Computational Physics - Exercise 3

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1 Numerov Algorithm for the Schrödinger Equation

We implement the numerov algorithm as a 3-dimensional Vector. Like that, we can store the Value y_{n+1}, y_n and y_{n-1} simultaneously. For each step, we store the calculated values in another array:

```
    def numerov(x0,y_n,h,n):
    x_n = np.zeros(n)
    x_n[0] = x0
    x_n[1] = x_n[0] + h
    output = np.zeros(n)
    output[0] = y_n[0] # = y_(n-1)
    output[1] = y_n[1] # = y_n

    for i in range(2, n):
        x_n[i] = x_n[i-1] + h

        y_n[2] = 2 * (1 - 5/12 * h**2 * k(x_n[i-1])) * y_n[1]
        y_n[2] -= (1 + 1/12 * h**2 * k(x_n[i-2])) * y_n[0]
        y_n[2] /= (1 + 1/12 * h**2 * k(x_n[i]))

        output[i] = y_n[2]
        y_n[0] = y_n[1]
        y_n[1] = y_n[2]

    return (x_n,output)
```

The equation to solve is the dimensionless form of the Schrödinger equation:

$$\psi''(x) + (2\varepsilon - x^2)\psi(x) = 0$$

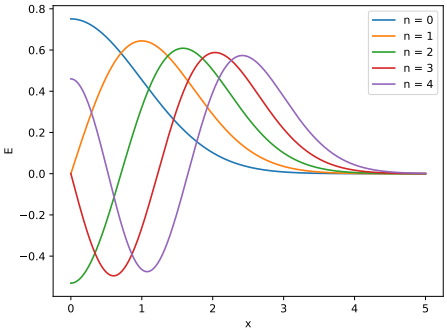
To be able to compare our results, we integrate the analytical solution into our code. For that we need a factorial and a Hermite Polynom function:

```
def H(x,n):
    if (n==0): return 1
    elif (n==1): return 2*x
    else: return 2*x*H(x,n-1)-2*(n-1)*H(x,n-2)

def factorial(n):
    if (n==0): return 1
    else: return n*factorial(n-1)
```

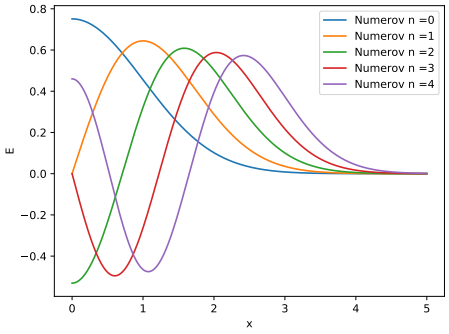
The analytical solution is:

$$\varphi(x) = \frac{H_n(x)}{(2^n n!\sqrt{\pi})^{\frac{1}{2}}} \exp\left(-\frac{x^2}{2}\right)$$

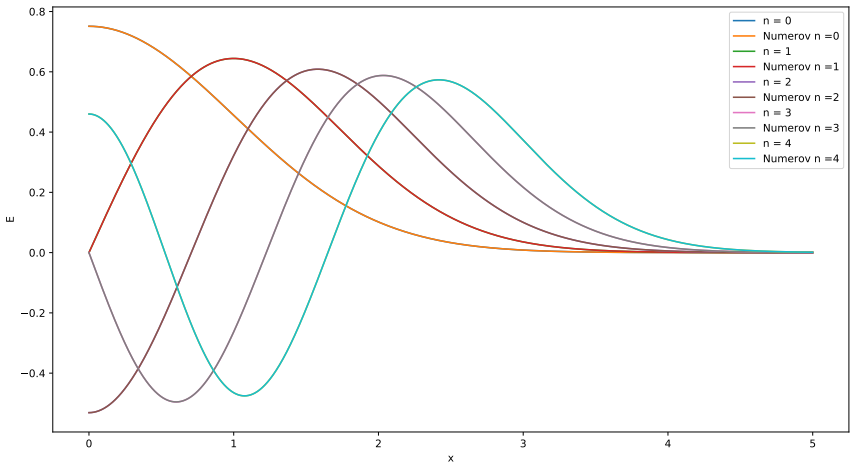
These Functions are solutions for the energy eigenvalues $\varepsilon = n + \frac{1}{2}$. For the Numerov algorithm we have to differentiate between symmetric (even n) and antisymmetric (odd n) solutions. For the symmetric solutions we have to choose $\psi(0) = a$ and $\psi(h) = \psi(0) - h^2 k_0 \psi(0)/2$ and for antisymmetric ones $\psi(0) = 0$ and $\psi(h) = a$. Plotting it for different orders of the Hermite Polynom n will yield:



(a) Analytical Solution



(b) Numeric Solution



(c) Overlay of Solutions

Figure 1: Comparison of Solutions

As seen above, the Plot resulting from our Numerov Algortihm barely differs from our analytical solution.

Neutrons in the gravitational field

We apply our Numerov Algorithm to the equation

$$\psi''(x) + (\varepsilon - x)\psi(x) = 0$$

As starting values we choose $\psi(0) = 0$ and $\psi(h) = a$. We calculate the outcome for 5 different ε. From that we will take two particularily interesting solutions (the symmetrical ones). Those solutions with $\varepsilon = \frac{5}{2}$ and $\frac{9}{2}$ show similar behaviour, except that one goes towards infinity and the other one towards minus infinity:

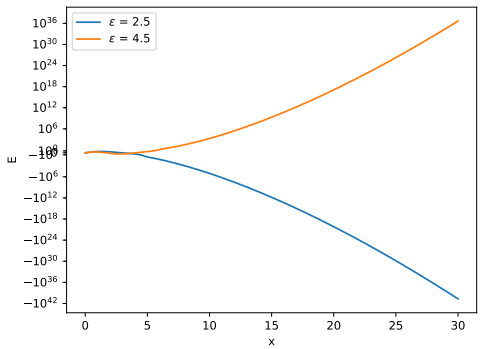


Figure 2: Neutrons in the gravitational field for different ε

Now we know, that at some value ε, the Function changes its sign. To find an eigenvalue, we need to find an ε_e, where the function ψ doesn't diverge, i.e. $\psi(x) \to 0$ for $x \to \infty$. First, we roughly try to find a few values, where the sign changes. For that, we let the program run roughly over a couple of ε in the interval [1,10], and print the value of $\psi(x)$ at large x . Console output for that reads:

```
Testing... y = 6.280723694044417e+40 & epsilon =  2.2727272727272725
Testing... y = -1.5235973614650188e+40 & epsilon =  2.3636363636363638
...
Testing... y = -1.2707732952939073e+37 & epsilon =  4.0
Testing... y = 2.7078206339593106e+35 & epsilon =  4.090909090909091
...
Testing... y = 6.977276804418008e+33 & epsilon =  5.454545454545455
Testing... y = -1.6852381320228214e+33 & epsilon =  5.545454545454546
...
Testing... y = -1.3309549719682978e+31 & epsilon =  6.7272727272727275
Testing... y = 4.5655959930342876e+30 & epsilon =  6.818181818181818
...
Testing... y = 2.9832517516046943e+28 & epsilon =  7.909090909090909
Testing... y = -3.0992991223435245e+28 & epsilon =  8.0
...
Testing... y = -1.2773923050848915e+26 & epsilon =  9.0
Testing... y = 2.526144567821359e+26 & epsilon =  9.090909090909092
```

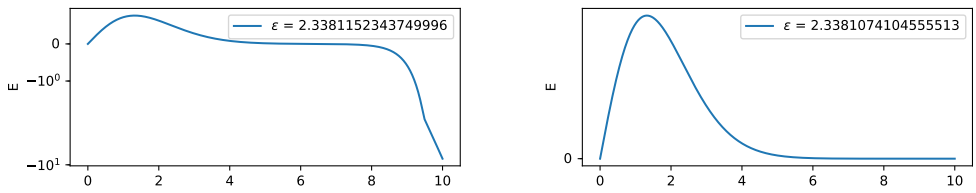
Next we implement a bisection algorithm, to estimate ε. That algorithm works in the following way:

1. Choose a minimum and maximum value $(\lambda_{\min}, \lambda_{\max})$ for ε that defines our interval $[\lambda_{\min}, \lambda_{\max}]$.
2. Cut that interval in half and set $\varepsilon = \lambda_{\text{half}}$.
3. Let's assume $\psi(x) \to -\infty$ for $\varepsilon = \lambda_{\min}$. We need to do the following:
4. If $y < 0$ for $\varepsilon = \lambda_{\text{half}}$, our new interval will be $[\lambda_{\text{half}}, \lambda_{\max}]$. Likewise, if $y > 0$ for $\varepsilon = \lambda_{\text{half}}$, our new interval will be $[\lambda_{\min}, \lambda_{\text{half}}]$.
5. Repeat from Step 2.

Let's implement that method into our code:

```
# Choose the Interval, in which you assume epsilon, and the amount of attempts
lambda_min = 2.27
lambda_max = 2.36
attempts = 100

# Check for the sign at lambda_min
x_vector, y_vector = numerov(x0,y_init,stepsize,steps,lambda_min)
sign_0 = int(np.sign(y_vector[testx]))

#start the Bisection Procedure
for n in range(attempts):
    epsilon = (lambda_min+lambda_max)/2
    y_init=np.ndarray((3))
    y_init[0] = 0
    y_init[1] = a
    x_vector, y_vector = numerov(x0,y_init,stepsize,steps,epsilon)

    sign = int(np.sign(y_vector[testx]))

    if sign is sign_0:
        lambda_min = epsilon
    if sign is not sign_0:
        lambda_max = epsilon
print(r"Approximation for $\varepsilon$: ", epsilon)
```

Let's choose the first example of the eigenvalue $epsilon_e \approx 2.3$. We set $\lambda_{\min} = 2.27$ and $\lambda_{\max} = 2.36$. With only 10 Attempts, we can calculate the Eigenvalue with an accuracy of 0.00001. If we choose to go higher, we will find the solution, where $\psi(x) \to 0$ for $x \to \infty$.



(a) 10 Iterations (b) 200 Iterations

Figure 3: Determining Epsilon with a Bisection Procedure

Doing the same for the remaining ε_e up to 10, we find 6 Functions ψ with $\psi(x) \to 0$ for $x \to \infty$, together with their corresponding eigenvalues ε:

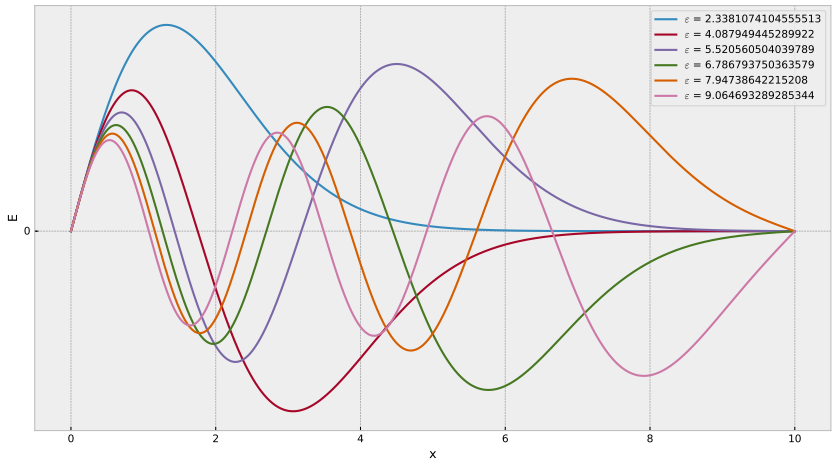


Figure 4: The first 6 Eigenvalues ε