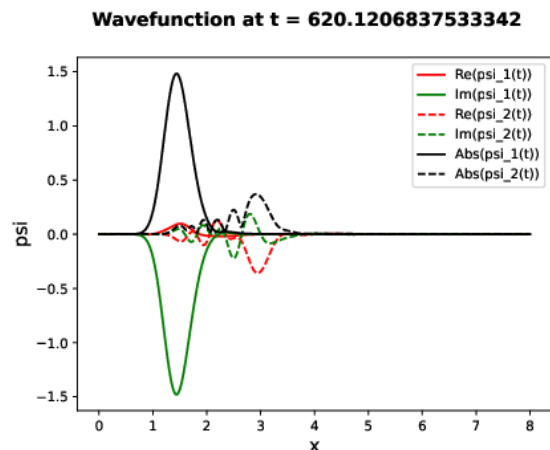# quantumGrid Documentation
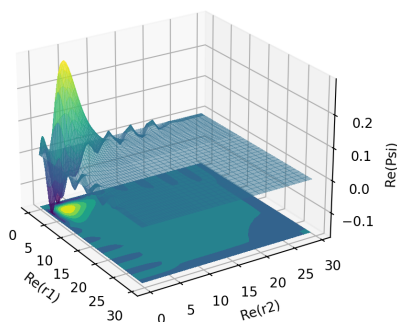
Zachary Streeter

Apr 26, 2021

CONTENTS:

Real_Psi_on_2D_ECS_grid

Brought to you by the AMO theory group at Berkeley National Lab.

Note: The image above is for a scattered wave on a 2D FEM-DVR grid which was created with POV-Ray. The next two figures were created with the example scripts time_dep_two_potential_excitation and two_electron, respectively.

quantumGrid is a package for solving a 1-D Schrödinger equation for an arbitrary potential on any interval. The heart of this package is using a Finite Element Method with a Discrete Variable Representation (FEM-DVR) grid to solve the time-dependent or time-independent Schrödinger equation. This grid provides a compact supported foundation for numerically accurate integration and also allows for a natural application of outgoing scattering boundary conditions by adding a complex tail as the last finite element of the FEM-DVR grid, called *exterior complex scaling* (ECS). Therefore, this grid can be applied to scattering problems where the resonances become square integrable under this complex rotation of the Hamiltonian.

ONE

MOTIVATION

This python package was created for a graduate course in time-dependent quantum mechanics at UC Davis. Given the generality and usefulness of a Finite Element Method - Discrete Variable Representation (FEM-DVR) grid for solving the Schrödinger equation and simple scattering problems, we wanted to go open source and provide this numerical tool for others in the name of science!

TWO

CONTRIBUTORS 👥

Thanks goes to these wonderful people ([emoji key](#)):

Willaim (Bill) McCurdy 🖥 📖 🐛

Zachary Streeter🖥 🐛 🤔

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This project follows the [all-contributors](#) specification. Contributions of any kind welcome!

INSTALLATION

3.1 Recommended

Before going further using conda, you should always update your conda package system:

```
$ conda update -y conda
```

First, we always recommend to create a conda environment for using our package. This is the general recommended procedure so there are no dependency issues and systemic issues that could break other parts of your computer. To create a conda environment named "DVRenv" run this command in your terminal:

```
$ conda create -n DVRenv
```

Now we want all the rest of the packages to only be installed into this environment so activate it before moving forward:

```
$ conda activate DVRenv
```

If you have Anaconda intergrated with your shell, you should see *(DVRenv)* in the front of your prompt, indicating you are now in the *DVRenv* environment. If you do not have Anaconda integrated with your shell, then run the following command and confirm you see *DVRenv* on the next line in your terminal:

```
$ echo $CONDA_DEFAULT_ENV
$ DVRenv
```

Now the quantumgrid package is on the PyPI index so we need to install pip to access that index.

```
(DVRenv) $ conda install pip
```

(Note that this pip will only be installed in our *DVRenv* environment!)

Now we can install quantumgrid!

```
(DVRenv) $ pip install quantumgrid
```

Now you should be able to use the quantumgrid package in your *DVRenv* conda environment! You can also run the example scripts simply by executing (see example directory for more details):

```
(DVRenv) $ ecs_femdvr_time_indep_h2
(DVRenv) $ ecs_femdvr_time_indep_h2 --want_to_plot=true
```

3.2 From sources

The sources for quantumGrid can be downloaded from the Github repo.

You can either clone the public repository:

```
$ git clone git://github.com/zstreeter/quantumGrid
```

Or download the tarball:

```
$ curl -OJL https://github.com/zstreeter/quantumGrid/tarball/master
```

Once you have a copy of the source, you can install it with:

```
$ python setup.py install
```

FOUR

BACKGROUND

These notes are an introduction to Discrete Variable Representations (DVRs) using an example that has particularly general applicability. The Finite Element Method with a Discrete Variable Representation (FEM-DVR) provides a way to solve the time-independent or time-dependent Schrödinger equation that, like all DVR methods, is more accurate and faster than finite difference. This method is one of a family of Discrete Variable Representations that are in common use today in chemistry and physics. It can be applied to problems with any potential on any interval. These notes explain the FEM-DVR method using Gauss-Lobatto quadrature, and also outline the Crank-Nicolson propagator for solving the time-dependent Schrödinger equation.

4.1 Introduction

Here we describe a method for solving the Schrödinger equation for a particle moving in one dimension with coordinate x for any potential $V(x)$ on any interval of x. The variational method of course provides a way to do so, but its application generally poses a practical problem we would like to overcome: If we expand the unknown wave function in $H|\Psi\rangle = E|\Psi\rangle$ in a finite set of basis functions

$$|\Psi\rangle \approx \sum_{n=1}^{N} c_n |\varphi_n\rangle$$

substitute it into the Schrödinger equation, and project from the left with $\langle\varphi_m|$, we come quickly to the familiar matrix representation

$$\mathbf{H}\vec{c} = E\vec{c}$$

$$\text{with} \quad H_{mn} = \langle\varphi_m|\hat{T}|\varphi_n\rangle + \langle\varphi_m|\hat{V}|\varphi_n\rangle$$

that we can also get from the variational theorem. This is a variational basis representation of the Schrödinger equation.

To construct this matrix eigenvalue problem we need the matrix elements of both the kinetic energy and potential energy operators $\hat{T}$ and $\hat{V}$. If we choose a basis for which the kinetic energy matrix elements are easy to evaluate, energy operators T and then try to apply it to solving this problem for various potentials, we generally find that the matrix elements are difficult to perform for many of those potential functions. The DVR is a way of getting around this problem. It is described in an extensive literature on many kinds of DVR that began in the 1980s with seminal work by John Light in the Chemistry Department at the University of Chicago and his coworkers [[**?**]]. The central idea is this: We choose a particular form of basis functions, no matter what the potential, that are constructed based on a Gaussian quadrature. Then we use that Gaussian quadrature to do every integral in the problem of both the kinetic and potential energy operators. The result is that the potential energy matrix is diagonal

$$\langle\varphi_m|\hat{V}|\varphi_n\rangle = \delta_{nm}V(x_n)$$

where x_n is a Gauss quadrature point. In other words, in this basis set method the potential energy matrix is always diagonal, and there are no potential energy integrals to be evaluated. We only have to evaluate the potential on a grid of