Including the classes from the lecture. First the potential:

In [1]:

```
# for simplicity, we define the OBE exchange by numerical integration
# and add one contact term to be determined using either a bound state or a scattering length

import numpy as np
import math as m
from numpy.polynomial.legendre import leggauss
from scipy.special import legendre


class OBEpot:
    """Provides a method for the partial wave representation of the OBE potential.

       The matrix elements are obtained by numerical intergration.
       The mass of the exchanged boson, the strength of the
       interaction and the couter term is given on initialization.
       The interaction is regularized using a cutoff that is also
       given on init.
    """

    # this are common parameters for all instances
    hbarc=197.327

    # init interaction
    def __init__(self, cutoff=500.0, C0=1.0, nx=12,mpi=138.0,A=-1.0):
        """Defines the one boson exchange for a given regulator, coupling strength and short distance parameter

        Parameters:
        cutoff -- regulator in MeV
        C0 -- strength of the short distance counter term (in s-wave)
        A -- strength of OBE
        nx -- number of angular grid points for numerical integration
        mpi -- mass of exchange boson in MeV"""

        self.mpi = mpi/self.hbarc
        self.cutoff = cutoff/self.hbarc
        self.C0=C0
        self.A=A
        self.nx=nx

        self.xp=np.empty((self.nx),dtype=np.double)
        self.xw=np.empty((self.nx),dtype=np.double)
```

```
        self.xp,self.xw=leggauss(self.nx)



    # function defines the x integral
    def _g(self,pp,p,k):
        """Calculates g function of the partial wave decomposition of OBE.

           pp -- outgoing momentum
           p -- incoming momentum
           k -- angular momentum"""

        # define prefact
        # get the corresponding legendre polynomial
        Pk = legendre(k)
        # define momentum transfer dependent on angles
        qval=np.sqrt(p**2+pp**2-2*p*pp*self.xp)

        # build integral of regularized OBE
        return float(np.sum(Pk(self.xp)/((qval**2+self.mpi**2))*self.xw*np.exp(-(qval**2+self.mpi**2)/self.cutoff**2)))

    # determines complete, regularized interaction
    def v(self,pp,p,l):
        """Potential matrix element in fm**2

           pp -- outgoing momentum in fm**-1
           p -- incoming momentum in fm**-1
           l -- angular momentum"""

        # first overall prefact of 1pi exchange part  (cancel 2pi factors!)
        prefact=self.A

        mat=prefact*self._g(pp,p,l)

        if (l==0):   # add s-wave counter term
          mat+=self.C0*np.exp(-(pp**2+p**2)/self.cutoff**2)  # 4pi is take into account by spherical harmonics for l=0

        return mat
```

And then the TwoBody class:

In [2]:
```
import numpy as np
from numpy.polynomial.legendre import leggauss
from scipy.special import spherical_jn
```

```python
from scipy.interpolate import interp1d

class TwoBody:
    """Methods to obtain eigenvalues and eigenvectors for the bound state problem and for searches of the binding energy."""
    # define hbarc for unit conversion
    hbarc=197.327

    def __init__(self, pot, np1=20, np2=10, pa=1.0, pb=5.0, pc=20.0, mred=938.92/2,l=0,
                            nr1=20, nr2=10, ra=1.0, rb=5.0, rc=20.0,
                            np1four=200,np2four=100):
        """Initialization of two-body solver.

           The initialization defines the momentum grids and the interaction and partial wave to be used.
           At this time, also the grid for Fourier transformation and for the Fourier transformed
           wave function is given.

           Parameters:
           pot -- object that defines the potential matrix elements (e.g. of class OBEpot).
           np1 -- number of grid points in interval [0,pb]
           np2 -- number of grid points in interval [pb,pc]
           pa  -- half of np1 points are in interval [0,pa]
           pb  -- interval boundary as defined above
           pc  -- upper integration boundary for the solution of the integral equation
           mred -- reduces mass of the two bosons in MeV

           nr1 -- number of r points in interval [0,rb]
           nr2 -- number of r points in interval [rb,rc]
           ra  -- half of np1 points are in interval [0,pa]
           rb  -- interval boundary as defined above
           rc  -- upper integration boundary for the solution of the integral equation

           np1four -- number of p points in interval [0,pb] for Fourier trafo
           np2four -- number of p points in interval [pb,pc] for Fourier trafo"""

        # store parameters (if necessary convert to fm)
        self.np1 = np1
        self.np2 = np2
        self.npoints  = np1+np2
        self.mred=mred/self.hbarc
        self.pa=pa
        self.pb=pb
        self.pc=pc
        self.l=l
```

```
        self.nr1 = nr1
        self.nr2 = nr2
        self.nrpoints  = nr1+nr2
        self.ra=ra
        self.rb=rb
        self.rc=rc

        self.np1four = np1four
        self.np2four = np2four
        self.npfour  = np1four+np2four

        # store grid points and weights for integral equations
        self.pgrid,self.pweight = self._trns(self.np1,self.np2,self.pa,self.pb,self.pc)

        # store grid points and weights for r space wave functions
        self.rgrid,self.rweight = self._trns(self.nr1,self.nr2,self.ra,self.rb,self.rc)

        # store grid points and weights for Fourier trafo
        self.pfourgrid,self.pfourweight = self._trns(self.np1four,self.np2four,self.pa,self.pb,self.pc)

        # store underlying interaction
        self.pot=pot

    def _trns(self,np1,np2,pa,pb,pc):
      """Auxilliary method that provides transformed Gaus-Legendre grid points and integration weights.

         This is using a hyperbolic trafo shown in the lecture.
         Parameter:
         np1 --  grid points in ]0,pb[
         np2 --  grid points are distributed in ]pb,pc[ using a linear trafo

         pa  -- half of np1 points are in interval [0,pa]
         pb  -- interval boundary as defined above
         pc  -- upper integration boundary """

      x1grid,x1weight=leggauss(np1)
      x2grid,x2weight=leggauss(np2)

      # trafo (1.+X) / (1./P1-(1./P1-2./P2)*X) for first interval
      p1grid=(1.+x1grid) / (1./pa-(1./pa-2./pb)*x1grid)
      p1weight=(2.0/pa-2.0/pb)*x1weight / (1./pa-(1./pa-2./pb)*x1grid)**2

      # linear trafo
      p2grid=(pc+pb)/2.0 + (pc-pb)/2.0*x2grid
```

```
      p2weight=(pc-pb)/2.0*x2weight

      pgrid=np.empty((self.npoints),dtype=np.double)
      pweight=np.empty((self.npoints),dtype=np.double)

      pgrid = np.concatenate((p1grid, p2grid), axis=None)
      pweight = np.concatenate((p1weight, p2weight), axis=None)

      return pgrid,pweight

# set up set of equations and calculate eigenvalues

    def eigv(self,E,neigv):
      """Solve two-body integral equation and return n-th eigenvalue, momentum grid and wave function.

         Parameters:
         E -- energy used in the integral equation in fm**-1
         neigv -- number of the eigenvalue to be used"""

    # set up the matrix amat for which eigenvalues have to be calculated
      amat=np.empty((self.npoints,self.npoints),dtype=np.double)
      for i in range(self.npoints):
        for j in range(self.npoints):
          amat[i,j]=np.real(1.0/(E-self.pgrid[i]**2/(2*self.mred))*self.pot.v(self.pgrid[i],self.pgrid[j],self.l)*self.pweight[j]*

    # determine eigenvalues using numpy's eig method
      evalue,evec=np.linalg.eig(amat)

    # I now assume that the relevant eigenvalues are real to avoid complex arithmetic
      evalue=np.real(evalue)

    # remove neigv-1 largest eigenvalues
      for n in range(neigv-1):
        maxpos=np.argmax(evalue)
        evalue[maxpos]=0.0

    # take the next one
      maxpos=np.argmax(evalue)
      eigv=evalue[maxpos]
    # define solution as unnormalized wave function
      wf=evec[:,maxpos]
    # and normalize
      norm=np.sum(wf**2*self.pweight[0:self.npoints]*self.pgrid[0:self.npoints]**2)
      wf=1/np.sqrt(norm)*wf
```

```
    return eigv,self.pgrid[0:self.npoints],wf


  def esearch(self,neigv=1,e1=-0.01,e2=-0.0105,elow=0.0,tol=1e-8):
      """Perform search for energy using the secant method.

         Parameters:
         neigv -- number of the eigenvalue to be used
         e1 -- first estimate of binding energy (should be negative)
         e2 -- second estimate of binding energy (should be negative)
         elow -- largest energy to be used in search (should be negative)
         tol -- if two consecutive energies differ by less then tol, the search is converged

         Energies are given in fm**-1. """

      # determine eigenvalues for starting energies
      eta1,pgrid,wf=self.eigv(e1,neigv)
      eta2,pgrid,wf=self.eigv(e2,neigv)

      while abs(e1-e2) > tol:
        # get new estimate (taking upper value into account)
        enew=e2+(e1-e2)/(eta1-eta2)*(1-eta2)
        enew=min(elow,enew)

        # get new eigenvalue and replace e1 and e2 for next iteration
        eta,pgrid,wf=self.eigv(enew,neigv)
        e2=e1
        eta2=eta1
        e1=enew
        eta1=eta

      return e1,eta1,pgrid,wf

  def fourier(self,wfp):
      """Calculates the Fourier transform of the partial wave representation of the wave function.

         Parameter:
         wfp -- wave function in momentum space

         Note that the factor I**l is omitted."""

      # calculate spherical bessel functions based dense Fourier trafo momentum grid and rgrid
      # prepare matrix based on r,p points
```

```
        rpmat = np.outer(self.rgrid,self.pfourgrid)
        # evaluate jl
        jlmat = spherical_jn(self.l,rpmat)

        # interpolate of wave to denser Fourier trafo grid
        wfinter = interp1d(self.pgrid, wfp, kind='cubic',fill_value="extrapolate")
        # interpolate wf and multiply my p**2*w elementwise
        wfdense = wfinter(self.pfourgrid)*self.pfourgrid**2*self.pfourweight*np.sqrt(2/m.pi)

        # now the Fourier trafo is a matrix-vector multiplication
        wfr = jlmat.dot(wfdense)

        return self.rgrid,wfr


    def rms(self,wfr):
        """Calculates the norm and rms radius for the given r-space wave function.

           Normalization of the wave function is assumed.
           Parameter:
           wfr -- wave function in r-space obtained by previous Fourier trafo"""


        norm=np.sum(wfr**2*self.rweight*self.rgrid**2)
        rms=np.sum(wfr**2*self.rweight*self.rgrid**4)


        rms=np.sqrt(rms)

        return norm,rms
```

In [3]:

```
import numpy as np
import math as m
import pandas as pd
from lmfit.models import ExpressionModel
from numpy.polynomial.legendre import leggauss
from scipy.special import legendre
import matplotlib.pyplot as plt
from scipy.interpolate import CubicSpline
from scipy.special import sph_harm
from scipy.special import spherical_jn
from scipy.integrate import simps
from scipy.integrate import quad
```

Homework 7 from Richard Baumann

The Lippmann-Schwinger equations have been rewritten into the form

$$t_l(p,p') = V_l(p,p') + \int_0^\infty dp\,''\ \frac{f(p\,'') - f(q)}{q^2 - p\,''^2} + f(q)\int_0^\infty dp\,''\ \frac{1}{q^2 - p\,''^2} - i\pi\frac{f(q)}{2q} \tag{1}$$

This again can be discretized using grid points p_i with $i \in [0,\ldots,N-1]$ and the corresponding integration weights w_i. This defines a set of matrix elements $t_l(p_i,p_j)$. These matrix elements do not contain the half on shell elements $t_l(q,p_j)$ and $t_l(p_i,q)$ and therfore also not $t_l(q,q)$.

In order to get this matrix elements list of grid points is append with $p_N = q$. Using this gridpoints I can calculate $t_l(q,q)$ = $t_l(p_N,p_N)$.

1 Using these grid points, show that the Lippmann-Schwinger equation can be written in the form:

$$A_{ik} = \begin{cases} \delta_{ij} - \frac{2\mu V_{ik} p_k^2}{q^2 - p_k^2} w_k, & \text{for k \uneq N} \\ \delta_{ij} + \sum_{m=0}^{N-1} \frac{2\mu V_{iN} q^2}{q^2 - p_m^2} w_m - \mu q V_{iN} \ln\left(\frac{p_{max}+q}{p_{max}-q}\right) + i\pi\mu q V_{iN}, & \text{for k = N} \end{cases} \tag{2}$$

Where p_{max} is the upper boundary of the integration as used for the discretization.

With

$$f(p\,'') = 2\mu V_l(p,p\,'')t_l(p\,'',p') \tag{3}$$

The original equation can be rewritten to:

$$\begin{aligned} t_l(p,p') &= V_l(p,p') + \int_0^\infty dp\,''\ \frac{f(p\,'') - f(q)}{q^2 - p\,''^2} + f(q)\int_0^\infty dp\,''\ \frac{1}{q^2 - p\,''^2} - i\pi\frac{f(q)}{2q} \\ &= V_l(p,p') + \int_0^\infty dp\,''\ \frac{2\mu p\,''^2\ V_l(p',p\,'')t_l(p',p\,'') - 2\mu q^2 V_l(p',q)t_l(q,p)}{q^2 - p\,''^2} + 2\mu q^2 V_l(p',q)t_l(q,p)\int_0^\infty dp\,''\ \frac{1}{q^2 - p\,''^2} - i\pi\frac{2\mu q^2 V_l(p',q)t_l(q, \\ &= V_l(p,p') + \int_0^\infty dp\,''\ \frac{2\mu p\,''^2\ V_l(p',p\,'')t_l(p',p\,'') - 2\mu q^2 V_l(p',q)t_l(q,p)}{q^2 - p\,''^2} + 2\mu q^2 V_l(p',q)t_l(q,p)\int_0^\infty dp\,''\ \frac{1}{q^2 - p\,''^2} - i\pi\mu q V_l(p',q)t_l(q,p \end{aligned}$$

I don't really know how to continue from here. I can definitly see that different parts of the right side represent different parts from the Matrix element A_{ik} . Therefore, I will give some expressions of proportionallity. Note that this expressions are most likely not proportional, but I just want to make the point that I think the given terms for A_{ik} will be derived from these terms in the equation above.

$$\frac{2\mu V_{ik} p_k^2}{q^2 - p_k^2} w_k \propto \int_0^\infty dp\,'' \, \frac{2\mu p\,''^2 \, V_l(p', p\,'') t_l(p', p\,'')}{q^2 - p\,''^2} \tag{5}$$

$$\frac{2\mu V_{iN} q^2}{q^2 - p_m^2} w_m \propto \int_0^\infty dp\,'' \, \frac{2\mu q^2 V_l(p', q) t_l(q, p)}{q^2 - p\,''^2} \tag{6}$$

$$\mu q V_{iN} \ln\left(\frac{p_{max} + q}{p_{max} - q}\right) \propto 2\mu q^2 V_l(p', q) t_l(q, p) \int_0^\infty dp\,'' \, \frac{1}{q^2 - p\,''^2} \tag{7}$$

$$i\pi\mu q V_{iN} \propto 2\mu q^2 V_l(p', q) t_l(q, p) \int_0^\infty dp\,'' \, i\pi\mu q V_l(p', q) t_l(q, p) \tag{8}$$

For some expressions the apperance is already very similar, for others the expression is very much different.

2. Implement the discretized form of the Lippmann-Schwinger equation to obtain the onshell matrix element t_{NN}.

For the implementation I can define a class for the T Matrix. For that I will:

- Generate a momentum grid with weights
- Calculate the A and V matrix with the correct potential
- Use a function to solve the Lippmann-Schwinger equation:

$$A_{ik} t_{kj} = V_{ij} \tag{9}$$

With that I will be able to calculate the onshell matrix element t_{NN}.

In [4]:
```
# next extend the class for twobody to scattering
from scipy.special import legendre
import cmath

class TwoBodyTMat(TwoBody):
    """This class defines the off-shell t-matrix for a three-body bound state.
```

```
   The class assumes three identical particles. It also contains the
   initialization of grid points for the three-body problem.
"""

def __init__(self, pot, np1=20, np2=10, pa=1.0, pb=5.0, pc=20.0,
                        nq1=20, nq2=10, qa=1.0, qb=5.0, qc=20.0,
                        nr1=20, nr2=10, ra=1.0, rb=5.0, rc=20.0,
                        lmax=0,mred=938.92,mass=938.92,
                        np1four=200,np2four=100):
    """Initialization of grid points and interaction for the solution of the three-body problem.

       Parameter:
       pot -- object that defines the potential matrix elements (e.g. of class OBEpot).
       np1 -- number of p grid points in interval [0,pb]
       np2 -- number of p grid points in interval [pb,pc]
       pa  -- half of np1 points are in interval [0,pa]
       pb  -- interval boundary as defined above
       pc  -- upper integration boundary for the solution of the integral equation
       nq1 -- number of q grid points in interval [0,qb]
       nq2 -- number of q grid points in interval [qb,qc]
       qa  -- half of np1 points are in interval [0,qa]
       qb  -- interval boundary as defined above
       qc  -- upper integration boundary for the solution of the integral equation
       mass -- particle mass of the three identical bosons in MeV

       np1four -- number of p or q  points in interval [0,pb] or[0,qb]   for Fourier trafo
       np2four -- number of p or q points in interval [pb,pc] or [qb,qc] for Fourier trafo

       lmax  -- maximal two-body angular momentum to be taken into account
       """


    # first use the TwoBody class to keep the main parameters
    super().__init__(pot,np1,np2,pa,pb,pc,mass/2,0,nr1,nr2,ra,rb,rc,np1four,np2four)
    self.pot = pot
    # Assigning the number of points in the first and second intervall
    self.np1 = np1
    self.np2 = np2

    # The number of total points is the number of points in each intervall added.
    self.npoints = np1+np2

    # Assigning the parameters from above
```

```
        self.pa=pa
        self.pb=pb
        self.pc=pc

        # The reduced mass is assigned
        self.mred=mred/self.hbarc

        # And also lmax
        self.lmax=lmax

        # Setting up grid points for the p grid, as well as weights
        self.pgrid,self.pweight = self._trns(self.np1,self.np2,self.pa,self.pb,self.pc)

    """
    Calculation of the t matrix
    """
    # Now I want to solve the t-Matrix as defined above in the formula:
    def prep_tmat(self,E):

        # First q is calculated
        q=(2*self.mred*E)**(1/2)

        # And appended to the p grid array
        self.pgrid=np.append(self.pgrid, q)

        # This changes the total number of grid points, so I
        # increase the number here. Then I don't have to do it
        # later in all loops.
        self.npoints = self.npoints + 1

        """
        Now it is time to calculate the t-matrix
        """

        # for every l I want to calculate I need a NxN big array to store the
        # results
        tmat=np.empty((self.lmax+1,self.npoints,self.npoints),dtype=np.double)

        # now I need to solve the Lippmann-Schwinger equation for each etmat and each l =0,..,lmax
        for l in range(self.lmax+1):

            # For calculating the A matrix I first have to initilize it.
            amat=np.zeros(self.npoints * self.npoints).reshape(self.npoints, self.npoints)
```

```
        # Now I can calculate every grid point in the A matrix,
        # and because of this I look over all entries
        for i in range(self.npoints):
            for k in range(self.npoints):

                # Determining the delta function
                if i==k:
                    delta = 1
                else:
                    delta = 0

                # If k =/= N, calculate
                if (k < self.npoints-1):
                    amat[i,k] = delta - (2 * self.mred * self.pot.pot.v(self.pgrid[i],self.pgrid[k],l)*self.pgrid[k]**2 \
                                / (q**2 - self.pgrid[k]**2) *self.pweight[k])

                # If k == N, calculate
                else:
                    sum=0
                    # This is the summation part of the calculation
                    for m in range(self.npoints-2):
                        sum = sum + 2 * (self.mred * self.pot.pot.v(self.pgrid[i],self.pgrid[self.npoints-1],l)*q**2 / (q**2 -
                                  + 1j * np.pi * self.mred * q * self.pot.pot.v(self.pgrid[i],self.pgrid[self.npoints-1],l) \
                                  - self.mred * q * self.pot.pot.v(self.pgrid[i],self.pgrid[self.npoints-1],l) * np.log((self.
                    amat[i,k] = delta + sum

        # Now all what is left is defining the potential matrix:
        vmat=np.empty((self.npoints,self.npoints),dtype=np.double)
        for i in range(self.npoints):
            for j in range(self.npoints):
                vmat[i,j]=self.pot.pot.v(self.pgrid[i],self.pgrid[j],l)

        # Finally I can solve A*t=V. This function returns the tmatrix.
        tmat[l]=np.linalg.solve(amat,vmat)

    # And with that I can return the tmatrix with the onshell
    # and the offshell matrix elements. (tmatrix is NxN big and
    # contains t_l(q, q))
    return tmat

"""
Calculation of the t matrix for p_max->inf
"""
# Now I want to solve the t-Matrix as defined above in the formula:
```

```
def prep_tmat_pmax_inf(self,E):

    # First q is calculated
    q=(2*self.mred*E)**(1/2)

    # And appended to the p grid array
    self.pgrid=np.append(self.pgrid, q)

    # This changes the total number of grid points, so I
    # increase the number here. Then I don't have to do it
    # later in all loops.
    self.npoints = self.npoints + 1

    """
    Now it is time to calculate the t-matrix
    """

    # for every l I want to calculate I need a NxN big array to store the
    # results
    tmat=np.empty((self.lmax+1,self.npoints,self.npoints),dtype=np.double)

    # now I need to solve the Lippmann-Schwinger equation for each etmat and each l =0,..,lmax
    for l in range(self.lmax+1):

        # For calculating the A matrix I first have to initilize it.
        amat=np.zeros(self.npoints * self.npoints).reshape(self.npoints, self.npoints)

        # Now I can calculate every grid point in the A matrix,
        # and because of this I look over all entries
        for i in range(self.npoints):
            for k in range(self.npoints):

                # Determining the delta function
                if i==k:
                    delta = 1
                else:
                    delta = 0

                # If k =/= N, calculate
                if (k < self.npoints-1):
                    amat[i,k] = delta - (2 * self.mred * self.pot.pot.v(self.pgrid[i],self.pgrid[k],l)*self.pgrid[k]**2 \
                                / (q**2 - self.pgrid[k]**2) *self.pweight[k])

                # If k == N, calculate
```

```
                    else:
                        sum=0
                        # This is the summation part of the calculation
                        for m in range(self.npoints-2):
                            sum = sum + 2 * (self.mred * self.pot.pot.v(self.pgrid[i],self.pgrid[self.npoints-1],l)*q**2 / (q**2 -
                                    + 1j * np.pi * self.mred * q * self.pot.pot.v(self.pgrid[i],self.pgrid[self.npoints-1],l)
                        amat[i,k] = delta + sum

            # Now all what is left is defining the potential matrix:
            vmat=np.empty((self.npoints,self.npoints),dtype=np.double)
            for i in range(self.npoints):
                for j in range(self.npoints):
                    vmat[i,j]=self.pot.pot.v(self.pgrid[i],self.pgrid[j],l)

            # Finally I can solve A*t=V. This function returns the tmatrix.
            tmat[l]=np.linalg.solve(amat,vmat)

        # And with that I can return the tmatrix with the onshell
        # and the offshell matrix elements. (tmatrix is NxN big and
        # contains t_l(q, q))
        return tmat
```

In [5]:

```
def t_N_N(lower_p, upper_p, points, Energy):

    # Setting up the relevant parameters.
    c_0 = 2.470795E-02
    lamda = 800

    # Determining the potential, and two body parameters.
    potential=OBEpot(nx=24,mpi=138.0,C0=c_0,A=-1.0/6.474860194946856,cutoff=lamda)
    system=TwoBody(pot=potential,np1=int(points/2),np2=int(points/2),pa=1,pb=lower_p,pc=upper_p,mred=938.92,l=0,
                        nr1=40, nr2=20, ra=1.0, rb=5.0, rc=20.0,
                        np1four=400,np2four=200)

    # Based on that I set up the t Matrix
    tmat=TwoBodyTMat(system, np1=int(points/2),np2=int(points/2),pa=1,pb=lower_p,pc=upper_p,mred=938.92) #(upper_p+lower_p)/2

    # And calculate
    element=tmat.prep_tmat(Energy)[0][tmat.npoints-1][tmat.npoints-1]
    return(element)

print(t_N_N(1., 100., 50., -2.225))
```

```
-0.0003113532634330139
```

The algorithm seems to be doing something, but I have now way of verifying that the result is correct.

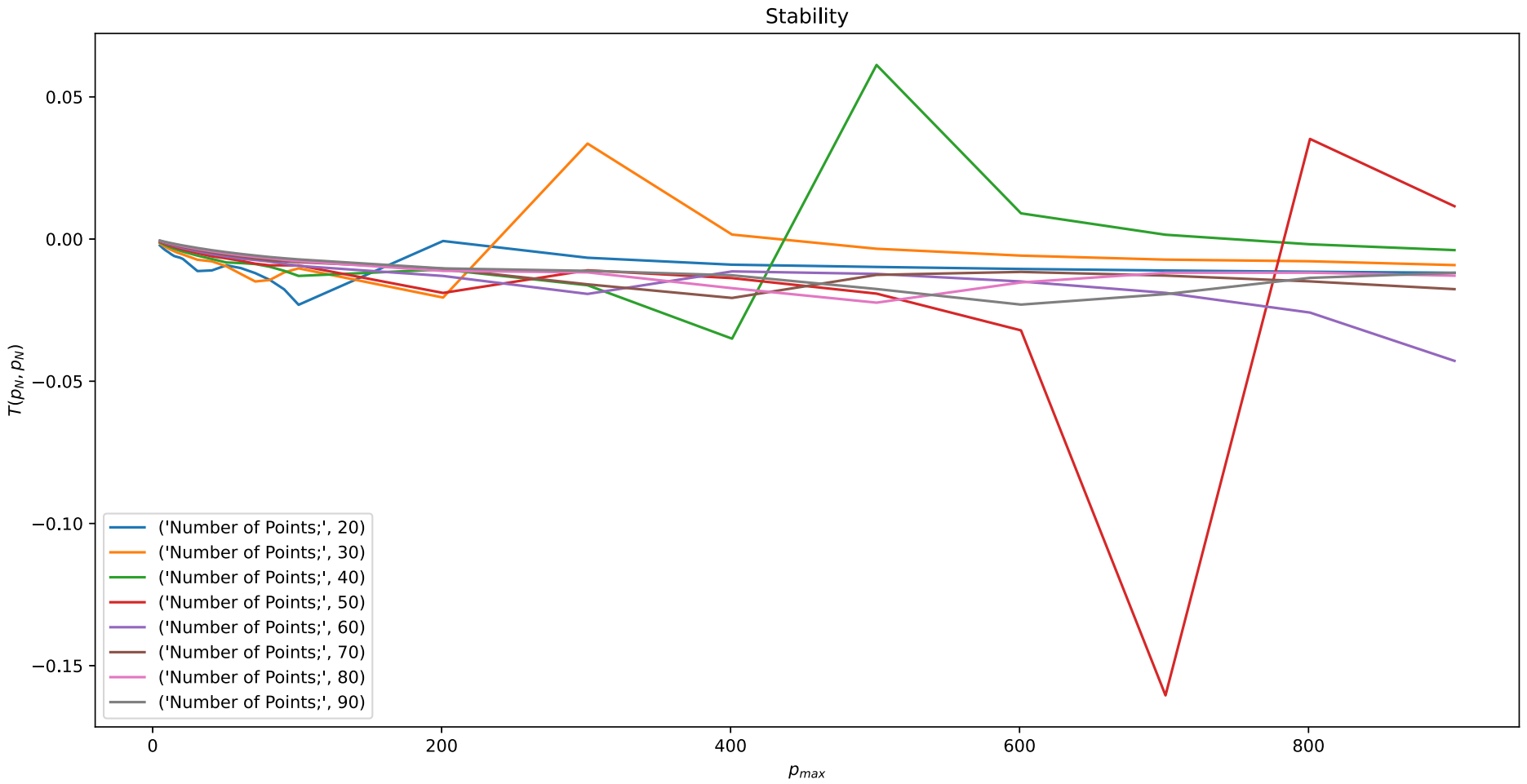
3: By variations of the number of grid points and the upper bound of integration p_{max}, quantify the numerical accuracy of your result for $t_0(q,q)$ for E = 1 MeV. The contribution A_{ik} includes a term that vanishes for $p_{max} \to \infty$. Neglect this term and vary p_{max} again. What do you observe? Why is the behavior different in this case?

First I can take a look at the difference, the number of points makes: For that I calculate the matrix element $t_l(q,q)$ for

- E= 1 MeV
- Number of grid points $\in [3, 5, 7, 9, 11, 13, 15, 17, 19, 21, 31, 41, 51, 61, 71, 81, 91, 101, 201, 301, 401, 501, 601, 701, 801, 901]$
- $p_{max} \in [20, 30, 40, 50, 60, 70, 80, 90]$

In [6]:
```
"""Function for finding the number of points that result in a stable solution"""
def p_test():

    # Initilizing the arrays. The number of points and p_max values are in accordance to the
    # values stated above
    points_array=np.arange(20, 100, 10)
    p_max_array=np.append(np.append(np.arange(3, 20, 2), np.arange(21, 100, 10)), np.arange(101, 1000, 100))
    t_l_l_array=np.zeros(len(p_max_array)*len(points_array)).reshape(len(points_array), len(p_max_array))

    # Calculate t_l_l for every combination of points and p_max values
    for j in range(len(points_array)):
        for i in range(len(p_max_array)):
            t_l_l_array[j][i]=t_N_N(1, p_max_array[i], points_array[j], 1)

    # The results are plotted with some cosmetics.
    plt.figure(figsize=(15,7.5))
    for j in range(len(points_array)):
        plt.plot(p_max_array, t_l_l_array[j], label=("Number of Points;", points_array[j]))
    plt.legend(loc="best")
    plt.xlabel(r"$p_{max}$")
    plt.ylabel(r"$T(p_N, p_N)$")
    plt.title("Stability")
    plt.savefig("pictures/stability.png", dpi=300)
```

```
p_test()
```



It can be seen, that the number of grid points has a great influence on the stability of the matrix element. Starting at 60-70 points the simulation for the matrix element seems to be stable. The computation times goes up a lot with increasing number of points. Therefore 60 points will be used from now on since this value seems to combine stability and low computation time.

Now, if I look at the term for A_{ik}:

$$A_{ik} = \begin{cases} \delta_{ij} - \frac{2\mu V_{ik} p_k^2}{q^2 - p_k^2} w_k, & \text{for k \uneq N} \\ \delta_{ij} + \sum_{m=0}^{N-1} \frac{2\mu V_{iN} q^2}{q^2 - p_m^2} w_m - \mu q V_{iN} \ln\left(\frac{p_{max}+q}{p_{max}-q}\right) + i\pi\mu q V_{iN}, & \text{for k = N} \end{cases} \tag{10}$$

I can see, that only one term is depended on p_{max}:

$$lim_{p_{max}\to\infty}\ \mu q V_{iN} \ln\left(\frac{p_{max}+q}{p_{max}-q}\right) = \mu q V_{iN} \ln(1) = 0 \tag{11}$$

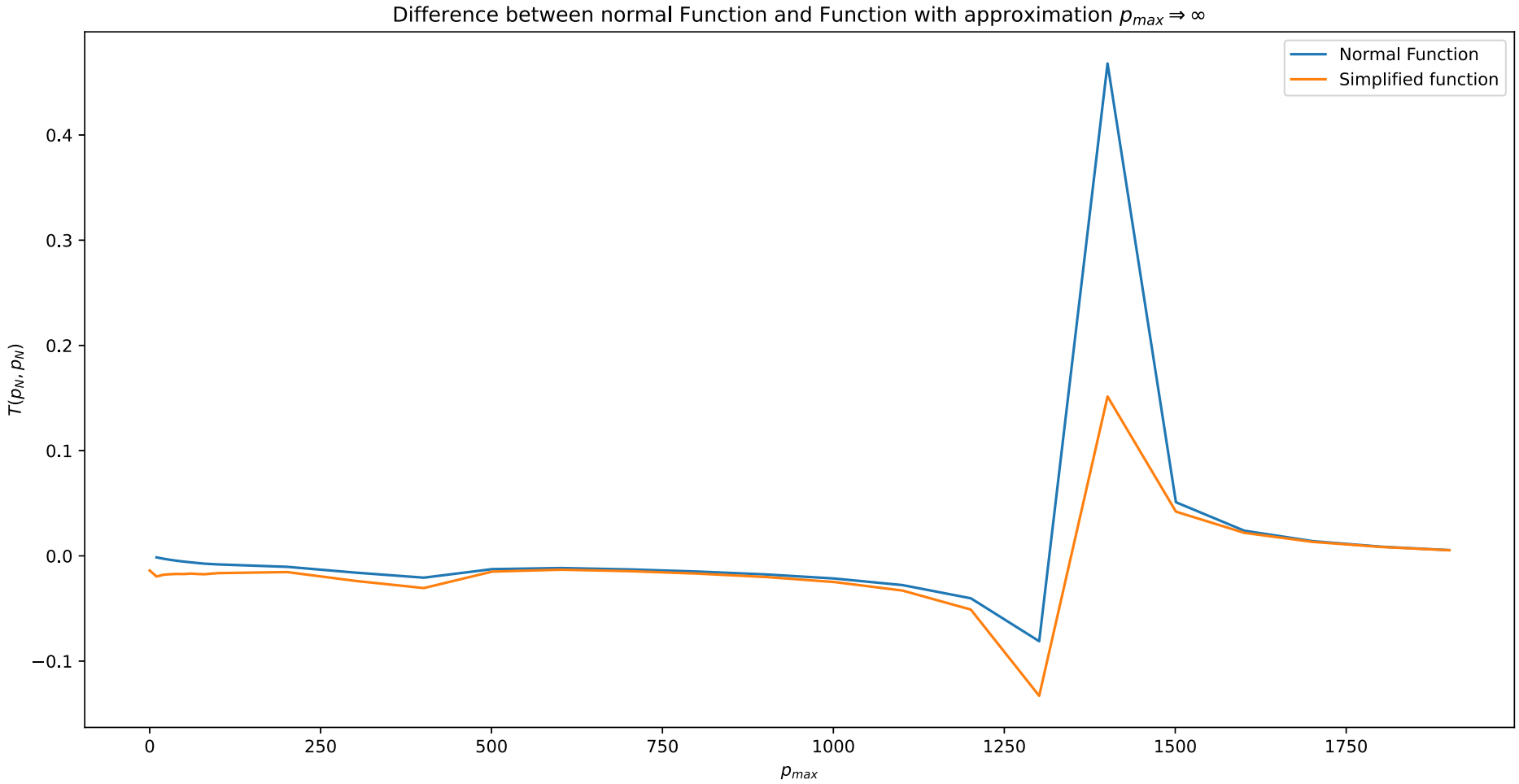
Therefore A_{ik} becomes:

$$A_{ik\,,\,p_{max}} = \begin{cases} \delta_{ij} - \frac{2\mu V_{ik} p_k^2}{q^2 - p_k^2} w_k, & \text{for k \uneq N} \\ \delta_{ij} + \sum_{m=0}^{N-1} \frac{2\mu V_{iN} q^2}{q^2 - p_m^2} w_m + i\pi\mu q V_{iN}, & \text{for k = N} \end{cases} \tag{12}$$

This has already been implemented in the t-Matrix class above. Therefore I will try out, if the two methods of computing $t_l(q,q)$ are similar at high momenta.

In [7]:
```
""" Function for getting the matrix element for p_max -> inf """
# (Identical to above only with different calculation for the
# matrix element)
def t_N_N_p_max(lower_p, upper_p, points, Energy):

    # Setting up the relevant parameters.
    c_0 = 2.470795E-02
    lamda = 800

    # Determining the potential, and two body parameters.
    pot=OBEpot(nx=24,mpi=138.0,C0=c_0,A=-1.0/6.474860194946856,cutoff=lamda)
    system=TwoBody(pot=pot,np1=int(points/2),np2=int(points/2),pa=1,pb=lower_p,pc=upper_p,mred=938.92,l=0,
                       nr1=40, nr2=20, ra=1.0, rb=5.0, rc=20.0,
                       np1four=400,np2four=200)

    # Here the Matrix element is calculated again, but with the routine that looks at p_max->inf
    tmat=TwoBodyTMat(system,np1=int(points/2),np2=int(points/2),pa=1,pb=lower_p,pc=upper_p,mred=938.92) #(upper_p+lower_p)/2

    # And calculate
    element=tmat.prep_tmat_pmax_inf(Energy)[0][tmat.npoints-1][tmat.npoints-1]
    return(element)
```

```python
""" Function that plots the t matrix with and without approximation for p_max->inf"""
def agreeance_for_p_max(points=70):

    # Initilizing the arrays. The p_max array contains some low values
    # and then with a bigger stepwidth values up to 2000
    p_max_array=np.append(np.arange(0, 100, 10), np.arange(101, 2000, 100))
    t_l_l_array=np.zeros(len(p_max_array))
    t_l_l_array_p_max_inf=np.zeros(len(p_max_array))

    # Calculate t_l_l and t_l_l with approximation for every momentum
    for i in range(len(p_max_array)):
        t_l_l_array[i]=t_N_N(1, p_max_array[i], points, 1)
        t_l_l_array_p_max_inf[i]=t_N_N_p_max(1, p_max_array[i], points, 1)

    # Plotting the values with some cosmetics
    plt.figure(figsize=(15,7.5))
    plt.plot(p_max_array, t_l_l_array, label="Normal Function")
    plt.plot(p_max_array, t_l_l_array_p_max_inf, label="Simplified function")
    plt.legend(loc="best")
    plt.xlabel(r"$p_{max}$")
    plt.ylabel(r"$T(p_N, p_N)$")
    plt.title(r"Difference between normal Function and Function with approximation $p_{max} \Rightarrow \infty$")
    plt.savefig("pictures/difference_function_approximation.png", dpi=300)

agreeance_for_p_max()
```



In that picture I can see, that the agreeance between the approximated solution and the normal solution is good at high energies.

4: The partial wave decomposed $S_l(q) = 1 - 2\pi i \mu q t_l(q,q)$ fulfills the unitarity relation |S_l(q)| = 1. Check that your code reproduces this property for l = 0 and selected q. Because of this property, the S- (and t)-matrix can be represented in terms of a real phase shift $\delta_l(q)$.

$$S_l(q) = exp(i2\delta_l(q)) \tag{13}$$

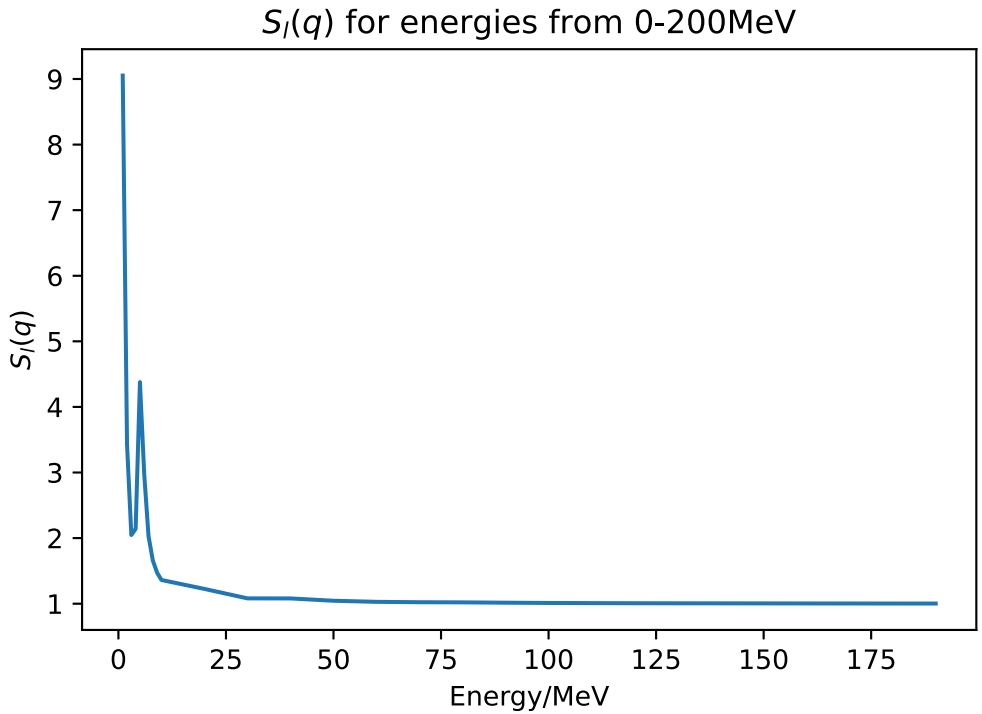
Note that changing δ by 180 deg does not change S_l use this feature to plot $\delta_l$for l = 0 in the range E = 0 . . . 200 MeV such that the function is continues and approaches zero at large E.

$$\begin{aligned} |S_l(q)| = |1 - 2\pi i\mu q t_l(q,q)| &= (1 - 2\pi i\mu q t_l(q,q)) \cdot (1 - 2\pi i\mu q t_l(q,q))^* \\ &= (1 - 2\pi i\mu q t_l(q,q)) \cdot (1 + 2\pi i\mu q t_l(q,q)) \\ &= 1 + 4\pi^2\mu^2 q^2 t_l(q,q)^2 \end{aligned} \tag{14}$$

In [8]:

```
"""Function for calculating s_l"""
def s_l(Energy, lower_p = 1, upper_p = 400, points = 70):
    # Setting up the relevant parameters.
    c_0 = 2.470795E-02
    lamda = 800

    # Determining the potential, and two body parameters.
    pot=OBEpot(nx=24,mpi=138.0,C0=c_0,A=-1.0/6.474860194946856,cutoff=lamda)
    system=TwoBody(pot=pot,np1=int(points/2),np2=int(points/2),pa=1,pb=lower_p,pc=upper_p,mred=938.92,l=0,
                       nr1=40, nr2=20, ra=1.0, rb=5.0, rc=20.0,
                       np1four=400,np2four=200)

    # Here the Matrix element is calculated again, but with the routine that looks at p_max->inf
    tmat=TwoBodyTMat(system,np1=int(points/2),np2=int(points/2),pa=1,pb=lower_p,pc=upper_p,mred=938.92)
    q=(2*tmat.mred*Energy)**(1/2)

    # And calculate the t-Matrix
    t_matrix=(tmat.prep_tmat_pmax_inf(Energy)[0][tmat.npoints-1][tmat.npoints-1])

    return (1+(4*np.pi**2*tmat.mred**2*q**2*t_matrix**2))

"""Calculating and plotting S_l"""
def test_s_l():

    # setting up arrays for energies and s-values.
    # There are more points in the low energy area and less in the high energy area
    energy_array=np.append(np.arange(1, 10, 1), np.arange(10, 200, 10))
    s_array=np.zeros(len(energy_array))

    # Here the s-values are calculated
    for i in range(len(s_array)):
        s_array[i]=s_l(energy_array[i])

    # and plotted
    plt.plot(energy_array, s_array)
```

```
    plt.xlabel("Energy/MeV")
    plt.ylabel(r"$S_l(q)$")
    plt.xlabel(r"Energy/MeV")
    plt.title(r"$S_l(q)$ for energies from 0-200MeV")
    plt.savefig("pictures/S_l(q)_energies.png", dpi=300)

test_s_l()
```



The picture seems not correct. I had expected a flat line at 1, since |S_l(q)| was supposed to equal 1. However, the function looks very much like a delta function at q=0, which it was supposed to look like. It seems that there might be a normaization factor, that I am not taking into account.