# My Project

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# Chapter 1

# **Class Index**

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Here are the classes, structs, unions and interfaces with brief descriptions:	
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2 Class Index

# **Chapter 2**

# File Index

## 2.1 File List

Here is a list of all files with brief descriptions:

ConstantGridSolver.cpp
Definitions of ConstantGridSolver class methods
ConstantGridSolver.h
Definition of ConstantGridSolver class
main.cpp
Parameters.cpp
Definitions of Parameters class methods
Parameters.h
Definition of Parameters class

File Index

# **Chapter 3**

## **Class Documentation**

### 3.1 ConstantGridSolver Class Reference

```
#include <ConstantGridSolver.h>
```

#### **Public Member Functions**

```
    arma::cx_mat calculateT (int j, double E) const
```

Calculates  $T(x_i, E)$  matrix.

arma::cx\_mat calculateU (int j, double E)

Calculates  $U(x_i, E)$  matrix.

• arma::cx\_mat calculateEP (int j, double E)

Calculates  $\mathbf{E}^+(x_i, E)$  matrix.

arma::cx\_mat calculateEM (int j, double E)

Calculates  $\mathbf{E}^-(x_j, E)$  matrix.

• void modifyCCnj (arma::cx\_mat &n1, arma::cx\_mat &n0, arma::cx\_mat &j1, arma::cx\_mat &j0, double E)

Modifies closed channels elements.

arma::cx\_mat fwdIteration (const arma::cx\_mat &B, double E)

Iterates Numerov algorithm forward up to N-1 and returns  $\mathbf{R}_{N-1}$  matrix for a given energy.

arma::cx\_mat calculateS (const arma::cx\_mat R\_N, double E)

Calculates S matrix for given  $\mathbf{R}_{N-1}$ .

void saveS (const arma::cx\_mat &S, const int E, const std::string directory)

Saves S matrix (Im and Re part separately).

- void setParameters (const Parameters &parameters)
- ConstantGridSolver ()=default
- $\sim$ ConstantGridSolver ()=default
- ConstantGridSolver (const Parameters &params)

Constructor.

void solveForEnergies (std::string directory)

Performs Numerov calculations for a given set of parameters for all energies.

#### 3.1.1 Constructor & Destructor Documentation

```
3.1.1.1 ConstantGridSolver::ConstantGridSolver() [default]
```

#### **3.1.1.2** ConstantGridSolver::~ConstantGridSolver( ) [default]

3.1.1.3 ConstantGridSolver::ConstantGridSolver (const Parameters & params) [explicit]

Constructor.

#### 3.1.2 Member Function Documentation

3.1.2.1 arma::cx\_mat ConstantGridSolver::calculateEM ( int j, double E )

Calculates  $\mathbf{E}^-(x_i, E)$  matrix.

This method calculates  $\mathbf{E}^-$  matrix for for a given point  $x_j$  on the grid and given energy. The matrix is diagonal and its elements are calculated the following way:

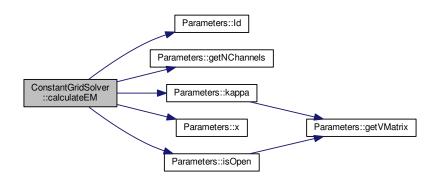
- $\mathbf{E}_{n,n}^-(x_j,E) = \exp(-ikx_j)$  if channel n is open
- $\mathbf{E}_{n,n}^-(x_j,E) = \cosh(kx_j)$  if channel n is closed
- $\mathbf{E}_{n,m}^{-}(x_{i},E) = 0$  for  $n \neq m$

#### **Parameters**

j	
Ε	

Returns

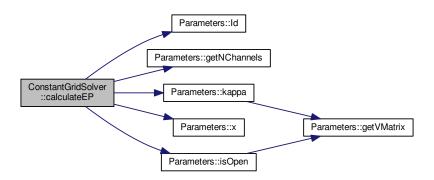
Here is the call graph for this function:



3.1.2.2 arma::cx\_mat ConstantGridSolver::calculateEP ( int j, double E )

Calculates  $\mathbf{E}^+(x_j, E)$  matrix.

Here is the call graph for this function:



#### 3.1.2.3 arma::cx\_mat ConstantGridSolver::calculateS ( const arma::cx\_mat R\_N, double E )

Calculates S matrix for given  $\mathbf{R}_{N-1}$ .

This method calculates the scattering matrix  $\mathbf{S}(E)$ . Its value is given by

$$\mathbf{S} = (\mathbf{R}_{N-1}\mathbf{e}_{N-1}^{+} - \mathbf{e}_{N}^{+}) - 1(\mathbf{R}_{N-1}\mathbf{e}_{N-1}^{-} - \mathbf{e}_{N}^{-})$$
(3.1)

where  $\mathbf{e}_i^\pm = (\mathbf{I} - \mathbf{T}_i) \mathbf{E}_i^\pm.$ 

**Parameters** 

R_N	$-\mathbf{R}_{N-1}$
Ε	- energy

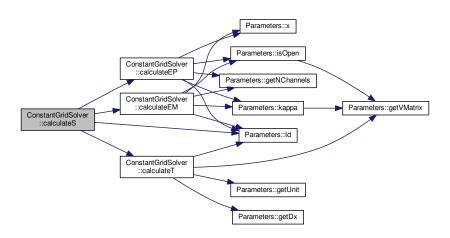
**Returns** 

S

**Exceptions** 

std::runtime_error   if there is a problem with calculating	sta::runtime error	if there is a problem with calculating
---	--------------------	--

Here is the call graph for this function:



### 3.1.2.4 arma::cx\_mat ConstantGridSolver::calculateT ( int j, double E ) const

Calculates  $T(x_j, E)$  matrix.

This method calculates T matrix for a given point  $x_j$  on the grid and given energy according to the formula:

$$\mathbf{T}_{j} = -\frac{dx}{12}\mathbf{Q}_{j}.\tag{3.2}$$

#### **Parameters**

j	- index of the value on the grid
Ε	- energy

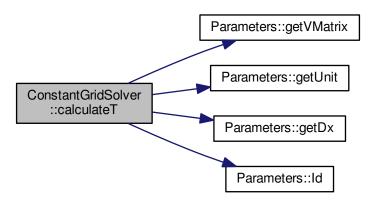
#### Returns

$$\mathbf{T}(x_j, E)$$

### **Exceptions**

std::invalid_argument	if the index $j$ is wrong
-----------------------	---------------------------

Here is the call graph for this function:



#### 3.1.2.5 arma::cx\_mat ConstantGridSolver::calculateU ( int j, double E )

Calculates  $U(x_i, E)$  matrix.

This method calculates  $\mathbf{U}$  matrix for given index j using the set of parameters provided to the ConstantGridSolver object according to the following formula:

$$\mathbf{U}_{i} = 12(\mathbf{I} - \mathbf{T}_{i}) - 1 - 10\mathbf{I}. \tag{3.3}$$

#### **Parameters**

in	j	- index on the grid of x value	
in	E	- energy value	

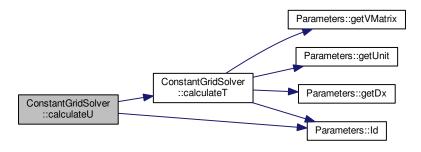
Returns

$$\mathbf{U}(x_i, E)$$

#### **Exceptions**

std::invalid_argument	if $x_j$ does not exist

Here is the call graph for this function:



3.1.2.6 arma::cx\_mat ConstantGridSolver::fwdIteration ( const arma::cx\_mat & B, double E )

Iterates Numerov algorithm forward up to N-1 and returns  $\mathbf{R}_{N-1}$  matrix for a given energy.

This method performs the Numerov iteration for a given energy for a case of some particular symmetry.

The initial value  $\mathbf{R}_0^{-1}$ :

- $\mathbf{R}_0^{-1} = \mathbf{0}$  if no symmetries
- +  ${f R}_0^{-1} = {f U}_0^{-1}({f I} + {f B})$  if the symmetry is described by  ${f B}$

Every value depends on the previous one:  $\mathbf{R}_j = \mathbf{U}_j - \mathbf{R}_{j-1}^{-1}$ .

#### Parameters

in	В	- B matrix to calculate the initial value	
in	Ε	- energy	

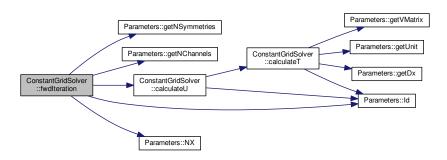
Returns

 $\mathbf{R}_{N-1}$ 

#### **Exceptions**

std::invalid_argument	if $\mathbf{U}_i$ cannot be calculated for given iteration $i$
std::runtime_error	

Here is the call graph for this function:



3.1.2.7 void ConstantGridSolver::modifyCCnj ( arma::cx\_mat & n1, arma::cx\_mat & n0, arma::cx\_mat & j1, arma::cx\_mat & j0, double E )

Modifies closed channels elements.

Here is the call graph for this function:



3.1.2.8 void ConstantGridSolver::saveS ( const arma::cx\_mat & S, const int E, const std::string directory )

Saves S matrix (Im and Re part separately).

This method saves the scattering matrix in a given directory. The real and imaginary part of S are saved in separate files.

Paths:

 $Re(\mathbf{S})$ : directory/re\_SE.dat (E is the value of the energy)  $Im(\mathbf{S})$ : directory/im\_SE.dat (E is the value of the energy) Parameters

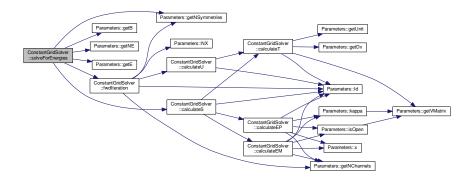
S	- scattering matrix to be saved	
Е	- energy	
directory	- where to save the files	

3.1.2.9 void ConstantGridSolver::setParameters ( const Parameters & parameters ) [inline]

3.1.2.10 void ConstantGridSolver::solveForEnergies ( std::string directory )

Performs Numerov calculations for a given set of parameters for all energies.

Here is the call graph for this function:



The documentation for this class was generated from the following files:

- ConstantGridSolver.h
- · ConstantGridSolver.cpp

#### 3.2 Parameters Class Reference

#include <Parameters.h>

#### **Public Member Functions**

void loadParams (std::string="Params.txt")

Reading the values of parameters from the file generated in Mathematica.

• void setXValues ()

Setting xValues.

- FRIEND\_TEST (ParametersInputTest, setXValues\_failsIfXMaxLessOrEqualXMin)
- FRIEND TEST (ParametersInputTest, setXValues failsIfInvalidDX)
- FRIEND\_TEST (ParametersInputTest, setXValues\_failsIfInvalidCombinationOfXMinXMaxDx)
- FRIEND\_TEST (ParametersInputTest, setXValues\_worksGoodForCorrectValues)
- void loadE (std::string filename="E.dat")

Reading the values of energies from the file generated in Mathematica.

void loadV (std::string filename="V.dat")

Reading the values of V from the file generated in Mathematica.

- FRIEND\_TEST (Parameters\_loadV\_Test, failsForIncorrectNumberOfRows)
- FRIEND TEST (Parameters loadV Test, worksGoodForGoodFileOneChannel)
- FRIEND\_TEST (Parameters\_loadV\_Test, worksGoodForGoodFileTwoChannels)

void loadB (std::string filename="B")

Reading the values of B from the file generated in Mathematica.

- FRIEND\_TEST (ParametersInputTest, loadB\_failsIfAnyFileDoesNotExistAndPositiveNSymmetries)
- FRIEND\_TEST (ParametersInputTest, loadB\_worksGoodForGoodFilesOneChannel)
- FRIEND TEST (ParametersInputTest, loadB failsIfAnyFileIsIncorrect)
- bool checkNumberOfRowsInFile (std::string filename, const int required\_number\_of\_columns)
- Parameters ()=default
- ∼Parameters ()=default
- Parameters (std::vector< std::string > filenames)

From a given directory takes all the needed values and creates Parameters object.

• arma::cx\_mat getVMatrix (int) const

V matrix for a given x\_i.

- double getE (int) const
- int NX () const
- double getXMin () const
- double getXMax () const
- double getDx () const
- double x (int i) const
- FRIEND\_TEST (ParametersOutputTest, x\_worksCorrectForNegativeIndices)
- · double getUnit () const
- int getNChannels () const
- int getNE () const
- arma::cx\_mat getB (int i) const
- int getNSymmetries () const
- int getGrid\_points\_per\_lambda () const
- · arma::cx\_mat ld () const
- · bool isOpen (int nChannel, double energy) const

Check if the channel is open.

- double kappa (int n1, int n2, int i, double E) const
- double kappa (int n1, int n2, double x, double E) const
- arma::cx mat getV (double x) const

Linear interpolation of V (works also for V given on non-constant grid if needed)

• double lambda (double x, double E) const

de Broglie length for a given potential and x

• double requiredDx (double x, double E) const

#### **Friends**

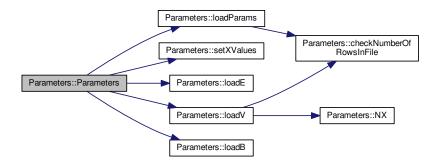
- class Parameters\_loadV\_Test
- class Parameters\_isOpen\_Test
- · class Parameters\_kappaInt\_Test
- · class Parameters\_kappaDouble\_Test
- class Parameters\_getV\_Test
- · class Parameters lambda Test
- class Parameters\_requiredDX\_Test

#### 3.2.1 Constructor & Destructor Documentation

- **3.2.1.1 Parameters::Parameters()** [default]
- **3.2.1.2** Parameters::~Parameters() [default]
- **3.2.1.3 Parameters::Parameters ( std::vector** < std::string > filenames ) [explicit]

From a given directory takes all the needed values and creates Parameters object.

Here is the call graph for this function:



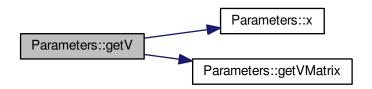
#### 3.2.2 Member Function Documentation

- 3.2.2.1 bool Parameters::checkNumberOfRowsInFile ( std::string filename, const int required number of columns )
- 3.2.2.2 Parameters::FRIEND\_TEST ( ParametersInputTest , setXValues\_failsIfXMaxLessOrEqualXMin )
- 3.2.2.3 Parameters::FRIEND\_TEST ( ParametersInputTest , setXValues\_failsIfInvalidDX )
- 3.2.2.4 Parameters::FRIEND\_TEST ( ParametersInputTest , setXValues\_failsIfInvalidCombinationOfXMinXMaxDx )
- 3.2.2.5 Parameters::FRIEND\_TEST ( ParametersInputTest , setXValues\_worksGoodForCorrectValues )
- 3.2.2.6 Parameters::FRIEND\_TEST ( Parameters\_loadV\_Test , failsForIncorrectNumberOfRows )
- 3.2.2.7 Parameters::FRIEND\_TEST ( Parameters loadV Test , worksGoodForGoodFileOneChannel )
- 3.2.2.8 Parameters::FRIEND\_TEST ( Parameters\_loadV\_Test , worksGoodForGoodFileTwoChannels )
- 3.2.2.9 Parameters::FRIEND\_TEST ( ParametersInputTest , loadB\_failsIfAnyFileDoesNotExistAndPositiveNSymmetries )
- 3.2.2.10 Parameters::FRIEND\_TEST ( ParametersInputTest , loadB\_worksGoodForGoodFilesOneChannel )
- 3.2.2.11 Parameters::FRIEND\_TEST ( ParametersInputTest , loadB\_failsIfAnyFileIsIncorrect )
- 3.2.2.12 Parameters::FRIEND\_TEST ( ParametersOutputTest , x\_worksCorrectForNegativeIndices )
- **3.2.2.13** arma::cx\_mat Parameters::getB ( int i ) const [inline]
- 3.2.2.14 double Parameters::getDx ( ) const [inline]

```
3.2.2.15 double Parameters::getE( int i) const
3.2.2.16 int Parameters::getGrid_points_per_lambda( ) const [inline]
3.2.2.17 int Parameters::getNChannels( ) const [inline]
3.2.2.18 int Parameters::getNE( ) const [inline]
3.2.2.19 int Parameters::getNSymmetries( ) const [inline]
3.2.2.20 double Parameters::getUnit( ) const [inline]
3.2.2.21 arma::cx_mat Parameters::getV ( double x ) const
```

Linear interpolation of V (works also for V given on non-constant grid if needed)

Here is the call graph for this function:



3.2.2.22 arma::cx\_mat Parameters::getVMatrix ( int i ) const

V matrix for a given x\_i.

3.2.2.23 double Parameters::getXMax( ) const [inline]

3.2.2.24 double Parameters::getXMin() const [inline]

3.2.2.25 arma::cx\_mat Parameters::ld( )const [inline]

3.2.2.26 bool Parameters::isOpen (int nChannel, double energy) const

Check if the channel is open.

Here is the call graph for this function:



3.2.2.27 double Parameters::kappa (int n1, int n2, int i, double E) const

Here is the call graph for this function:



3.2.2.28 double Parameters::kappa (int n1, int n2, double x, double E) const

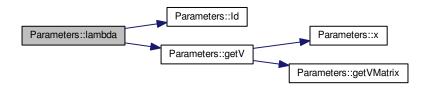
Here is the call graph for this function:



3.2.2.29 double Parameters::lambda ( double x, double E ) const

de Broglie length for a given potential and x

Here is the call graph for this function:



3.2.2.30 void Parameters::loadB ( std::string filename = "B" )

Reading the values of B from the file generated in Mathematica.

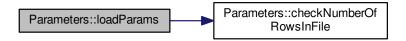
3.2.2.31 void Parameters::loadE ( std::string filename = "E.dat" )

Reading the values of energies from the file generated in Mathematica.

3.2.2.32 void Parameters::loadParams ( std::string filename = "Params.txt" )

Reading the values of parameters from the file generated in Mathematica.

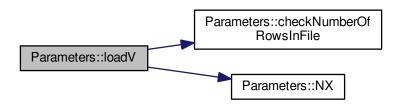
Here is the call graph for this function:



3.2.2.33 void Parameters::loadV ( std::string filename = "V.dat" )

Reading the values of V from the file generated in Mathematica.

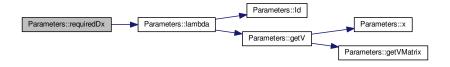
Here is the call graph for this function:



3.2.2.34 int Parameters::NX ( ) const

3.2.2.35 double Parameters::requiredDx ( double x, double E ) const

Here is the call graph for this function:



3.2.2.36 void Parameters::setXValues ( )

Setting xValues.

```
3.2.3.7 double Parameters::x (int i) const [inline]
3.2.3 Friends And Related Function Documentation
3.2.3.1 friend class Parameters_getV_Test [friend]
3.2.3.2 friend class Parameters_isOpen_Test [friend]
3.2.3.3 friend class Parameters_kappaDouble_Test [friend]
3.2.3.4 friend class Parameters_kappaInt_Test [friend]
3.2.3.5 friend class Parameters_lambda_Test [friend]
3.2.3.6 friend class Parameters_loadV_Test [friend]
3.2.3.7 friend class Parameters_requiredDX_Test [friend]
```

The documentation for this class was generated from the following files:

- · Parameters.h
- Parameters.cpp

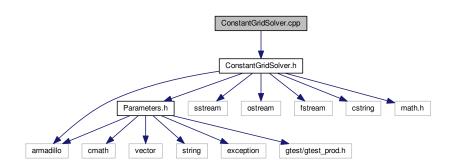
# **Chapter 4**

# **File Documentation**

## 4.1 ConstantGridSolver.cpp File Reference

Definitions of ConstantGridSolver class methods.

```
#include "ConstantGridSolver.h"
Include dependency graph for ConstantGridSolver.cpp:
```



#### 4.1.1 Detailed Description

Definitions of ConstantGridSolver class methods.

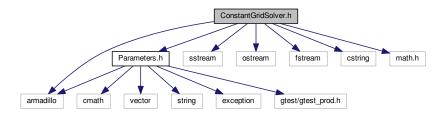
### 4.2 ConstantGridSolver.h File Reference

Definition of ConstantGridSolver class.

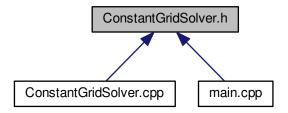
```
#include "armadillo"
#include "Parameters.h"
#include <sstream>
#include <fstream>
#include <cstring>
#include <math.h>
```

20 File Documentation

Include dependency graph for ConstantGridSolver.h:



This graph shows which files directly or indirectly include this file:



#### Classes

· class ConstantGridSolver

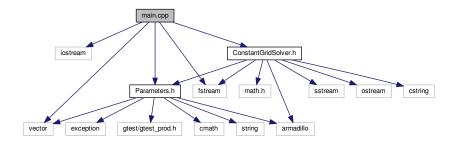
### 4.2.1 Detailed Description

Definition of ConstantGridSolver class. This file contains a definition of ConstantGridSolver class, performing the calculations for a given set of parameters (Parameters object).

## 4.3 main.cpp File Reference

```
#include <iostream>
#include <vector>
#include <fstream>
#include "Parameters.h"
#include "ConstantGridSolver.h"
```

Include dependency graph for main.cpp:



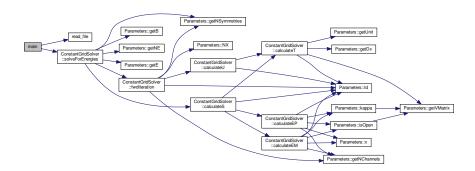
#### **Functions**

- std::vector< std::string > read\_file (std::string filename)
- int main ()

#### 4.3.1 Function Documentation

#### 4.3.1.1 int main ( )

Here is the call graph for this function:



4.3.1.2 std::vector<std::string> read\_file ( std::string filename )

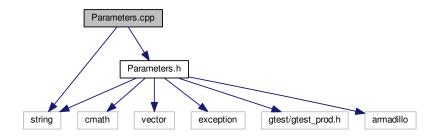
## 4.4 Parameters.cpp File Reference

Definitions of Parameters class methods.

```
#include <string>
#include "Parameters.h"
```

22 File Documentation

Include dependency graph for Parameters.cpp:



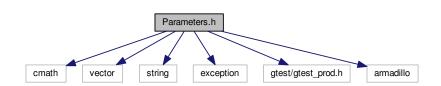
#### 4.4.1 Detailed Description

Definitions of Parameters class methods.

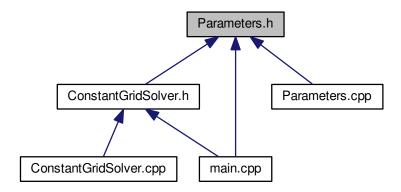
### 4.5 Parameters.h File Reference

Definition of Parameters class.

```
#include <cmath>
#include <vector>
#include <string>
#include <exception>
#include <gtest/gtest_prod.h>
#include "armadillo"
Include dependency graph for Parameters.h:
```



This graph shows which files directly or indirectly include this file:



#### Classes

• class Parameters

## 4.5.1 Detailed Description

Definition of Parameters class. This file contains the definition of Parameters class.

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