ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Programming Techniques for Scientific Simulations Exercise 11

HS 10
Prof. M. Troyer

Problem 11.1 Numerical integration

BLAS/LAPACK Installation In case you don't have these libraries on your system yet here are some hints:
If you work on your laptop, install BLAS and LAPACK (e.g. ATLAS, which you can obtain from http://www.netlib.org/atlas/). If you work on one of the computers in the exercise room, BLAS and LAPACK should already be installed. If you work with Mac OS X, you can either install ATLAS or use the pre-installed `veclib` framework by linking with `-framework veclib` instead of the standard BLAS/LAPACK linker options.

Anharmonic oscillator In this exercise we will consider the first quantum mechanical problem in this lecture: we will calculate properties of the anharmonic oscillator. The quantum mechanical description is based on an eigenvalue problem (the stationary Schrödinger equation),

$$H|\Psi\rangle = E|\Psi\rangle \tag{1}$$

where

- $|\Psi\rangle \in \mathcal{H}$ is a vector in some Hilbert space $\mathcal{H}$. It is the *wave function* that describes the properties of a quantum mechanical state.
- H is the Hamilton operator which acts on vectors in $\mathcal{H}$.
- E are the energy eigenvalues.

Further explanations will be given in the exercise class. To solve this problem, we will set up the eigenvalue problem numerically and find the eigenvalues using a LAPACK routine. The Hamiltonian of the anharmonic oscillator is given by

$$\begin{aligned} H &= H_{\text{kinetic}} + H_{\text{harmonic}} + H_{\text{anharmonic}} & (2)\\ &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + Kx^4, & (3) \end{aligned}$$

where x and p are operators that generally do not commute, $xp - px \neq 0$.
The harmonic part of this Hamiltonian can be written as

$$H_{\text{harmonic}} = \hbar\omega(a^\dagger a + \frac{1}{2}) \tag{4}$$

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

$$a = \sqrt{\frac{m\omega}{2\hbar}}x + \frac{ip}{\sqrt{2m\hbar\omega}} \tag{5}$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}x - \frac{ip}{\sqrt{2m\hbar\omega}} \tag{6}$$

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

$$Kx^4 = \frac{K\hbar^2}{4m^2\omega^2}(a + a^\dagger)^4 \tag{7}$$

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

$$\begin{aligned}
\langle n+4|(a+a^\dagger)^4|n\rangle &= \sqrt{(n+1)(n+2)(n+3)(n+4)} &(8)\\
\langle n+2|(a+a^\dagger)^4|n\rangle &= (4n+6)\sqrt{(n+1)(n+2)} &(9)\\
\langle n|(a+a^\dagger)^4|n\rangle &= 3[n^2+(n+1)^2] &(10)
\end{aligned}$$

Numerical solution Store the matrix representation M_{ij} of $H = H_{harm} + H_{anharm}$ in a matrix and diagonalize it with LAPACK routine DSYEV (see the documentation in http://www.netlib.org/lapack/double/dsyev.f). Of course, you will need to choose a finite cutoff for n in order to make the matrix finite. It is also probably a good idea to keep K small - do you understand why?
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 might 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.