0 m2 0 0 0 0 ;
         0 0 m1 0 0 0 ;
         0 0 0 m2 0 0 ;
         0 0 0 0 m1 0 ;
         0 0 0 0 0 m2 ] ;
minv = inv(mass);

% The terms of the dynamical matrix D.
% First, all the diagonal elements

D1x1x = 4*alpha_phi + 4*(alpha_s - alpha_phi)/3;
D1y1y = D1x1x;
D1z1z = D1x1x;
D2x2x = D1x1x;
D2y2y = D1x1x;
D2z2z = D1x1x;

D1x1y = 0;
D1x1z = 0;

```

```

D1y1z = 0;

D2x2y = 0;
D2x2z = 0;
D2y2z = 0;

% Now, the crossterms D1_2_ and stuff

Da = -(alpha_s + 2*alpha_phi)/3;
Db = (alpha_phi - alpha_s)/3;
eka1 = exp(-i*k*a1);
eka2 = exp(-i*k*a2);
eka3 = exp(-i*k*a3);
C = 1 + eka1 + eka2 + eka3;

D1x2x = Da*C';
D1y2y = Da*C';
D1z2z = Da*C';

D1x2y = Db + Db*eka1' - Db*eka2' - Db*eka3';
D1x2z = Db - Db*eka1' + Db*eka2' - Db*eka3';
D1y2z = Db - Db*eka1' - Db*eka2' + Db*eka3';

D2x1y = Db + Db*eka1 - Db*eka2 - Db*eka3;
D2x1z = Db - Db*eka1 + Db*eka2 - Db*eka3;
D2y1z = Db - Db*eka1 - Db*eka2 + Db*eka3;

% The Dynamical Matrix -- the form from the notes
% Remember that ' acting on a scalar takes the complex conjugate
%      1x      2x      1y      2y      1z      2z

D = [ D1x1x  D1x2x  D1x1y  D1x2y  D1x1z  D1x2z ;
      D1x2x' D2x2x  D2x1y  D2x2y  D2x1z  D2x2z ;
      D1x1y' D2x1y' D1y1y  D1y2y  D1y1z  D1y2z ;
      D1x2y' D2x2y' D1y2y' D2y2y  D2y1z  D2y2z ;
      D1x1z' D2x1z' D1y1z' D2y1z' D1z1z  D1z2z ;
      D1x2z' D2x2z' D1y2z' D2y2z' D1z2z' D2z2z ];

% The output of this script is (Inverse of the mass matrix)*(D) thus we
% can just find the eigenfrequencies by using eig() on the output of this
% script, e.g. eig(dyngaas(0,0,0))

MD = minv*D;

```