Computational Quantum Physics – Exercise 3

Problem 1 *Calculate the energy eigenvalues of the anharmonic oscillator numerically*

The Hamiltonian of the anharmonic oscillator is given by

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + Kx^4$$

The harmonic part of this Hamiltonian can be written as

$$H_{harm} = \hbar\omega(a^\dagger a + \frac{1}{2})$$

with the operators a and $a^\dagger$ defined by

$$a = \sqrt{\frac{m\omega}{2\hbar}}x + \frac{ip}{\sqrt{2m\hbar\omega}}$$
$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}x - \frac{ip}{\sqrt{2m\hbar\omega}}$$

The eigenstates $|n\rangle$ of the count operator $N = a^\dagger a$ build a natural set of basis states for the harmonic oscillator. Their energy eigenvalues are given by $\langle n|H_{harm}|n\rangle = \hbar\omega(n + \frac{1}{2})$. Using the definitions of a and $a^\dagger$ one can write the anharmonic part of the hamiltonian as

$$Kx^4 = \frac{K\hbar^2}{4m^2\omega^2}(a + a^\dagger)^4$$

Using the commutaion relation $[a, a^\dagger] = 1$ one can obtain the nonzero matrix elements of H_{anharm}

$$\begin{aligned}\langle n+4|(a+a^\dagger)^4|n\rangle &= \sqrt{(n+1)(n+2)(n+3)(n+4)} \\ \langle n+2|(a+a^\dagger)^4|n\rangle &= (4n+6)\sqrt{(n+1)(n+2)} \\ \langle n|(a+a^\dagger)^4|n\rangle &= 3[n^2 + (n+1)^2]\end{aligned}$$

Store the matrix representation M_{ij} of $H = H_{harm} + H_{anharm}$ using a two dimensional array (e.g. using a `boost::ublas::matrix`) and diagonalize it with LAPCK routinne DSYEV (see man page below).

To use the LAPACK routine, you have to link your program with some additional libraries (g++ -lblas -llapack). As the LAPACK routines are FORTRAN routines, you have to link your program also with some additional FORTRAN runtime libraries. The names and paths of these libraries can be found by using the verbose option (−−verbose) of the g77 FORTRAN compiler.

```
      SUBROUTINE DSYEV( JOBZ, UPLO, N, A, LDA, W, WORK, LWORK, INFO )

  -- LAPACK driver routine (version 3.0) --
     Univ. of Tennessee, Univ. of California Berkeley, NAG Ltd.,
     Courant Institute, Argonne National Lab, and Rice University
     June 30, 1999

     .. Scalar Arguments ..
```

```
    CHARACTER          JOBZ, UPLO
    INTEGER            INFO, LDA, LWORK, N
   ..
   .. Array Arguments ..
    DOUBLE PRECISION   A( LDA, * ), W( * ), WORK( * )
   ..

Purpose
=======

DSYEV computes all eigenvalues and, optionally, eigenvectors of a
real symmetric matrix A.

Arguments
=========

JOBZ    (input) CHARACTER*1
        = 'N':  Compute eigenvalues only;
        = 'V':  Compute eigenvalues and eigenvectors.

UPLO    (input) CHARACTER*1
        = 'U':  Upper triangle of A is stored;
        = 'L':  Lower triangle of A is stored.

N       (input) INTEGER
        The order of the matrix A.  N >= 0.

A       (input/output) DOUBLE PRECISION array, dimension (LDA, N)
        On entry, the symmetric matrix A.  If UPLO = 'U', the
        leading N-by-N upper triangular part of A contains the
        upper triangular part of the matrix A.  If UPLO = 'L',
        the leading N-by-N lower triangular part of A contains
        the lower triangular part of the matrix A.
        On exit, if JOBZ = 'V', then if INFO = 0, A contains the
        orthonormal eigenvectors of the matrix A.
        If JOBZ = 'N', then on exit the lower triangle (if UPLO='L')
        or the upper triangle (if UPLO='U') of A, including the
        diagonal, is destroyed.

LDA     (input) INTEGER
        The leading dimension of the array A.  LDA >= max(1,N).

W       (output) DOUBLE PRECISION array, dimension (N)
        If INFO = 0, the eigenvalues in ascending order.

WORK    (workspace/output) DOUBLE PRECISION array, dimension (LWORK)
        On exit, if INFO = 0, WORK(1) returns the optimal LWORK.

LWORK   (input) INTEGER
        The length of the array WORK.  LWORK >= max(1,3*N-1).
        For optimal efficiency, LWORK >= (NB+2)*N,
        where NB is the blocksize for DSYTRD returned by ILAENV.

        If LWORK = -1, then a workspace query is assumed; the routine
        only calculates the optimal size of the WORK array, returns
        this value as the first entry of the WORK array, and no error
        message related to LWORK is issued by XERBLA.
```

```
INFO    (output) INTEGER
        = 0:  successful exit
        < 0:  if INFO = -i, the i-th argument had an illegal value
        > 0:  if INFO = i, the algorithm failed to converge; i
              off-diagonal elements of an intermediate tridiagonal
              form did not converge to zero.
```