Massachusetts Institute of Technology

Mathematical Methods for Materials Scientists and Engineers

3.016 Fall 2010

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Problem Set 5: **Out: 4 Oct.** and **Due: 12 Oct.**

Individual assigments should be a combination of your hand-worked solutions and other printed material—they should be placed in the mailbox outside Prof. Carter's door. Email group assignments to 3016-psets(the symbol at)pruffle.mit.edu

For the individual problems indicated as "Handworked", you should work your solutions by hand and show your work. Print the results of software-worked solutions, and staple them to your hand-worked assignments before turning them in.

The following are this week's randomly assigned homework groups. The first member of the group is the "Jomework Jefe" who will be in charge of setting up work meetings and have responsibility for turning in the group's homework notebook. If some some reason, the first member in the list is incapacitated, recalcitrant, or otherwise unavailable, then the second member should take that position. *Attention slackers:* The Jefe should include a line at the top of your notebook listing the group members that participated in the notebook's production; only those listed will receive credit. Group names are boldfaced text.

Allobroges: *jschein, ckopp, eperry4, ssluo*

Aquitani: *jchenlia, ronrose, vtrevino, aliciac*

Carnutes: *spuranam, m_gibson, nsinatra, changey*

Catalauni: *tsmickel, elomeli, amelanie, ernmart*

Helvetii: *andy_c, dimitri_, viviand, pmelo*

Lexovii: *ezuniga, llena, mcjasso, aypark*

Petrocorii: *tsarathi, jrm90, chandrak, sojung*

Redones: *yhelen,hekopp, bwee, msee*

Individual (Handworked) Exercise I5-1

For matrix given below, find its form in a coordinate system after it has undergone two sequential rotations: first it is rotated by θ around the x-axis and then followed by a θ rotation around the z-axis.

$$\begin{pmatrix} 1 & 4 & -2 \\ 4 & 1 & 2 \\ -2 & 2 & -2 \end{pmatrix}$$

Compute its eigenvalues and eigenvectors in the initial and in the final (i.e., after both rotations) coordinate systems.

Do the same exercise, but exchange the order of the rotations (i.e., first rotated by θ around the z-axis and then θ around the x-axis.

Individual Exercise I5-2

Purple is half blue and half red. Yellow is half red and half green. Cyan is half green and half blue. Define a unit normal vector in the $r - g - b$ space as $\hat{n} = (r, g, b)/\sqrt{r^2 + b^2 + g^2}$ Find a matrix that converts a vector given as $\hat{n}$ to a vector given as purple, yellow, cyan (p, o, c). Is the magnitude of the vector changed by the matrix transformation? Find the eigenvectors of this matrix. Visualize the properties of these eigenvectors.

Individual Exercise I5-3

Experimental analysis of the processes that take place as a battery is charged or discharged is commonly obtained with impedance spectroscopy. In impedance spectroscopy the electronic behavior of a material is analyzed by observing its voltage/current response as a function of frequency For example, the voltage will be changed with some frequency ω: $V(t;\omega) = V_o + V_{\text{amp}} \cos(\omega t)$, and the current is measured as a function of time and frequency: $I(t;\omega) =$. The impedance is the ratio of the voltage to the current $Z(\omega) = V(t;\omega)/I(t,\ omega)$. The impedance is a complex number: the magnitude of the impedance is the circuit's resistance and the imaginary part is the "lag" of the current's oscillation behind the that of the voltage.

The simplest model the behavior of an electrode/electrolyte interface is the simple circuit of a resistor and a capacitor in parallel, see Fig. 2 at `http://en.wikipedia.org/wiki/Electrochemical_impedance_spectroscopy` which also has an example of a Nyquist plot).

The impedance of this simple circuit is given by

$$Z(\omega) = \frac{R}{1 + \imath RC\omega}$$

In a Nyquist plot, the negative of the imaginary part of $Z(\omega)$ is plotted on the vertical axis and the real part is plotted on the horizontal axis for all values of ω.

1. Visualize the Nyquist plots for different values of RC. It is probably a good idea to non-dimensionalize the Z by dividing by R.

2. Because information about the measurement's driving frequency, ω, is not plotted, I believe the Nyquist plots are not as informative as they might be. Find a way to improve the Nyquist plot by introducing a means of displaying frequency along with the real and imaginary parts of the impedance.

Group Exercise G5-1

The electrical conductivity, σ, is a second-rank tensor property that relates the current density vector, $\vec{j}$, to the electric field, $\vec{E}$ by

$$\vec{j} = \sigma \vec{E} \tag{1}$$

In a particular coordinate system, the electrical conductivity of a tetragonal tin single crystal was measured to be:

$$\sigma = \begin{pmatrix} 8.55 & 1.55 & 0 \\ 1.55 & 8.55 & 0 \\ 0 & 0 & 10.1 \end{pmatrix} \times 10^6 \quad (\text{ohm} \cdot \text{m})^{-1} \tag{2}$$

1. Find the current density vector and its magnitude when an electric field of 0.1 V/m is applied parallel to the "2" axis in this coordinate frame.

2. Find the electric field, $\vec{E}$, which will create a current density $\vec{j}$ of magnitude 10^{-6} coulomb $\text{s}^{-1}\,\text{m}^{-2}$ flowing *in the directions* x- y-, and z-directions.

3. The vector

   $$\hat{E} = \begin{pmatrix} \cos\phi \cos\theta \\ \cos\phi \sin\theta \\ \sin\phi \end{pmatrix}$$

   represents electric fields with unit magnitude in all directions (i.e., the unit sphere). The angle, α, between two vectors $\vec{j}$ and $\vec{E}$ is given by

   $$\cos\alpha = \frac{\vec{j} \cdot \vec{E}}{|\vec{E}|\,|\vec{j}|}$$

   Plot the angle between the current density and the electric field for for all the unit vectors, $\hat{E}$, given above. In other words, plot $\alpha(\theta, \phi)$.

4. Find the eigenvalues and eigenvectors of tin's electrical conductivity.

5. Demonstrate that, if an electric field is applied in the direction of one of the eigenvectors calculated above, the current density will be parallel to the electric field.

6. The heating rate density (or power dissipation density) is given by $\vec{E} \cdot \vec{j}$. A tensor can be represented by the surface that gives, for any direction, the magnitude of the applied field that produces a unit density (in this case unit power dissipation density). For this problem, this surface is a quadratic form $\vec{E} \cdot \sigma \cdot \vec{E} = 1$, and for all tensors is called "the representation surface." Plot this surface for tin in the original coordinate system and in the principle coordinate system (the eigensystem).

7. Find the conductivity tensors for a cubic single crystal and an orthorhombic single crystal and illustrate their representation surface.