Assignment 4

SCP8082721 - QUANTUM INFORMATION AND COMPUTING

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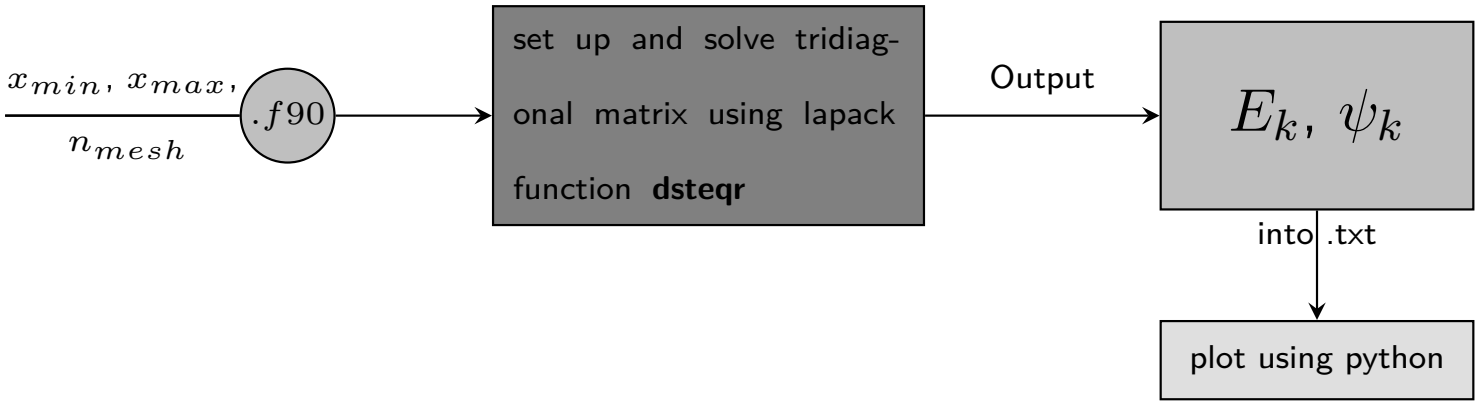
Exc 1: Intro and theory

- solving one dimensional harmonic oscillator

$$\hat{H} = \hat{p}^2/2m + m\omega^2\hat{q}^2/2$$
$$\Rightarrow -\frac{\hbar^2}{2m}\nabla^2\psi(x) + \frac{1}{2}m\omega^2 x^2\psi(x) = E\psi(x)$$

- with $\hat{p} = -i\hbar\partial_x$ and $\hat{q} = x$
- analytic solution for eigenvalues $E_n = (n + 1/2)\omega\hbar$
- using finite differences to solve it numerically
- $-\frac{\hbar^2}{2m}\frac{1}{h^2}\left(\psi_{k+1} + \psi_{k-1}\right) + \frac{\hbar^2}{2m}\frac{2}{h^2}\psi_k + \frac{m\omega^2}{2}x_k^2\psi_k = E\psi_k,$
- (with $h = \Delta x$) $\Rightarrow$ tridiagonal matrix diagonalization

Exc 1: The code




```
xmesh(1) = xmin
h = (xmax-xmin)/DBLE(n_mesh)

do i=1,n_mesh
    xmesh(i+1) =  xmesh(i) + h
end do

sd(:) = -hbar*hbar/(2*m*h*h)

do i=1,n_mesh
    d(i) = hbar*hbar/(2.0*m*h*h)*2 + 1.0/2*m*omega*omega*xmesh(i)*xmesh(i)
end do

call dsteqr('I', n_mesh, d, sd, Z, LDZ, WORK, INFO)
```

Frame: Here I show the main part of the code: setting up of the two vectors corresponding to diagonal and subdiagonal and putting them into the diagonalization function dsteqr, where d is the vector corresponding to the diagonal and sd the subdiagonals; $\hbar, m, \omega = 1$, xmin = -6, xmax = 6, $n_{mesh} = 250$.

Exc 1: Results

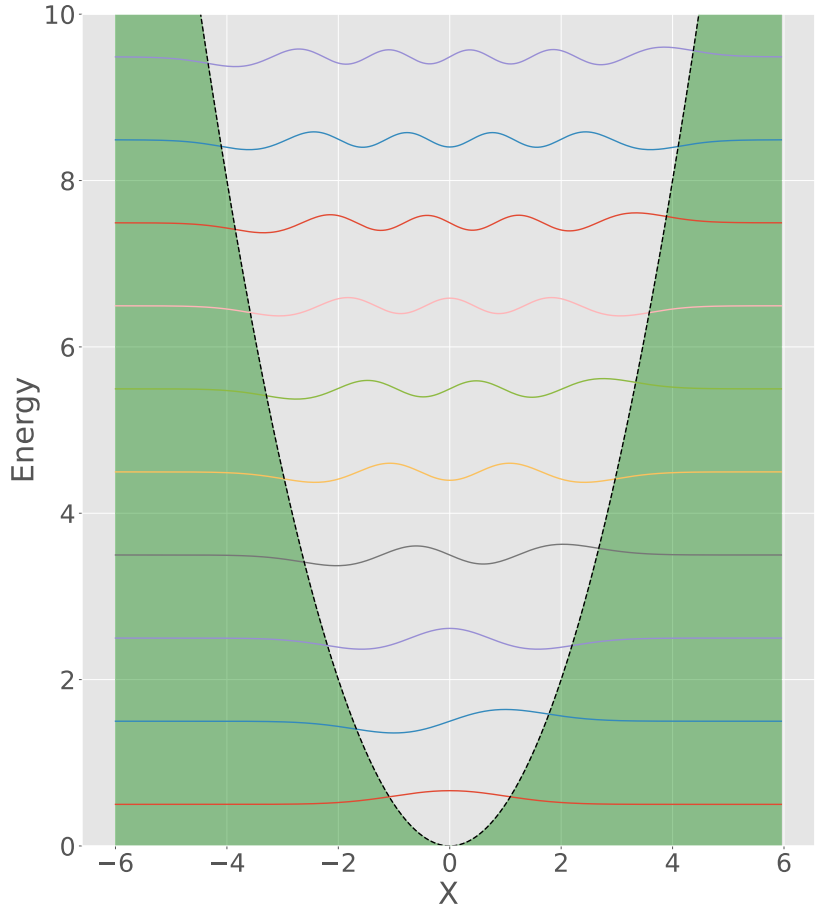
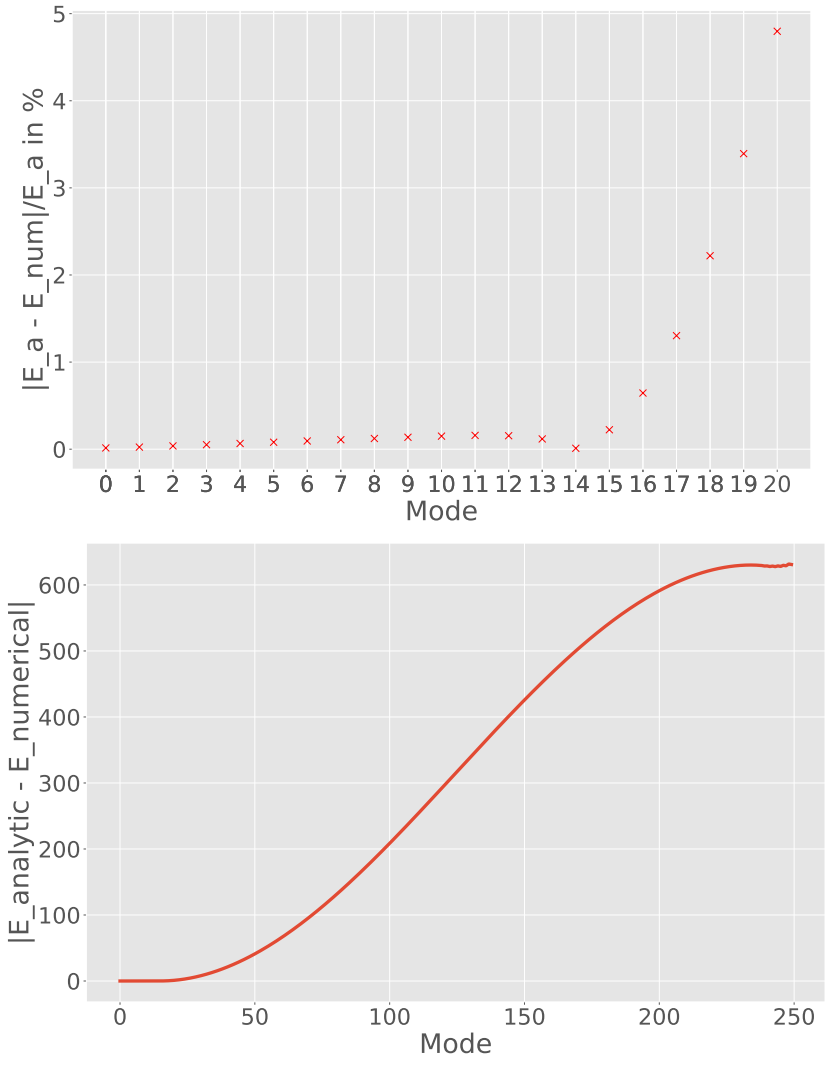


Figure: The first 10 wavefunctions and the potential..

Table: The numerical calculated value using finite differences and the energy determined from the analytic formula.

Mode	E_{num}	E_a
1	0.49992799	0.5
2	1.49963991	1.5
3	2.49906364	2.5
4	3.49819906	3.5
5	4.49704604	4.5
6	5.49560447	5.5
7	6.49387432	6.5
8	7.49185614	7.5
9	8.48955416	8.5
10	9.48699111	9.5

Exc 1: Comment on the quality of the code



- Correctness: Looking at the analytic results the low modes are very accurate, higher modes not as much but can be improved by increasing the x-range and discretization mesh, which makes sense since I supplied a mesh from $x \in [-6, 6]$ while high order wavefunctions extend above this range so will yield inaccurate results.
- Flexibility: The code is flexible with respect to choosing different values for frequency, mass etc. However, it fails if a more complex Hamiltonian wants to be supplied (e.g. a hermitian instead of symmetric one)
- Efficiency: The finite difference method is a lot better and faster in this example than numerov, which has an additional problem of reliably finding every eigenvalue (actually in my code it does not work at all but I have not had the time to solve this problem).
  Also, the dsteqr Lapack function is nice, since it is supplied only two vectors, so not a full matrix has to be created.

Figure: The absolute difference between the numerical evaluated eigenvalues and the eigenvalues from the analytic formula. Top: the first 20 modes, bottom: All 250 modes of the particular computation ($n_{mesh} = 250$).