

# PHYS 501: Mathematical Physics I

Fall 2011

## Homework #2

(Due: October 21, 2011)

1. An electrical network consists of  $N$  interconnected nodes. Each pair of nodes  $(i, j)$  is connected by a resistor of resistance  $R_{ij} = \min(i, j) + 2\max(i, j)$ , for  $i, j = 1, \dots, N$ . Let  $V_i$  be the electrical potential of node  $i$ , and choose the zero level of potential to set  $V_1 = 0$ . Then Kirchoff's laws for the other nodes in the network can be conveniently written as

$$\sum_{\substack{j=1 \\ j \neq i}}^N \frac{V_j - V_i}{R_{ij}} = I_i,$$

for  $i = 2, \dots, N$ , where  $I_i$  is the current flowing from node  $i$  to some external circuit. Suppose  $N = 100$  and the external connection is such that current flows out of node 2 and back into node 1, so  $I_1 = -1$ ,  $I_2 = 1$ , and  $I_i = 0$  for  $i > 2$ . By solving the above  $(N - 1)$ -dimensional matrix equation (e.g. using the *Numerical Recipes* routine `gaussj`, or `solve` in Python, or `linsolve` in Matlab), calculate the total resistance between nodes 1 and 2.

2. (a) Using the routines described in *Numerical Recipes* (provided online on `newton`), or the `lu` function in Python or Matlab, apply LU decomposition to the  $n \times n$  matrix  $A$  stored (one element per line, in row order, with the dimension  $n$  preceding the data) in the file <http://www.physics.drexel.edu/students/courses/physics-501/hw2.2.dat> on the course Web page. Carry out the following operations:
  - (i) Calculate the determinant of  $A$ .
  - (ii) Calculate the inverse of  $A$  and print out the first 20 elements of the first row and the last 20 elements of the last row. (Don't print out the entire inverse matrix!)
  - (iii) Multiply  $A$  by its inverse and call the product  $P$ . This should be the unit matrix. Quantify the overall error in the inversion procedure by calculating the largest deviation of any diagonal element of  $P$  from 1, and also the magnitude of the largest off-diagonal element.
3. The data file <http://www.physics.drexel.edu/students/courses/physics-501/hw2.3.dat> on the course Web page contains (hypothetical) experimental data on the measurement of a function  $y(x)$ . The  $N$  data points are arranged, one measurement per line, in the format

$x_i$

$y_i$  (measured)

$\sigma_i$

where  $\sigma_i$  is an estimate of the uncertainty in the  $i$ -th measurement. It is desired to find the least-square fit to the data by polynomials of the form

$$y(x) = \sum_{j=1}^m a_j x^{j-1},$$

for specified values of  $m$ , by minimizing the quantity

$$\chi^2 = \sum_{i=1}^N \left[ \frac{y_i - \sum_{j=1}^m a_j x^{j-1}}{\sigma_i} \right]^2.$$

As discussed in class (and in *Numerical Recipes*, pp 671–676), write down the overdetermined design matrix equation that results from writing  $y(x_i) = y_i$ ,

$$\mathbf{A}\mathbf{a} = \mathbf{b},$$

where  $A_{ij} = x_i^{j-1}/\sigma_i$ ,  $b_i = y_i/\sigma_i$  (so the measurement uncertainties are included in each row), and  $\mathbf{a}$  is the vector of unknown coefficients. Solve this system using singular value decomposition (`svdcmp` in *Numerical Recipes*, `svd` in Python or Matlab) to obtain the best fitting polynomial for each of the cases  $m = 2, 4, 7$ , and  $13$ . For each  $m$ , give the values of  $a_j$  and  $\chi^2$ , and plot the data and the best fit on a single graph.

4. We wish to approximate the energy eigenfunctions of a one-dimensional square well by expanding them in terms of a *finite* ( $N$ -dimensional) subset of harmonic oscillator wavefunctions. The square well is defined by the potential

$$V(x) = \begin{cases} 0 & (|x| < a), \\ V_0 & (|x| > a). \end{cases}$$

The harmonic oscillator potential is  $V_{ho}(x) = \frac{1}{2}kx^2$ , where we will take  $k = 2V_0/a^2$  here. As discussed in class, solving the problem entails diagonalization (e.g. using the *Numerical Recipes* functions `tred2` and `tqli`) of the Hamiltonian matrix  $H = (h_{nm})$ , where

$$h_{nm} = \langle n|H|m\rangle = \int dx \phi_n^*(x) \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \phi_m(x)$$

and  $\phi_n(x)$  is the  $n$ -th harmonic oscillator wavefunction:

$$\phi_n(x) = \left( \frac{\beta^2}{\pi} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-\frac{1}{2}\beta^2 x^2} H_n(\beta x),$$

with  $\beta^4 = mk/\hbar^2$ .

Use the recurrence relations given in Riley & Hobson, p. 373, to generate the  $H_n$ , and the differential relations (same page) along with the trapezoidal rule, where needed, to compute the matrix elements  $h_{nm}$ .

Hence, by diagonalizing the matrix  $H$ , determine the first (and only) two energy levels  $E_0$  and  $E_1$  of a square well with  $V_0 a^2 = 2\hbar^2/m$ , for three different values of  $N$ : (a) use  $\phi_0, \dots, \phi_4$  as a basis ( $N = 5$ ); (b) use  $\phi_0, \dots, \phi_9$  ( $N = 10$ ); and (c) use  $\phi_0, \dots, \phi_{19}$  ( $N = 20$ ). In each case, compare your answers with the exact values

$$E_0 = 0.53 \frac{\hbar^2}{ma^2}, \quad E_1 = 1.80 \frac{\hbar^2}{ma^2}.$$