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SQuIDS: A Tool to Solve Time Evolution in finite dimensional (open) Quantum Systems

An Application to Neutrino Oscillations

arxiv:1412.3832

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Outline:

Motivation

Task: Solve time evolution of finite dimensional quantum (sub-)systems:

- Flavor oscillations
- Quantum computation
- Systems with finitely many energy levels
- Spins

Time evolution of closed quantum system: Schrödinger equation

$$i\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle \qquad (\hbar = 1) \tag{1}$$

Density matrices instead of state vectors

Often: finite dimensional system S coupled to a complicated (but uninteresting) environment E

$\rightarrow$ Get rid of Environment (keyword: partial trace)

$\rightarrow$ Just consider degrees of freedom of interest

Consequence: Decoherence

- Subsystem cannot be described by pure state $|\psi\rangle$
- Mixed state: Described by density matrix $\varrho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$

Example: Neutrino oscillations in matter

$S \simeq \mathbb{C}^3$	E
flavor degrees of freedom $\lvert\psi\rangle = \sum_{\alpha=e}^{\tau} \psi_\alpha \lvert\nu_\alpha\rangle$	all remaining d.o.f (momenta, spins, ...) $\rightarrow$ infinite dimensional

- We are not at all interested in E
- Only the ν flavor composition is interesting to us
- **But**: E significantly influences flavor d.o.f.

$\Rightarrow$ Need effective description!

Time evolution of the density matrix

Master equation(s): (multiple density matrices possible)

$$\frac{\mathrm{d}\varrho_j}{\mathrm{d}t} = -i[\hat{H}_j(t), \varrho_j(t)] + \{\Gamma_j(t), \varrho_j(t)\} + F_j[\{\varrho_k\}_k, t]$$

- Why multiple ϱ_j? E.g.: One per energy bin!
- $\hat{H} = \hat{H}_0 + \hat{H}_1(t)$: Unitary evolution
- Γ: Decoherence
- F: Other non-linear effects (coupling between ϱ_j)

Simple Example: ν Oscillations in Vacuum

Neutrino Experiment:

- Fixed baseline L
- N energy bins $\{E_j\}_j$
- $\hat{H}^j = \hat{H}_0^j = E_j \cdot \mathbb{I} + \frac{1}{2E_j}\mathbb{M}^2$
- $\Gamma \equiv 0$
- $F \equiv 0$
- $\varrho_j(t) = \sum_{\alpha=e}^{\tau} \phi_\alpha^j(t)|\nu_\alpha\rangle\langle\nu_\alpha|$

$$\mathbb{M} = \sum_{j,k=1}^{3} (\mathbb{M}_0)_{jk}|\nu_j\rangle\langle\nu_k| = \sum_{\alpha,\beta=e}^{\tau} (\mathbb{M}_1)_{\alpha\beta}|\nu_\alpha\rangle\langle\nu_\beta|$$

$$\mathbb{M}_0 = \begin{pmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{pmatrix}$$

$$\mathbb{M}_1 = U_{\mathrm{PMNS}}^\dagger \mathbb{M}_0 U_{\mathrm{PMNS}}$$

Some Important Considerations

The master equation simplifies to

$$\frac{\mathrm{d}\varrho_j}{\mathrm{d}t} = -i[\hat{H}_0^j, \varrho_j(t)]$$

Further simplifications

- Consider in mass basis: $\hat{H}_0^j$ is diagonal
- Depends only on commutator!
  - $[A, \mathbb{I}] = 0 \Rightarrow [\hat{H}_0^j, \varrho_j(t)] = [\hat{H}_0^j - \epsilon_j \mathbb{I}, \varrho_j(t)]$
  - $\epsilon_j := E_j + {m_1^2}/{2E_j}$

$$\tilde{H}^j = \frac{1}{2E_j} \begin{pmatrix} 0 & 0 & 0 \\ 0 & \Delta m_{21}^2 & 0 \\ 0 & 0 & \Delta m_{31}^2 \end{pmatrix}$$

Some Important Considerations (ctd.)

Can solve H_0 evolution analytically!

- Pass to interaction picture:

$$\tilde{\varrho}(t) := \exp(iH_0 t)\varrho \exp(-iH_0 t)$$
$$\Rightarrow \dot{\varrho} = -i[H_0, \rho] + \exp(-iH_0 t)\dot{\tilde{\varrho}} \exp(iH_0 t)$$

- Can subtract $-i[H_0, \varrho]$ on both sides of master equation
- Must transform all terms to interaction picture (SQuIDS does that automatically and efficiently)

Some Important Considerations (ctd.)

All matrices in our system are hermitian: $A^\dagger = A$

- Hermitian $n \times n$ matrices form $N = n^2$ dimenional real vector space
- Convenient basis: $SU(n)$ generators σ_i (e.g. $n = 2$: Pauli matrices $+$ identity)
- Decompose: $\varrho = \sum_{i=0}^{n^2-1} \rho_i \cdot \sigma_i$
- Components ρ_i form n^2 dimensional vector called `SU_vector` in the following

Summary

What did we learn so far (in general):

1. We passed to density matrix formulation (allows for mixed states)
2. Formulated master equation
3. Can subtract $\epsilon_0 \cdot \mathbb{I}$ from $\hat{H}$ (only energy diff. important)
4. Can solve $\hat{H}_0$ exactly (interaction picture) $\varrho \to e^{i\hat{H}_0 t}\varrho e^{-i\hat{H}_0 t}$
5. Can represent $\varrho, H, \ldots$ as n^2 dimensional, real vector (`SU_vector`)!
   $\rightarrow$ Efficient and preserves hermiticity automatically!

SQuIDS

Clone the Repo!

Git Repository includes all needed files (slides, code templates)

Instructions

`cd` to the location where you want to place the repo

```
git clone https://github.com/B0bsen/sm_to_bsm_neutrino.git
cd sm_to_bsm_neutrino
```

Overview

SQuIDS mainly consists out of 3 interconnected classes:

1. `squids::Const`
   - Implements all sorts of constants of nature
   - Conversion between natural units and other unit systems
   - Stores system parameters (mixing angles, energy differences, . . .)

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   - Represents hermitian matrices efficiently
   - Implements all sorts of operations on them (Unitary transformations, trace, commutator, ...)

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2. `squids::SU_vector`
   - Represents hermitian matrices efficiently
   - Implements all sorts of operations on them (Unitary transformations, trace, commutator, . . .)
3. `squids::SQuIDS`
   - Abstract base class, uses `squids::Const` and `squids::SU_vector`
   - Implements time evolution of the system of density matrices
   - Includes methods for taking expectation values etc

SQuIDS - The Const Class

Const - Construction of objects

Can only be default constructed:

```
squids::Const units;
```

- Constructs `squids::Const` object called `units`
- This object contains
  - Different physical constants ($G_F, N_A, G, m_p, \dots$)
  - Values of km, s, J, kg, etc. in natural units
  - Yet unspecified values for:
    - basis change from B_0 to B_1 (e.g. mass and flavor basis)
    - energy differences which can be used for the hamiltonian $\hat{H}_0$

Const - Unit conversion

Easily convert between SI and natural units:

```
squids::Const units;
double L = 10 * units.cm; \\ 506773 eV^{-1}
double T = 1 * units.year; \\ 4.79116e+22 eV^{-1}
double GF = units.GF * (units.GeV * units.GeV); \\
1.16638e-05 GeV^{-2}
```

The units are to be read as `[unit we want]` / [eV$^\alpha$], e.g.:

`km` / [eV^{-1}]: `[Value in eV`$^{-1}$`]` $=$ `[Value in km]` $\cdot$ `km` / [eV^{-1}]

`[Value in km]` $= L$ / `km`

Const - Setting / Getting Mixing Angles

Furthermore you can store system parameters:

```
squids::Const params;
\\ Sets $\theta_{12} = 24^\circ$
params.SetMixingAngle(0, 1, 24 * params.degree);
\\ Sets $\delta_{13} = 2^\circ$
params.SetPhase(0, 2, 2 * params.degree);
\\ Sets $\Delta E_{10} = 7\mathrm{eV}$
params.SetEnergyDifference(1, 7 * params.eV);
```

- Substitute `Set` for `Get`: returns corresponding value
- Energy differences: Only convenience parameters simplifying definition of $\hat{H}_0$

SQuIDS - The Const Class: Exercise

Const class exercise

1. Declare a default constructed const class object
2. Answer the following questions:
   2.1 How many eV^{-1} correspond to $300\,\mathrm{km}$
   2.2 How many radians correspond to 25°
   2.3 If you are 24 years old, how many eV^{-1} are you old?
3. Set the mixing parameters for three neutrino generations to:
   - $\theta_{12} = 33.48^\circ$
   - $\theta_{13} = 8.55^\circ$
   - $\theta_{23} = 42.3^\circ$
4. Set the energy differences to:
   - $\Delta m^2_{21} = 7.5 \cdot 10^{-5}\,\mathrm{eV}^2$
   - $\Delta m^2_{31} = 2.45 \cdot 10^{-3}\,\mathrm{eV}^2$

SQuIDS - The SU_vector Class

SU Vector - Contructors

Construct a SU Vector:

- Default: No entries, no size

```
squids::SU_vector rho;
```

- Defined Dimension: entries are zero, size is $\texttt{dim}(\mathcal{H}) > 0$

```
squids::SU_vector rho(dim); \\size = dim^2
```

And more: construct from `array`, `gsl_matrix_complex`, `std::vector`

...

SU Vector - Special Matrices

Construct a SU Vector to Standard Form:

- Identity: Corresponding matrix is the identity $(Id)_{ij} = \delta_{ij}$

```
squids::SU_vector Id
= squids::SU_vector::Identity(dim);
```

- Projector on state k_0: only the (k_0, k_0) element is 1, i.e. $(\mathbb{P}_{k_0})_{ij} = \delta_{ik_0}\delta_{jk_0}$

```
squids::SU_vector P_k0
= squids::SU_vector::Projector(dim, k0);
```

And more: See documentation (also in the repo)

SU Vector - Functions

Manipulate a SU Vector:

- Rotate from one basis to another ($B_0 \leftrightarrow B_1$): (using angles specfied in params)

```
rho.RotateToB1(params); \\B0 to B1
rho.RotateToB0(params); \\B1 to B0
```

- Return dim of Hilbert space, Size of vector:

```
rho.Dim(); \\returns dim(H)
rho.Size(); \\returns number of elements
```

Furthermore: You can add, subtract multiply (also with scalars), assign, access elements via `rho[]` etc.

SQuIDS - The SU_vector Class: Exercise

SU vector exercise

1. Declare an empty SU vector corresponding to a 3D Hilbert space
2. Initialize an array of projectors for the three mass eigenstates (B_0)
3. Rotate them to the flavor basis (B_1)
4. Initialize a SU vector corresponding to the matrix (B_0)

$$\Delta\mathbb{M}^2 := \begin{pmatrix} 0 & 0 & 0 \\ 0 & \Delta m_{21}^2 & 0 \\ 0 & 0 & m_{31}^2 \end{pmatrix} \tag{2}$$

SQuIDS - The SQuIDS Class

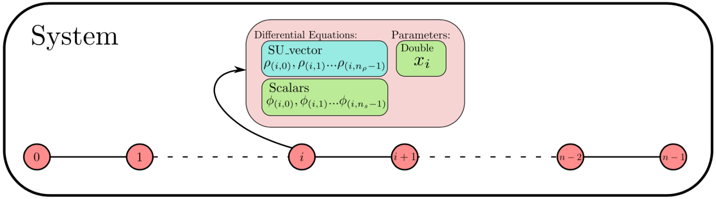
SQuIDS - General Overview pt. I

`squids::SQuIDS` is a so called base class:

- You derive your own class from it
- It provides fundamental functionality through member functions
    - Integration of the master equation
    - Efficient memory management and storage of density matrices
- Already includes several members storing basic data of your system
- Virtual member functions:
    - Some you have to define for the class to work (`H0`, constructors, `init`, ...)
    - Some you can ignore if your system doesn't need them

SQuIDS - General Overview pt. II

Distribution of density matrices across the nodes [arxiv:1412.3832]:


System
Differential Equations:
Parameters:
SU_vector
$\rho_{(i,0)}, \rho_{(i,1)} \cdots \rho_{(i,n_\rho-1)}$
Double
x_i
Scalars
$\phi_{(i,0)}, \phi_{(i,1)} \cdots \phi_{(i,n_s-1)}$
0
1
i
$i+1$
$n-2$
$n-1$

- `n` nodes x_i (energy bins, angles, whatever feature of your system)
- At each node:
  - `nrho` density matrices
  - `ns` scalars (not important for us)

$\rightarrow$ Specify initial data, `H0`, `HI`, `GammaRho`, etc.

$\Rightarrow$ `SQuIDS` evolves the whole system (+ can take expectation values of observables)

SQuIDS - Constructors

Constructors / Initializors: (Set bkg. params and allocate memory)

```
SQuDIS(); \\ default
SQuDIS(uint nx, uint dim, unit nrho, uint nscalar,
double ti = 0);
void ini(uint nx, uint dim, unit nrho, uint nscalar,
double ti = 0);
```

- `nx`: Number of x nodes `x_i`
- `dim`: Dimensions of Hilbert space
- `nrho` / `nscalar`: # density matrices / scalars *per node*
- `ti`: initial time, defaults to zero

Call them in your own constructor with the system parameters you need!

SQuIDS - Member variables

SQuIDS is set up to include the following member variables:

- `std::vector<double> x`: x range
- `uint nsun`: Dim. of Hilbertspace
- `Const params`: `squids::Const` object containing system parameters
- And many more!

You can (and should) access these from within your own member functions!

SQuIDS - Handy functions

Some very useful predefined member functions are:

```
int Set_xrange(double xini, double xend, std::string
scale); \\ Sets x = {xini, ..., xend} with lin or log
scale
```

SQuIDS - Handy functions

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```
int Set_xrange(double xini, double xend, std::string
scale); \\ Sets x = {xini, ..., xend} with lin or log
scale
double Get_x(uint i) const; \\ Returns x[i]
```

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double Get_x(uint i) const; \\ Returns x[i]
const * Const Get_params() const; \\ Returns Const member
```

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int Evolve(double dt); \\ Evolves System by dt
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int Evolve(double dt); \\ Evolves System by dt
double GetExpectationValue(SU_vector op, uint irho, uint
ix) const; \\ Calculates exp.  val.  of op at node ix with
density matrix irho at current time
```

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density matrix irho at current time
```

Of course there are more but these are most important for us!

SQuIDS - Evolution functions

Last but not least: The time independent Hamiltonian `H0`

```
SU_vector H0(double x, uint irho) const;
```

- Returns $\hat{H}_0$ as `SU_vector` object
- Assumes that $\hat{H}_0$ diagonal (i.e. given in mass basis `B0` for ν oscillations)
- Cannot modify but can read member variables (const)
- `irho`: `H0` for density matrix at node x_i

SQuIDS - The SQuIDS Class: Exercise

SQuIDS application: Neutrino oscillations in vacuum

General set up: Vacuum Oscillations Experiment with . . .

- Fixed baseline L ($\hat{=}$ time variable)
- `n` logarithmic energy bins: $E \in [10\,\mathrm{MeV}, 10\,\mathrm{GeV}]$
- All neutrinos are produced as electron neutrinos

Use: `x` nodes as energy nodes, one density matrix per node, no scalar functions, only `H0` non-zero

SQuIDS application: Neutrino oscillations in vacuum

1. Declare vacuum class publically derived from squids::SQuIDS class in `vac/src/vacuum.hpp` with methods
   - Default constructor
   - Initializing constructor
   - `H0`
   - `GetProbabilities`
   - Destructor if needed
2. Define the corresponding member functions in `vac/src/vacuum.cpp`
   - `nbins` x-nodes corresponding to number of E bins (log scaled)
   - One density function per node, no scalar functions
   - `nflavor` neutrino flavors
   - Initial condition $\varrho_i(t = 0) = \mathbb{P}_e$ for all $i \in \{1, \ldots, \texttt{nbins}\}$
   - Work in mass basis!!!

SQuIDS application: Neutrino oscillations in vacuum

3. Initialize an object from your class in `vac/src/main.cpp` (`nbins` $=$ 1000, `nflavor` $= 3$, $E \in [10\,\mathrm{MeV}, 10\,\mathrm{GeV}]$)
4. Evolve the system for $L = 300\ \mathrm{km}$
5. Save the oscillation probabilities $P_{e\alpha}(E_j, L)$ to file(s) $\alpha = e, \mu, \tau$
6. Plot them against the energy

Outlook

- So far we only scratched the surface of SQuIDS' abilities
- Setting $\hat{H}_1(t, \varrho), \Gamma(t, \varrho), F(t, \varrho) \neq 0$ opens up possibilities to include decoherence, interactions, etc.
- These extra terms are solved numerically (using `GSL`)
- Examples for neutrinos:
  - Wave packet decoherence
  - Neutrino propagation through the sun / earth
  - Collective neutrino oscillations (early universe, supernovae, ...)
  - Active sterile oscillations by using more than three generations

BACK UP

Installation

What do we need for this tutorial?

- A unix-like (sub-)system
  - Linux
  - Mac (+ Xcode developer tools!)
  - On Windows: WSL
- A C++ compiler
- Make, wget, Git

Use scripts `install_gsl.sh` and `install_SQuIDS.sh` from the repo!

Installation (GSL)

```
cd $HOME
mkdir -p smToBsmLibs/gsl
wget ftp://ftp.gnu.org/gnu/gsl/gsl-latest.tar.gz
tar -zxvf gsl-latest.tar.gz
rm gsl-latest.tar.gz
cd $(find gsl-* | head -n 1)
./configure --prefix=$HOME/smToBsmLibs/gsl
make
make check
make install
LD_LIBRARY_PATH=$HOME/smToBsmLibs/gsl/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH
cd $HOME
rm -rf $(find gsl-* | head -n 1)
```

Installation (SQuIDS)

```
cd $HOME
mkdir -p smToBsmLibs/SQuIDS
git clone https://github.com/jsalvado/SQuIDS.git
cd $(find SQuIDS* | head -n 1)
./configure --with-gsl-incdir=$HOME/smToBsmLibs/gsl/include \
--with-gsl-libdir=$HOME/smToBsmLibs/gsl/lib \
--prefix=$HOME/smToBsmLibs/SQuIDS
make
make test
make install
LD_LIBRARY_PATH=$HOME/smToBsmLibs/SQuIDS/lib:$LD_LIBRARY_PATH # linux only
export LD_LIBRARY_PATH # linux only
cd $HOME
rm -rf $(find SQuIDS* | head -n 1)
```