Problem Set #4

Due Friday, November 7, 2008

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 $V = \sum_{\textbf{neighbors}} V\left(\vec{\mathbf{r}}_{\text{neighbor}}\right)$ 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 $\mathbf{V}_2$?

(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.

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

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

2. RHB Problem 20.1.

