Homework #5 — PHYS 374 — Fall 2006 Professor Victor Yakovenko
Deadline: **Tuesday, October 17, 2006, in class** Office: 2115 Physics

Textbook: Roel Snieder, *A Guided Tour of Mathematical Methods for the Physical Sciences*, Cambridge University Press, 2nd edition, 2004, ISBN 0-521-83492-9

Web page: http://www2.physics.umd.edu/~yakovenk/teaching/

Do not forget to write your name and the homework number!

Ch. 13 Linear Algebra

1. **Projection operators and closure relation**

   Let us consider the vector space of two-component vectors.

   (a) [**2 points**] Calculate the operator $\hat{\mathbf{P}}_1$ of projection along the unit vector

   $$\hat{\boldsymbol{n}}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}. \tag{1}$$

   Write $\hat{\mathbf{P}}_1$ as a 2×2 matrix. See Problem 13.1.g in the textbook as an example.

   (b) [**2 points**] Calculate the operator $\hat{\mathbf{P}}_2$ of projection along the unit vector

   $$\hat{\boldsymbol{n}}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix}. \tag{2}$$

   Write $\hat{\mathbf{P}}_2$ as a 2×2 matrix.

   (c) [**2 points**] Show that the closure relation (13.13) is satisfied:

   $$\hat{\mathbf{P}}_1 + \hat{\mathbf{P}}_2 = \mathbf{I}, \tag{3}$$

   where $\mathbf{I}$ is the unity matrix.

2. **Eigenvalues and eigenvectors of a 2 × 2 matrix**

   (a) [**4 points**] Calculate the eigenvalues $\lambda_{1,2}$ of the matrix

   $$\begin{pmatrix} a & b \\ b & -a \end{pmatrix}. \tag{4}$$

   Sketch a plot of $\lambda_1(a)$ and $\lambda_2(a)$ as functions of a from negative $a \ll -|b|$ to positive $a \gg |b|$ for a fixed $b \neq 0$.

   (b) [**4 points**] Calculate the normalized eigenvectors $\hat{\boldsymbol{v}}_{1,2}$ of this matrix for general values of a and b.

   Obtain the eigenvectors $\hat{\boldsymbol{v}}_{1,2}$ in the limiting cases of negative $a \ll -|b|$, positive $a \gg |b|$, and $a = 0$. Write these vectors on top of your sketch in Part 2a in the corresponding limits. Describe qualitatively what happens to the eigenvectors when a changes from $-\infty$ to $+\infty$ for a fixed $b \neq 0$.

3. Exponential function of a matrix

(a) [**3 point**] Consider the matrix

$$\mathbf{M} = \begin{pmatrix} \theta & 0 \\ 0 & -\theta \end{pmatrix}. \tag{5}$$

Calculate the matrix $e^{\mathbf{M}}$. Write the answer as a 2×2 matrix.

(b) [**4 point**] Consider the matrix

$$\mathbf{N} = \begin{pmatrix} 0 & \theta \\ \theta & 0 \end{pmatrix}. \tag{6}$$

Calculate the matrix $e^{\mathbf{N}}$. Write the answer as a 2×2 matrix.

You can solve this problem using the method described in Ch. 13.5.

Alternatively, you can use the following trick. Calculate $\mathbf{N}^2$, $\mathbf{N}^3$, $\mathbf{N}^4$, etc. and observe a pattern. Use the Taylor expansions of $\cosh(\theta)$ and $\sinh(\theta)$ in powers of θ to obtain the answer (see HW#2 Problem 2).

4. Normal vibrational modes of the CO_2 molecule

Let us consider three masses connected by springs as shown in Fig. 13.6 in the textbook. This is a model of the CO_2 molecule, which is a linear molecule O=C=O with carbon at the center and oxygens on the sides. **Unlike in the textbook, we consider the case where the central mass is M, whereas the side masses are m, which is a more realistic model of CO_2 with $M \neq m$.** As in the textbook, we consider motion of the atoms only in the x direction.

(a) [**2 points**] Write down the equations of motion for the three atoms similar to Eq. (13.60) (but different!).

(b) [**8 points**] Consider motion of the atoms without external forces $\boldsymbol{F} = 0$. Find the frequencies $\omega_{1,2,3}$ and the vectors $\boldsymbol{v}_{1,2,3}$ of the normal modes of vibration. Make sure that your results, calculated for $M \neq m$, agree with the results in the textbook for $M = m$.

(c) [**8 points**] Answer the questions (e), (f), (g), (h) from Ch. 13.6 of the textbook, as applied to our problem with $M \neq m$.

(d) [**6 points**] Find out what happens to the frequencies and vectors of the normal modes in the cases $M \gg m$ and $M \ll m$. Explain the results qualitatively.

(e) [**4 points**] The considered system has a reflection symmetry with respect to the central atom (carbon in O=C=O). Show that the reflection operator $\hat{R}$ can be written as

$$x_1 \to -x_3, \quad x_2 \to -x_2, \quad x_3 \to -x_1. \tag{7}$$

Apply the operator $\hat{R}$ to the vectors $\boldsymbol{v}_{1,2,3}$ of the normal modes and observe how they transform upon reflection. Which vectors are symmetric and which antisymmetric upon reflection?

(f) [**6 points**] Suppose a periodic in time force

$$\boldsymbol{F} = \begin{pmatrix} F_1 \\ F_2 \\ F_3 \end{pmatrix} e^{-i\omega t} \tag{8}$$

is applied to the three atoms. Let us introduce the "acceleration" vector

$$\boldsymbol{A} = \begin{pmatrix} F_1/m \\ F_2/M \\ F_3/m \end{pmatrix} \tag{9}$$

Shown that the displacements of the atoms in response to the external force can be written as

$$\boldsymbol{x} = \sum_{n=1}^{3} \frac{\hat{\boldsymbol{v}}_n(\hat{\boldsymbol{v}}_n \cdot \boldsymbol{A})}{\omega_n^2 - \omega^2}. \tag{10}$$

This formula is similar, but different from Eq. (13.67), because in our case $M \neq m$. Describe qualitatively what happens when ω approaches to one of the frequencies $\omega_{1,2,3}$ of the normal modes. What is the name of this phenomenon?