Problem Set #4

Solutions

1. The electric field gradient tensor.

In nuclear magnetic resonance and related spectroscopies in solids, the nuclear electric quadrupole interaction often plays an important role. The interaction energy involves a tensor that describes the gradient of the electric field at a lattice point. The field is produced by neighboring ionic charges. The field gradient tensor is a second order tensor (3 x 3 matrix) whose elements are the second partial derivatives of the electrostatic potential $V = \sum_{\textbf{neighbors}} V(\vec{\mathbf{r}}_{\text{neighbor}})$ at a lattice point:

$$\mathbf{V}_2 = \begin{pmatrix} V_{xx} & V_{xy} & V_{xz} \\ V_{yx} & V_{yy} & V_{yz} \\ V_{zx} & V_{zy} & V_{zz} \end{pmatrix} \text{ where, for example, } V_{xx} = \frac{\partial^2 V}{\partial x^2}, \quad V_{xy} = \frac{\partial^2 V}{\partial x \, \partial y} \text{ etc.}$$

(a) What does Laplace's law imply about Tr $\mathbf{V}_2$?

Laplace's law: $\nabla^2 V = \dfrac{\partial^2 V}{\partial x^2} + \dfrac{\partial^2 V}{\partial y^2} + \dfrac{\partial^2 V}{\partial z^2} = V_{xx} + V_{yy} + V_{zz} = \text{Tr}\,\mathbf{V}_2 = 0$.

(It is assumed that there are no charges at the point where the electric field gradient is being evaluated.)

(b) In a particular coordinate system, the field gradient tensor has the following form for a certain crystal:

$$\mathbf{V}_2 = \frac{1}{4}\begin{pmatrix} 3a+b & \sqrt{3}(a-b) & 0 \\ \sqrt{3}(a-b) & a+3b & 0 \\ 0 & 0 & -4(a+b) \end{pmatrix}$$

Find the eigenvalues and corresponding eigenvectors in this coordinate system.

Set up and solve the secular equation (taking into account the factor ¼):

$$\begin{vmatrix} 3a+b-4\lambda & \sqrt{3}(a-b) & 0 \\ \sqrt{3}(a-b) & a+3b-4\lambda & 0 \\ 0 & 0 & -4(a+b)-4\lambda \end{vmatrix} = 0$$

$$-(4a+4b+4\lambda)(3a+b-4\lambda)(a+3b-4\lambda) + (4a+4b+4\lambda)\cdot 3(a-b)^2 = 0$$

$$-(4a+4b+4\lambda)\left(3a^2+3b^2+9ab+ab-16\lambda(a+b)+16\lambda^2-3a^2-3b^2+6ab\right) = 0$$

$$-(4a+4b+4\lambda)\left(16\lambda^2 - 16(a+b)\lambda + 16ab\right) = 0$$

$$-(a+b+\lambda)\left(\lambda^2 - (a+b)\lambda + ab\right) = 0$$

The first factor gives the root $\lambda_3 = -(a+b)$.

The remaining two eigenvalues are the roots of the quadratic:

$$\lambda = \frac{(a+b) \pm \sqrt{(a+b)^2 - 4ab}}{2} = \frac{(a+b) \pm \sqrt{(a-b)^2}}{2} = \frac{(a+b) \pm (a-b)}{2}$$

Thus, $\lambda_1 = a$ and $\lambda_2 = b$.

To get the eigenvector for $\lambda_1 = a$,

$$\frac{1}{4}\begin{pmatrix} 3a+b & \sqrt{3}(a-b) & 0 \\ \sqrt{3}(a-b) & a+3b & 0 \\ 0 & 0 & -4(a+b) \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = a\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

$$(3a+b-4a)c_1 + \sqrt{3}(a-b)c_2 = 0$$

$$-(a-b)c_1 + \sqrt{3}(a-b)c_2 = 0 \qquad \Rightarrow \qquad c_2 = \frac{1}{\sqrt{3}}c_1$$

$$c_1^2 + c_2^2 = c_1^2 + \frac{1}{3}c_1^2 = \frac{4}{3}c_1^2 = 1 \;\Rightarrow \qquad c_1 = \frac{\sqrt{3}}{2}$$

$$\mathbf{x}^1 = \frac{\sqrt{3}}{2}\hat{\mathbf{e}}_1 + \frac{1}{2}\hat{\mathbf{e}}_2$$

To get the eigenvector for $\lambda_2 = b$,

$$\frac{1}{4}\begin{pmatrix} 3a+b & \sqrt{3}(a-b) & 0 \\ \sqrt{3}(a-b) & a+3b & 0 \\ 0 & 0 & -4(a+b) \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = b\begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

$$(3a+b-4b)c_1 + \sqrt{3}(a-b)c_2 = 0$$

$$3(a-b)c_1 + \sqrt{3}(a-b)c_2 = 0 \quad \Rightarrow \quad c_2 = -\sqrt{3}\,c_1$$

$$c_1^2 + c_2^2 = c_1^2 + 3c_1^2 = 4c_1^2 = 1 \quad \Rightarrow \quad c_1 = -\frac{1}{2}$$

$$\mathbf{x}^2 = -\frac{1}{2}\hat{\mathbf{e}}_1 + \frac{\sqrt{3}}{2}\hat{\mathbf{e}}_2$$

The sign of $\mathbf{x}^2$ is chosen so that the matrix **S** (next section) takes the form of a rotation.

The eigenvector for $\lambda_3 = -(a+b)$ is simply $\mathbf{x}^3 = \hat{\mathbf{e}}_3$.

(c) Use your eigenvectors to construct the transformation matrix that diagonalizes $\mathbf{V}_2$ and verify by a similarity transformation that your matrix works.

The matrix is $\mathbf{S} = \begin{pmatrix} * & * & * \\ \mathbf{x}^1 & \mathbf{x}^2 & \mathbf{x}^3 \\ * & * & * \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Then the similarity transformation is

$$\mathbf{S}^{-1}\mathbf{V}_2\mathbf{S} = \frac{1}{4}\begin{pmatrix} \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 3a+b & \sqrt{3}(a-b) & 0 \\ \sqrt{3}(a-b) & a+3b & 0 \\ 0 & 0 & -4(a+b) \end{pmatrix}\begin{pmatrix} \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \frac{1}{4}\begin{pmatrix} \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} (3a+b)\frac{\sqrt{3}}{2}+(a-b)\frac{\sqrt{3}}{2} & -(3a+b)\frac{1}{2}+(a-b)\frac{3}{2} & 0 \\ (a-b)\frac{3}{2}+(a+3b)\frac{1}{2} & -(a-b)\frac{\sqrt{3}}{2}+(a+3b)\frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & -4(a+b) \end{pmatrix}$$

$$= \frac{1}{4}\begin{pmatrix} (3a+b)\frac{3}{4}+(a-b)\frac{3}{4} + (a-b)\frac{3}{4}+(a+3b)\frac{1}{4} & -(3a+b)\frac{\sqrt{3}}{4}+(a-b)\frac{3\sqrt{3}}{4} - (a-b)\frac{\sqrt{3}}{4}+(a+3b)\frac{\sqrt{3}}{4} & 0 \\ -(3a+b)\frac{\sqrt{3}}{4}-(a-b)\frac{\sqrt{3}}{4} + (a-b)\frac{3\sqrt{3}}{4}+(a+3b)\frac{\sqrt{3}}{4} & (3a+b)\frac{1}{4}-(a-b)\frac{3}{4} - (a-b)\frac{3}{4}+(a+3b)\frac{3}{4} & 0 \\ 0 & 0 & -4(a+b) \end{pmatrix}$$

$$\mathbf{S}^{-1}\mathbf{V}_2\mathbf{S} = \frac{1}{4}\begin{pmatrix} 4a & 0 & 0 \\ 0 & 4b & 0 \\ 0 & 0 & -4(a+b) \end{pmatrix} = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & -(a+b) \end{pmatrix}$$

Thus, the similarity transformation diagonalizes the matrix and the diagonal elements are the eigenvalues, as expected.

(d) How is the coordinate system in which $\mathbf{V}_2$ is diagonal related to the original frame?

We can identify the transformation matrix with a rotation:

$$\mathbf{S} = \begin{pmatrix} \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\sin\theta = -\frac{1}{2},\ \cos\theta = \frac{\sqrt{3}}{2} \quad \Rightarrow \quad \theta = -\frac{\pi}{6}$$

Coordinate axes are rotated clockwise around the z-axis by 30^o.

2. RHB Problem 20.1

This problem was assigned in error. I apologize.