



Project6 Quantum: The Quantum Mechanical Package

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Project Report
(Group 6)



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Title
Introduction
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Problem Analysis:

Matrix-Matrix Multiplication

Matrix-Vector Multiplication

Vector-Vector Multiplication

Matrix & Vector Transpose

Eigen vector and Eigen Values

- Matrix Class
- Vector Class
- Math kernel library

[-libp6quantum.so](http://libp6quantum.so)



Task Allocation

Engine
-QMatrix
-QVector

Documentation

Problem
Implementation



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C++

Classes in separate files

mkl libraries

Makefile to compile the package

Shared library

- libp6quantum.so

Doxgyen : Documentation

Version Control

Mercurial (Hg)

<https://emenkah@bitbucket.org/project6quantum/repo6>

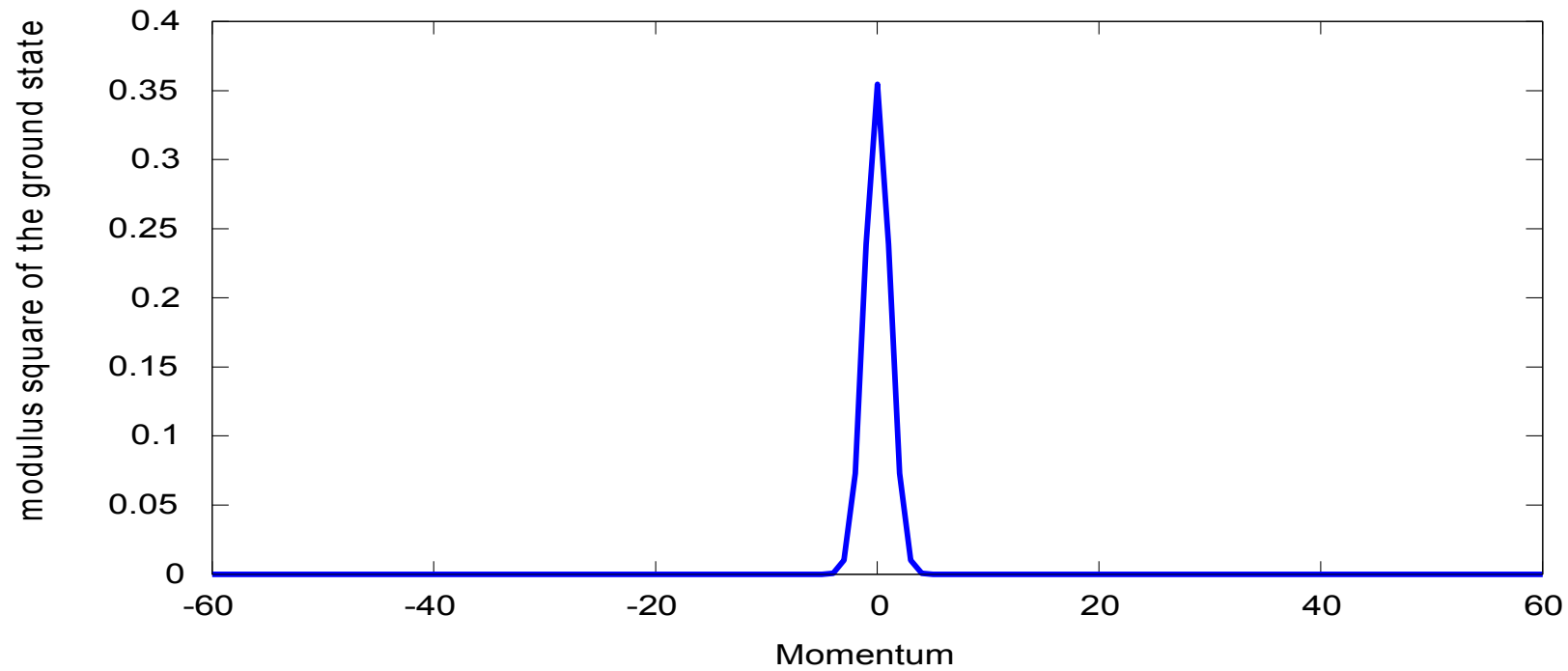
Hamiltonian of the quantum harmonic oscillator:

$$\frac{1}{2m} \left(\frac{2\bar{u}p}{L} \right)^2 \delta_{p,p'} + \frac{m\omega^2 L^2}{(2\bar{u}(p-p'))^2} \cos((p-p')\bar{u}) (1 - \delta_{p,p'}) + \frac{m\omega^2 L^2}{24} \delta_{p,p'}$$

$$\delta_{p,p'} = \begin{cases} 1 & p = p' \\ 0 & p \neq p' \end{cases}$$


Output

Modulus square of the ground state of harmonic oscillator in momentum space






Team Work

 repo6

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Author	Commit	Message	Date	Builds
ss	0f98de8	ssds	3 minutes ago	
Saeid	3482009	sss	8 minutes ago	
elliot	b6b2000	Mainpage for Documentation	an hour ago	
roya_moghadasi	203eada	Calculating the zero eigenstate and Energy expectation value	an hour ago	
roya_moghadasi	2fda6fc	merge	10 hours ago	
roya_moghadasi	e309153	Make Quantum input in main.cpp	10 hours ago	
elliot	110e0aa	Presentation Slide	10 hours ago	
alireza	206ae7b	improve multiplication $V=V(\text{transpose})^*M$	15 hours ago	
alireza	444b7c0	erge and fix mem error	16 hours ago	
Saeid	32d0541	I added ...	17 hours ago	
alireza	9aa7f81	fix comment errors	18 hours ago	
alireza	ca5ab57	merged	18 hours ago	
alireza	49f4c7c	deleted fried function	18 hours ago	
elliot	3c7763a	Text Correction in qvector.h file	18 hours ago	
Elliot Menkah	817bee6	merged	18 hours ago	
elliot	8a7cac7	Documentation generation	18 hours ago	
alireza	b7663f9	$V=Matrix^*V$	20 hours ago	
alireza	193d8aa	Add implemmentation of $V=M^*V$	yesterday	
saeid	098f767	Implimentin of * with cblas	yesterday	
alireza	0a7d92a	implement qvector::operator=	yesterday	



Project6 QAUNTUM 1.0

A project aimed at solving some quantum mechanical problems based on linear algebra library

Main Page	Data Structures	Files	
Data Structures	Data Structure Index	Class Hierarchy	

[Public Member Functions](#) | [Protected Member Functions](#) | [Protected Attributes](#)

QMatrix Class Reference

Declaration and Usage of the base class which shows the interface for implementation of program. [More...](#)

```
#include <qmatrix.h>
```

Inheritance diagram for QMatrix:



Public Member Functions

QMatrix (int nr, int nc)
QMatrix (const QMatrix &matrix)
QMatrix & operator= (const QMatrix &matrix)
QMatrix operator* (QMatrix &matrix)
operator double () const
double & operator() (int row_index, int col_index) const
double & operator() (int row_index, int col_index)
QVector EigenValues (QMatrix &A)
QMatrix Transpose ()
double Trace ()
void Save2File (char *filename)
void FillMatrix ()
int getDimensionSize (int dim) const



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- libp6quantum.so

$$H^{(op)} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$