A Simple Quantum Integro-Differential Solver (SQuIDS)

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Abstract

Simple Quantum Integro-Differential Solver (SQuIDS) is a C++ code designed to solve semi-analytically the evolution of a set of density matrices and scalar functions. This is done efficiently by expressing all operators in an SU(N) basis. SQuIDS provides a base class from which users can derive new classes to include new non-trivial terms from the right hand sides of density matrix equations. The code was designed in the context of solving neutrino oscillation problems, but can be applied to any problem that involves solving the quantum evolution of a collection of particles with Hilbert space of dimension up to six.

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\textsuperscript{a}The code can be found in \url{https://github.com/jsalvado/SQuIDS}

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1. Introduction

The evolution of an ensemble of neutrinos is a many body quantum mechanics problem, where every neutrino is represented by a state in a Hilbert space.

When all neutrinos are produced in the same quantum state and there are no interactions, a pure quantum state evolution is a good approximation. This can be implemented by solving the corresponding Schrödinger equation.

On the other hand, especially at high energies, there are interactions which can mix the states. In this case, the system is represented by a mixed state and therefore the evolution is more naturally described in the context of the density matrix formalism [1, 2, 3].

The possibility of using the symmetries of the problem in order to efficiently solve the evolution, i.e. differential equations, is a well studied topic in applied Mathematics [4]. In this paper, we apply this principle to make explicit the physical degrees of freedom, thus enabling us to solve analytically the evolution due to the time independent part of the
Hamiltonian \((H_0)\). This approach has been also used in the context of two neutrino flavor approximations [3].

The Simple Quantum Integro-Differential Solver (SQuIDS) is a code that implements the evolution of a set of density matrices and scalar functions using a semi-analytic approach. The code is written in object-oriented C++ and contains a base class which sets up the problem by means of virtual member functions. This allows the user to create a derived class which defines the right hand side terms of the differential equation via its implementation of these functions. Numerical integration is performed using the GNU Scientific Library [5].

The code works with a Hilbert space of dimension up to six and allows the inclusion of an arbitrary number of density matrices and scalar functions. The physical degrees of freedom in the problem can be represented in the basis of the generators of the \(SU(N)\) group plus the identity, where \(N\) is the dimension of the Hilbert space, so we write all operators in terms of this basis. The evolution generated by the time independent part of the Hamiltonian and basis changes can be thought as the action of the unitary group on the operators. These transformations are included as analytic expressions in the code. Then, in order to make the numerical solution efficient we solve the evolution of the entire system in the interaction picture [6].

The paper is structured in the following sections: In section 3 we introduce the density matrix formalism. In section 2, we comment on other approaches to solve similar problems. In section 4, we describe the evolution equations in the context of the \(SU(N)\) algebra. In section 5, we describe how this formulation is implemented in the code. Finally, in section 6, we include three simple examples to illustrate some applications: neutrino oscillations in vacuum, Rabi oscillations, and collective neutrino oscillations.

2. Related work

Solving quantum mechanics problems using computers has been a long standing topic of study. Examples of codes that solve the Schrödinger equation in the position representation have been published for both stationary [7] and time evolving [8, 9, 10] many body systems. On the other hand, representation of finite, quantum-mechanical, closed systems has been developed in order to perform quantum computing calculations (see e.g. [11]). In high energy particle physics the need for precise neutrino oscillation calculation has encouraged the development of ad hoc tools to solve two or three level closed quantum systems subject to time varying potentials (see e.g. [12, 13, 14]). This work goes beyond the pure state representation by using the density matrix formalism, which allows us to express in a natural way mixed states, as well as treating open quantum systems. To do this, we have developed a highly efficient representation of states and operators in terms of the generators of the \(SU(N)\) group.

3. Density matrix formalism

3.1. Definition

In quantum mechanics the state of system is given by a vector in a Hilbert space, i.e. \(|\phi_i\rangle \in \mathcal{H}_i\), where \(\mathcal{H}_i\) is the Hilbert space for the \(i\)-th particle. In general we can be interested
in solving a system of many particles and for that the Hilbert space is constructed as $\mathcal{H} = \bigotimes_i \mathcal{H}_i$. For a large number of particles the dimension of this space grows exponentially. Nevertheless in the limit where the different particles do not have quantum correlations and $\mathcal{H}_i$ is the same for all of the single particles of the system, we can approximate the system as a statistical ensemble of single particle quantum states, which is known as a mixed state.

To describe a system in this limit it is convenient to introduce the density matrix formalism. For a given set of states $\{\langle \psi_i | i = 1, ..., n \rangle\}$ and a set of positive real numbers $\{p_i | \sum_i p_i = 1\}$, that are physically interpreted as the probability of the system to be in the $i$-th state, the density operator, which represents the mixed state, is constructed as

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle \langle \psi_i|.$$  

(1)

For a particular basis $\{|u_1\rangle, |u_2\rangle, ..., |u_n\rangle\}$ of the Hilbert space the components of the density matrix can be written as

$$\rho_{lm} = \sum_i p_i \langle u_l | \psi_i \rangle \langle \psi_i | u_m \rangle,$$

(2)

in other words, for a given basis the density operator is represented by a $n \times n$ Hermitian matrix $\rho$.

Is also useful to define the projectors to the $i$-state of a basis,

$$\hat{\Pi}^{(i)} = |u_i\rangle \langle u_i|.$$  

(3)

The expectation value for any operator $\hat{O}$ when the system is described by $\hat{\rho}$ is given by the trace of the matrix product

$$\langle \hat{O} \rangle_\rho = \sum_{lm} O_{lm} \rho_{lm},$$

(4)

where $O_{lm}$ are the components that represent $\hat{O}$ in the same basis as $\rho_{lm}$.

In particular, the expectation value of the projector gives the probability of finding the system in the $i$-state, and is

$$\langle \hat{\Pi}^{(i)} \rangle_\rho = \sum_{lm} \Pi^{(i)}_{lm} \rho_{lm} = p_i.$$  

(5)

### 3.2. Unitary transformations

In general in quantum mechanics, the transformation from one basis to another is always given by a unitary transformation. In this section we describe a way of writing a general unitary transformation in terms of a set of mixing angles and phases. This parametrization is widely used in the context of neutrino physics and is included in the code.

This parametrization can be written as product of two dimensional rotations, in particular,

$$U(\theta_{ij}, \delta_{ij}) = R_{N-1 N} R_{N-2 N} ... R_{45} R_{35} R_{25} R_{15} R_{34} R_{24} R_{14} R_{23} R_{13} R_{12},$$

(6)
where each matrix \( R_{ij} \) is a rotation in the \( ij \) plane with rotation angle \( \theta_{ij} \) and complex phase \( \delta_{ij} \), namely

\[
R_{ij} = \begin{pmatrix}
\vdots \\
\cos \theta_{ij} & \cdots & \sin \theta_{ij} e^{-i\delta_{ij}} \\
\vdots \\
-\sin \theta_{ij} e^{i\delta_{ij}} & \cdots & \cos \theta_{ij} \\
\vdots \\
\vdots
\end{pmatrix}.
\] (7)

In a minimal description only a subset of the \( \delta_{ij} \) are required to be allowed to be non-zero.

An operator in the Hilbert space is transformed using the relation

\[
O_{lm} \rightarrow \sum_{kn} U_{lk}^* O_{kn} U_{nm}.
\] (8)

3.3. System Definition and Time Evolution

Consider a system corresponding to \( n \times n \) nodes, where a node is an object with \( n_{\rho} \) density matrices and \( n_s \) scalar functions, labeled by a parameter \( x \). For notational convenience we define \( \tilde{\rho} \) and \( \tilde{S} \) as the set of all density matrices with elements \( \rho_J \) and set of all scalar functions with elements \( S_K \), respectively, where \( J \) and \( K \) are general indices to label the elements of the sets, \( J \in \{(i,j)\mid i = 0, \ldots, n_x - 1; j = 0, \ldots, n_{\rho} - 1\} \) and \( K \in \{(i,k)\mid i = 0, \ldots, n_x - 1; k = 0, \ldots, n_s - 1\} \).

The evolution of the system is given by two coupled equations: one for the density matrices and another for the scalar functions. The first one is the Von Neumann equation which contains terms for coherent, decoherence, and other interactions. The second one is a Boltzmann-like differential equation for the scalar functions

\[
\frac{\partial \rho_J}{\partial t} = -i[H_J(t), \rho_J] + \{\Gamma_J(t), \rho_J\} + F_J(\tilde{\rho}, \tilde{S}; t),
\] (9)

\[
\frac{\partial S_K}{\partial t} = -\Gamma_K(t)S_K + G_K(\tilde{\rho}, \tilde{S}; t),
\] (10)

where \( H_J \) is the Hamiltonian, \( \Gamma_J \) is the decoherence and attenuation term, \( \Gamma_K \) is the attenuation for the scalar functions, and finally the functions \( F_J \) and \( G_K \) are general functions of the full sets \( \tilde{\rho} \) and \( \tilde{S} \) that may contain non-linear and interaction terms.

The scalar functions can be used to solve the evolution of populations of particles where there is no coherent quantum dynamics. These parameters can also be used to implement any other first-order differential equation.

3.3.1. Interaction Picture Evolution

The Hamiltonian can always be decomposed into one part that does not depend on time \( H_{0J} \) and another that contains the time dependence, \( H_{1J}(t) \)

\[
H_J(t) = H_{0J} + H_{1J}(t).
\] (11)
In a finite Hilbert space the evolution generated by \( H_{0J} \) can be solved analytically. This may dramatically speed up the numerical computation, particularly in the case where \( H_0 \) contains terms that produce very fast oscillations. This motivates expressing the problem in the interaction picture in which an operator \( \hat{O}_J \) is transformed into \( \bar{\hat{O}}_J \) by
\[
\bar{\hat{O}}_J(t) = e^{-iH_{0J}t}\hat{O}_Je^{iH_{0J}t}.
\]
Then, the evolution equations Eq.(9) are
\[
\frac{\partial \bar{\hat{p}}_J}{\partial t} = -i[\bar{H}_1(t), \bar{\hat{p}}_J] + \{\bar{\Gamma}_J(t), \bar{\hat{p}}_J\} + F'_J(\bar{\hat{p}}, \bar{\hat{S}}; t),
\]
\[
\frac{\partial S_K}{\partial t} = -\Gamma_K(t)S_K + G'_K(\bar{\hat{p}}, \bar{\hat{S}}; t),
\]
where \( \bar{H}_1(t) \) is known as the interaction Hamiltonian, and \( F'_J \) and \( G'_K \) are the corresponding \( F_J \) and \( G_K \) in the interaction picture.

4. Density matrix formalism using \( SU(N) \) generators

Every \( \rho_J \) is a Hermitian matrix therefore has, by construction, real eigenvalues and can always be decomposed as a linear combination of the \( SU(N) \) generators plus the identity with real coefficients, being \( N \) the dimension of the Hilbert space. The same applies to all the operators in the right hand side of Eq.(9). Using this decomposition we can write the operators as follows,
\[
\rho_J = \rho^\alpha_J\lambda_\alpha, \quad H_J = H^\alpha_J\lambda_\alpha, \quad \Gamma_J = \Gamma^\alpha_J\lambda_\alpha,
\]
where \( \{\lambda_\alpha|\alpha = 1, ..., N^2 - 1\} \) are the \( SU(N) \) generators, \( \lambda_0 = \mathbb{I} \), and we have use the Einstein convention, i.e. a sum over repeated indices is implicit.

We can use the commutator and anti-commutator relations in the lie algebra,
\[
i[\lambda_\alpha, \lambda_\beta] = -f^\gamma_{\alpha\beta}\lambda_\gamma \quad \text{(18)}
\]
\[
\{\lambda_\alpha, \lambda_\beta\} = d^\gamma_{\alpha\beta}\lambda_\gamma, \quad \text{(19)}
\]
in order to write down the evolution equations Eq.(9, 10)
\[
\frac{\partial \rho^\alpha_J}{\partial t} = H^\beta_J(t)\rho^\alpha_J + \Gamma^\beta_J(t)\rho^\beta_Jd^\gamma_J + F^\gamma_J(\bar{\hat{p}}, \bar{\hat{S}}; t),
\]
\[
\frac{\partial S_K}{\partial t} = -\Gamma_K(t)S_K + G_K(\bar{\hat{p}}, \bar{\hat{S}}; t).
\]
4.1. Unitary transformations and zero order time evolution

Since any hermitian operator $\hat{O}$ can be expressed as linear combination of $\{\lambda_\alpha\}$, then the effect of any linear transformation on $\hat{O}$ only depends on the effect on every element on the basis $\{\lambda_\alpha\}$. In particular, transformations of the form given in Eqs.(6, 12) fall into this category. For Eq.(6) we can write this explicitly

$$\lambda_\alpha \rightarrow U^\dagger(\theta_{ij}\delta_{ij})\lambda_\alpha U(\theta_{ij}\delta_{ij}),$$

(22)
given that Eq.(22) preserves hermiticity and that $\{\lambda_\alpha\}$ spans the hermitian operator space then

$$U^\dagger(\theta_{ij}\delta_{ij})\lambda_\alpha U(\theta_{ij}\delta_{ij}) = u^\beta_\alpha(\theta_{ij}\delta_{ij})\lambda^\beta_\alpha,$$

(23)
where $u^\beta_\alpha(\theta_{ij}\delta_{ij})$ are real functions that are solved analytically in the code.

The same procedure can be applied to the time evolution generated by $\hat{H}_0$ given by Eq.(12), i.e.

$$\bar{\lambda}_\alpha(t) = e^{-i\hat{H}_0 t}\lambda_\alpha e^{i\hat{H}_0 t} = u^\beta_\alpha(t)\lambda^\beta_\alpha,$$

(24)
as before the analytic expressions for $u^\beta_\alpha(t)$ are in the code.

4.2. Interaction Picture Evolution

Give the formalism in Sec. 4.1 a general hermitian operator $\hat{O}$ in the interaction picture is given by

$$\bar{\hat{O}}(t) = e^{-i\hat{H}_0 t}\hat{O} e^{i\hat{H}_0 t} = O^a e^{-i\hat{H}_0 t}\lambda^a_\alpha(t) e^{i\hat{H}_0 t} = O^a\bar{\lambda}^a_\alpha(t).$$

(25)

The commutator and anti-commutator relations holds for the time dependent generators with the same structure constants, which implies that the evolution equations in the interactions picture are the same, but with the $\tilde{H}_{1J}(t)$ instead of $H_J(t)$,

$$\frac{\partial\bar{\rho}^a_J}{\partial t} = \tilde{H}^\beta_{1J}(t)\bar{\rho}^\beta_J + \Gamma^\beta_{1J}(t)\bar{\rho}^\beta_J d\gamma,\quad F^a_J(\bar{\rho},\bar{\tilde{S}},t),$$

(26)
$$\frac{\partial S_K}{\partial t} = -\Gamma_K(t)S_K + G^a_K(\bar{\rho},\bar{\tilde{S}},t).$$

(27)

5. Description of the Code

SQuIDS is a code written in C++ to solve the set of equations specified in the previous section, specifically Eqs.(26, 27). In this section we will describe the classes, functions, and operations defined between the objects that compose the SQuIDS library.

The system structure is shown in Figure 5.1, each $i$-node contains a set of density matrices $\{\rho_{(ij)}\}$ and scalar functions $\{S_{(ik)}\}$ as well as a real number $x_i$ that can play the role of a parameter or label for the node. For example, when we are describing a system in which each node represents a given position $x$ then $x_i \equiv x$, on the other hand when we are describing
a system in which each state is characterized by energy or momentum, then \( x_i \equiv E \) in each node. Even though \( x_i \) can have a physical interpretation, in general it need not to be related to any physical quantity. Furthermore, each node can have an arbitrary number of scalars and density matrices, according to the problem at hand.

All of the classes are declared in the header files contained in the folder SQuIDS/inc/, and the corresponding source code that implements them is in SQuIDS/src/. In particular, the files that contain the analytic solutions for the evolution and rotation Eqs.\((23, 24)\) is included in SQuIDS/inc/SUinc/ up to dimension six. Finally, SQuIDS/resources contains a Mathematica notebook that can be used to generate higher dimension solutions.

5.1. Const

The Const class serves two purposes in the SQuIDS library. First, it contains transformation of physical units to natural units, which enable the user to work on a consistent unit system, as well as some fundamental constants such as Fermi constant, Avogadro number, proton mass, neutron mass, etc. These constant can be access as public members of the class. The full list of constant is listed in Table 1. Second, it manages the mixing angles \( (\theta_{ij}) \) and complex phases \( (\delta_{ij}) \) that define the transformation between the \( B_0 \) and \( B_1 \) basis as defined in Eq.\((6)\), which can be modified and obtained through public member functions. Finally, the class is declared in SQuIDS/inc/const.h and implemented in SQuIDS/inc/const.cpp.

5.1.1. Constructors

- Constructor;
  
  Const();

  Initializes all units and arrays.

5.1.2. Functions

- Set Mixing angle
  
  void SetMixingAngle(unsigned int i, unsigned int j, double theta);

  Sets the rotation angle \( \theta_{ij} \) to \( \theta \).

- Get Mixing angle
  
  double GetMixingAngle(unsigned int i, unsigned int j);

  Returns the rotation angle \( \theta_{ij} \).

- Set complex phase
  
  void SetPhase(unsigned int i, unsigned int j, double phase);

  Set the complex phase \( \delta_{ij} \) to \( \delta \).

- Get complex phase
double GetPhase(unsigned int i, unsigned int j);

Returns the complex phase $\delta_{ij}$.

- Set energy eigenvalue difference
  
  ```c
  void SetEnergyDifference(unsigned int i, double Ediff);
  ```

  Sets the energy eigenvalue difference $\Delta E_{i0} = E_i - E_0$ to `Ediff`. We require $i > 0$.

- Get energy eigenvalue difference
  
  ```c
  double GetEnergyDifference(unsigned int i);
  ```

  Returns the energy eigenvalue difference $\Delta E_{i0}$.

### Physical quantities

| Physical quantities | Description |
|---------------------|-------------|
| GF                  | Fermi constant in natural units |
| Na                  | Avogadro number |
| sw_sq               | $\sin^2(\theta_w)$ where $\theta_w$ is the weak mixing angle |
| G                   | gravitational constant |
| proton_mass         | proton mass |
| neutron_mass        | neutron mass |
| electron_mass       | $e$ mass |
| muon_mass           | $\mu$ mass |
| muon_lifetime       | $\mu$ lifetime |
| tau_mass            | $\tau$ mass |
| tau_lifetime        | $\tau$ lifetime |
| alpha               | fine structure constant |
| e_charge            | unit of electric charge (Lorentz-Heaviside) |

### Units in natural units ($\hbar = c = k_b = 1$)

| Unit       | Description           |
|------------|-----------------------|
| eV         | 1 electron-volt       |
| keV        | $10^4$ electron-volt  |
| MeV        | $10^6$ electron-volt  |
| GeV        | $10^9$ electron-volt  |
| TeV        | $10^{12}$ electron-volt |
| Joule      | 1 Joule               |
| kg         | 1 kilogram            |
| gr         | 1 gram                |
| sec        | 1 second              |
| hour       | 1 hour                |
| day        | 1 day                 |
| year       | 1 year                |
The SU
vector
class is a type that represents an operator in a N-dimensional Hilbert space as a linear combination of the SU(N) generators and is the building block of the SQuIDS library. The real coefficients of the generator plus the identity linear combination are stored as a private double pointer of size N^2. All the right hand side terms of the Von Neumann equation Eq. (26) must be constructed using SU
vector objects. In order to do this, the SU
vector class implements operations such as: addition, subtraction, scaling by a constant, rotation, time evolution, and traces. Of these the time evolution and rotation are the most computationally expensive. In order to improve the efficiency of the code we have implemented algebraic solutions of Eqs. (23, 24) that implement rotation and time evolution respectively, and can be found in the files located in SQuIDS/inc/SU
inc/.

The headers that declare the class and operations are in the files SQuIDS/inc/SUNalg.h and the source code in SQuIDS/inc/SUNalg.cpp. Details of the operation implementation can be found in SQuIDS/inc/detail/ and SQuIDS/inc/SU
inc/.

5.2.1. Constructors

Different constructors and initialization functions are added in order to make more flexible the object initialization.

• Default constructor.

SU
vector();

Table 1: Units and physics constants contained in Const.
Constructs an empty SU_vector with no size.

- Copy constructor.
  
  \[
  \text{SU}_\text{vector}(\text{const SU}_\text{vector}& \ V);
  \]

  The newly constructed SU_vector will allocate its own storage which it will manage automatically.

- Move constructor.
  
  \[
  \text{SU}_\text{vector}(&& \ V);
  \]

  If V owned its own storage, it will be taken by the newly constructed SU_vector, and V will be left empty, as if default constructed.

- Constructor of a zero vector in an N-dimensional Hilbert space.
  
  \[
  \text{SU}_\text{vector}(\text{unsigned int} \ dim);
  \]

  This constructor allocates the memory (which will be managed automatically) for the components of the SU_vector with size given by the argument and initializes it to zero.

- Constructor with a pointer to double.
  
  \[
  \text{SU}_\text{vector}(\text{int} \ dim, \text{double}*)
  \]

  This constructor initializes the SU_vector with dimension given by the value of dim and uses as the SU_vector components the values in the double*. The newly constructed SU_vector will treat the specified data buffer as its backing storage. The user is responsible for ensuring that this buffer is large enough (at least \( dim^2 \)), and has a lifetime at least as long as the constructed vector and any vectors which inherit the use of this buffer from it by move construction or assignment. The contents of the buffer will not be modified during construction.

- \text{gsl_matrix_complex} constructor
  
  \[
  \text{SU}_\text{vector}(\text{const} \ \text{gsl}_\text{matrix}_\text{complex}*)
  \]

  Constructs a SU_vector from a complex hermitian GSL matrix. The \text{gsl_matrix_complex}* contents will copied and not modified.

- Constructor with standard vector.
  
  \[
  \text{SU}_\text{vector}(\text{const std::vector<_double>&} \ \text{vector});
  \]

  Constructs SU_vector of dimension equal to the square root of size of the vector and components given by the contents of the vector. The newly constructed SU_vector will allocate its own storage, but it will copy its component information from vector.
For convenience we also provide factory functions to construct operators that are commonly used such as the identity, projectors, and generators. The following are available:

- **Identity.**

  ```c
  SU_vector Identity(unsigned int dim);
  ```

  Returns a `SU_vector` which represents the identity of a Hilbert space of dimension `dim`.

- **Generator.**

  ```c
  SU_vector Generator(unsigned int dim, unsigned int i);
  ```

  Returns a `SU_vector` that represents the `i`th generator ($\lambda_i$) of a Hilbert space of dimension `dim`.

- **Projector.**

  ```c
  SU_vector Projector(unsigned int dim, unsigned int i);
  ```

  Returns a `SU_vector` that represents the projector operator into the subspace spanned by the `i`-state. Namely, `Projector = diag(0, ..., 0, 1, 0, ..., 0)` where the one is in the `i`th entry.

- **PosProjector.**

  ```c
  SU_vector PosProjector(unsigned int dim, unsigned int i);
  ```

  Returns a `SU_vector` that represents a projector to the upper subspace of dimension `i`, i.e. `PosProjector = diag(1, ..., 1, 0, ..., 0)` where the last one is in the `i-1` entry.

- **NegProjector.**

  ```c
  SU_vector NegProjector(unsigned int dim, unsigned int i);
  ```

  Returns a `SU_vector` that represents a projector to the lower subspace of dimension `i`, i.e. `NegProjector = diag(0, ..., 0, 1, ..., 1)` where the first one is in the `d-i` entry.

### 5.2.2. Functions

In this section we will describe the general functions that are used to manipulate the objects, access the values and do different operations.

- **SetAllComponents.**

  ```c
  void SetAllComponents(double v);
  ```

  Sets all the components of the `SU_vector` to `v`.

- **SetBackingStore.**
void SetBackingStore(double * storage);

Sets the external storage used by the SU\_vector. If the SU\_vector had previously allocated automatically managed storage, that memory will be deallocated; but if it had previously used manually specified storage it will simply cease using that storage without attempting to deallocate it. All data previously stored in the SU\_vector is lost after this function is called.

• Rotate function.
  
  \texttt{SU\_vector} & Rotate(unsigned int \ i, unsigned int \ j, double \ theta, double \ delta) \ \textbf{const};

Returns the rotated SU\_vector by a rotation $R_{ij}$ in the $ij$-subspace by an angle $\theta_{ij}$ (in radians) and complex phase $\delta_{ij}$ (in radians) defined in Eq.(7). In order to make it efficient and general uses the analytic solution form Eq.(23) stored in SQuIDS/inc/SU\_inc.

• Change of basis.
  
  void RotateToB1(const Const& param);
  void RotateToB0(const Const& param);

This functions uses Rotate to transform the SU\_vector from a basis $B0$ to $B1$ or vice versa. The mixing matrix that defines the unitary transformation that relate $B0$ to $B1$, defined in Eqs.(7, 8), are given by the parameters in param. In particular, RotateToB0 transform a SU\_vector from the $B1$ basis to the $B0$ basis, whereas RotateToB1 does the opposite.

• Dimension.
  
  unsigned int Dim(void) \ \textbf{const};

Returns the dimension of the Hilbert space.

• Size of vector array.
  
  unsigned int Size(void) \ \textbf{const};

Returns the number of components of the SU\_vector.

• Evolution by time independent hamiltonian.
  
  SU\_vector Evolve(const SU\_vector& h0, double t) \ \textbf{const};

This function returns a SU\_vector after applying the time evolution driven by the operator $h0$ argument during a time interval $t$. The analytic solutions of Eq.(24) stored in SQuIDS/inc/SU\_inc/ are used. The SU\_vector& operator must be a diagonal operator, therefore a linear combinations of the projector in the $B0$ basis. This choice of the basis makes the evolution more efficient since is not necessary to diagonalize the operator every time.
5.2.3. Operators

Some of the standard C++ operators are overloaded to make more simple and natural writing mathematical expressions. Here we list the operators and how they are defined.

- Logical equality operator (==).
  
  ```cpp
  bool operator == (const SU_vector&)
  ```

  Returns true or false if both SU_vectors are equal.

- Scalar product operator (*).
  
  ```cpp
  double operator * (const SU_vector&)
  ```

  Returns the scalar product of the two vectors, which is equivalent to the trace of the product of the operators that they represent. This operation is useful to compute expectation values, see Eq.(4).

- Product by scalar (*).
  
  ```cpp
  SU_vector operator * (const double)
  ```

  Returns the SU_vector re-scaled by the double.

- Assignation operator (=)
  
  Assigns the value of the SU_vector on the right to the one on the left. The dimensions of the SU_vector must be the same.

- Sum operator (+).
  
  ```cpp
  SU_vector operator + (const SU_vector&)
  ```

  Returns the sum of two SU_vector objects.

- Subtraction operator (-).
  
  ```cpp
  SU_vector operator - (const SU_vector&)
  ```

  Returns the subtraction of two SU_vector objects.

- Negation operator (-)
  
  ```cpp
  SU_vector operator - ()
  ```

  Returns the additive inverse of an SU_vector object.

- Assignment and move assignment operators (=)
  
  ```cpp
  SU_vector & operator = (const SU_vector&);
  SU_vector & operator = (SU_vector&&);
  ```
The assignment operator as well as the move assignment operator are defined. In particular, for the move operator, if the vector is empty or owns its own storage it will switch to using whatever storage was used by other, causing other to relinquish any ownership of that storage. If, however, the vector is non-empty and uses external storage, it will copy other’s data rather than shifting its storage. In this case if the dimensions of the two vectors differ the assignment will fail.

- Assignment addition and subtraction operators (-= +=)
  
  ```cpp
  SU_vector & operator+=(const SU_vector&);
  SU_vector & operator-=(const SU_vector&);
  ```

  These operations combine the addition and subtraction with the assignment as usual in C++.

- Assignment multiplication and division operators (*= /=)
  
  ```cpp
  SU_vector & operator*=(double);
  SU_vector & operator/=(double);
  ```

  These operations combine the multiplication and division by scalars with the SU_vector assignment operation.

- Array like component access.
  
  ```cpp
  double& operator[](int);
  const double& operator[](int) const;
  ```

  Returns the component given by the int argument.

- Ostrem operator (<<).
  
  ```cpp
  friend ostream& operator<<(ostream&, const SU_vector&);
  ```

  Writes the components of the SU_vector in to the ostream object as human-readable text.

5.2.4. External functions

We have also defined quantum mechanical operations between two SU_vector. Furthermore, to optimize the code we have implemented the iCommutator and Anticommutator analytically and stored them in SQuIDS/inc/SU_inc.

- iCommutator.
  
  ```cpp
  SU_vector iCommutator(const SU_vector&, const SU_vector&);
  ```

  Returns the SU_vector result of $i$ times the commutator of the SU_vector objects given as an arguments Eq.(18).
• Anticommutator.

\[
\text{SU\_vector } \text{ACommutator} (\text{const SU\_vector}&, \text{const SU\_vector}&);
\]

Returns the SU\_vector result of the anti-commutator of the SU\_vectors objects given as an arguments Eq. (19).

• Trace function.

\[
\text{double } \text{SUTrace} (\text{const SU\_vector}&, \text{const SU\_vector}&);
\]

Returns the trace of the product of the two operators represented by the SU\_vectors given in the arguments. It is the same as the scalar product.

5.2.5. Usage and optimization

A SU\_vector of dimension N has \(N^2\) components that are stored as a private double*. By default SU\_vector will automatically allocate sufficient ‘backing storage’ to contain these. It is, however, possible to specify that an SU\_vector should treat some externally provided buffer as its backing storage. In this case the size and lifetime of that buffer are the responsibility of the user, so users are encouraged to avoid using this mode unless it is required by their application, as its use is more difficult and requires much greater care. The external storage mode is primarily useful because it allows interfacing with other, low-level numerical codes efficiently.

As described in the previous sections SU\_vector provides overloaded mathematical operators so that algebra can be written in a natural way. Furthermore, the SQuIDS library has a limited ability to optimize away temporary objects (via a partial expression template system). That is, all operations of the forms

\[
v1 \ [\text{Op1}]= v2 \ [\text{Op2}] \ v3;
v1 \ [\text{Op1}]= s \ * \ v2;
\]

where \(v1\), \(v2\), and \(v3\) are pre-existing objects of type SU\_vector (and \(s\) is a scalar) are performed without allocating memory. \(\text{Op1}\) may \(+\), \(-\), or nothing (normal assignment), and \(\text{Op2}\) may be \(+\), \(-\), time evolution, a commutator or an anticommutator.

This optimization is inhibited when \(v1\) aliases \(v2\) or \(v3\) (they are the same objects or they otherwise refer to the same backing storage) and the operation being performed involves components in the input and output vectors with different indices. This has no influence on the correctness of writing complex expressions in terms of subexpressions: These will still be correctly evaluated, but memory will be allocated for the results of the subexpressions, making the calculation slower than if this can be avoided. It is expected that users will write expressions in the form they find most natural, and only if performance optimization is required consider restructuring code to take deliberate advantage of this optimization. In that case, the following techniques may be useful:

• If a calculation involving subexpressions is performed in a loop, it is advantageous to manually create sufficient temporaries for all subexpressions outside of the loop and then split the complex expression into a series of basic operations whose results are
stored to the temporaries. This ensures that allocation will be performed only once per temporary before entering the loop, rather than once per temporary, per loop iteration. For example:

```c
//assuming size N arrays of SU_vector state, v1, v2, v3, and v4
//and a floating-point t
for(unsigned int i=0; i<N; i++)
    state[i] += v1[i].Evolve(v2[i],t)
          + v3[i].Evolve(v4[i],t);
```

In this code the addition on the right hand side can be performed without allocation, but each of the evolution operations must allocate a temporary, so 2*N allocations and deallocations must occur. This can be reduced to 2 allocations and deallocations by rewriting in this form:

```c
SU_vector temp1, temp2;
for(unsigned int i=0; i<N; i++){
    temp1 = v1[i].Evolve(v2[i],t);
    temp2 = v3[i].Evolve(v4[i],t)
    state[i] += temp1 + temp2;
}
```

- If a calculation has an SU_vector calculation as a subexpression, but otherwise operates on scalars, it can be useful to rewrite the expression so that the vector calculation forms the top level if possible:

```c
//assuming SU_vectors v1 and v2 and scalars s1 and s2
v1 = s1*(s2*v2);
//can be better reassociated as:
v1 = (s1*s2)*v2;
```

### 5.3. SQUIDS

This object implements the numerical solution for a set of density matrices plus a set of scalar functions in the interaction picture, where the evolution given by $H_0$ is solved analytically. The numerical calculation is done using the GNU Scientific Library, and different parameters for the numerical precision and integrator can be set through the SQuIDS interface.

As we described before in Sec. 3.3 the system consist of a set of nodes where every $i$-node contains $n_\rho$ density matrix expressed as SU_vector, $n_s$ scalar functions which are double, and a double parameter $x_i$. The scheme is shown in Fig.5.1.

The object is defined so that all of the terms in the right hand side of the differential equation are defined as virtual functions that by default return zero, and can be overridden by the user.

If the user does not activate the terms that are numerically solved, then the evolution will be done analytically.
5.3.1. Constructors and Initializing Functions
- Default constructor.
  
  \[
  \text{SQUIDS}();
  \]

  Constructs an uninitialized SQUIDS object.

- Constructor and initializing function.
  
  \[
  \text{SQUIDS}(\text{unsigned int } nx, \text{unsigned int } \text{dim}, \text{unsigned int } \text{nrho}, \\
  \text{unsigned int } \text{nscalar}, \text{double } \text{ti} = 0);
  \]

  \[
  \text{void ini}(\text{unsigned int } nx, \text{unsigned int } \text{dim}, \text{unsigned int } \text{nrho}, \\
  \text{unsigned int } \text{nscalar}, \text{double } \text{ti} = 0);
  \]

  Initializes the object, allocating all necessary memory for the density matrices and scalars. The arguments are described in Table 2.

| Argument | Type        | Description                                                                 |
|----------|-------------|-----------------------------------------------------------------------------|
| nx       | unsigned int| Number of nodes in the problem, each node has a set of density matrices and scalars as defined by the other arguments. |
| dim      | unsigned int| Dimension of the Hilbert space of the density matrices.                     |
| nrho     | unsigned int| Number of density matrices in each node.                                   |
| nscalar  | unsigned int| Number of scalars functions in each node.                                  |
| ti       | double      | Initial time of the system. (Defaults to zero.)                             |

Table 2: Arguments description of SQUIDS constructor and initialization function from left to right.

5.3.2. Functions
- Set the range for the array \( x \).
  
  \[
  \text{int Set_xrange(} \text{double } xini, \text{double } xend, \text{string scale});
  \]

  This function sets the values on the array \( x \). The array will start at \( xini \) and end at \( xend \) (inclusive) with either a uniform linear or logarithmic spacing.

- Get value of \( x \)
| Argument | type     | description                           |
|----------|----------|---------------------------------------|
| xini     | double   | smaller value of x.                   |
| xend     | double   | largest value of x.                   |
| scale    | string   | Either "lin" or "log" and sets the scale as a linear or logarithmic. |

Table 3: Arguments of the Set_xrange function.

```c
double Get_x(unsigned int i) const;
```

Returns the i-th value of the x array.

- Get the bin in a
  ```c
  int Get_i(double x) const;
  ```

  Returns the index of the x array whose value is closest to a. a must be between the values previously specified for xini and xend in the most recent call to Set_xrange.

- Get current system time
  ```c
  double Get_t() const;
  ```

  Returns the current time of the system.

- Get params object
  ```c
  double Get_t_initial() const;
  ```

  Returns the initial time of the system.

- Get initial time
  ```c
  const * Const Get_params() const;
  ```

  Returns a const reference to the params SQUIDS protected member.

- Derivative.
  ```c
  int Derive(double t);
  ```

  Computes the derivative, r.h.s. of Eq. (26, 27), of the system at a time t, including all of the terms defined by the user by overriding the virtual functions specified in section 5.3.3. Note that for each user-supplied interaction term the appropriate flag must be set true for that term to be included (see Sec. 5.3.4 and Table 4).

- Evolution function.
  ```c
  int Evolve(double dt);
  ```
Evolves the system by a time interval $dt$ given in natural units $^1$ (see Const class in Sec. 5.1 and, in particular, Table 1).

- Get expectation value.

  ```cpp
  double GetExpectationValue(SU_vector op, unsigned int irho, unsigned int ix) const;
  double GetExpectationValueD(SU_vector op, unsigned int irho, double x) const;
  ```

  The first function returns the expectation value of the operator represented by $\text{op}$ for the state in the $\text{irho}$ density matrix in that $\text{ix}$ node at the current time $t$. Notice that $\text{op}$ is evolved by the $H_{0(\text{ix,irho})}$ hamiltonian in order to go the interaction picture at time $t$.

  In general $H_{0J}$ may depend continuously in the parameter $x$, in that case in order to compute the expectation value it is very useful perform the evolution of the operator $\text{op}$ driven by $H_{0J}$ for the exact value of $x$. The second function uses this method together with a linear interpolation in $\rho$ over the parameter $x$ in order to give the expectation value.

5.3.3. Virtual Functions

All of these virtual functions return a zero SU_vector by default and may be overridden by the user in a derived class to define a problem. When implemented, each function’s return value must be in natural units (see Table 1).

- Time independent Hamiltonian $H_{0J}$.

  ```cpp
  virtual SU_vector H0(double x, unsigned int irho) const;
  ```

  This function returns the time independent hamiltonian that will be solved analytically, for a particular value of the parameter $x$ and density matrix $\text{irho}$. It is important to note that the analytic solution is implemented assuming that this operator is represented by a diagonal matrix; therefore the problem basis should be chosen to satisfy this condition. For example, in the case of neutrino oscillations this means that the operators are defined in the mass basis.

  The double $x$ gives the parameter corresponding to the node of the $x$ array. Notice that $H_{0J}$ must be defined as a continuous function of $x$ since $H_{0J}$ is solved analytically and thus its independent of the discrete nodes, as this allows GetExpectationValueD to calculate observables at arbitrary $x$.

- Time dependent Hamiltonian $H_{1J}$.

  ```cpp
  virtual SU_vector H1(unsigned int ix, unsigned int irho, double t) const;
  ```

$^1$We set $c = h = k_b = 1$. 
Returns the time dependent part of the Hamiltonian at the \(\text{ix}\) node for the density matrix \(\text{irho}\) at time \(t\). The result of this function is used to calculate the commutator that drives the quantum evolution, the first term in Eq.\((26)\).

This function is used only if \texttt{Set\_CoherentRhoTerms} has been called with a \texttt{true} argument.

- Non coherent terms \(\Gamma_J\).
  
  \[\text{virtual SU\_vector GammaRho(unsigned int ix, unsigned int irho, double t) const;}\]

  Returns the non-coherent interaction at the \(\text{ix}\) node for the density matrix \(\text{irho}\) at time \(t\). The result of this function is used to calculate the anticommutator, the second term in Eq.\((26)\).

  This function is used only if \texttt{Set\_NonCoherentRhoTerms} has been called with a \texttt{true} argument.

- Other \(\rho\) interactions \(F_J\).
  
  \[\text{virtual SU\_vector InteractionsRho(unsigned int ix, unsigned int irho, double t) const;}\]

  Returns the third term on the right hand side of Eq.\((26)\) at the \(\text{ix}\) node for the density matrix \(\text{irho}\) at time \(t\). For example, terms mixing different density matrices and scalar functions of different nodes can be included here.

  This function is used only if \texttt{Set\_OtherRhoTerms} has been called with a \texttt{true} argument.

- Scalar function attenuation \(\Gamma_K\).
  
  \[\text{virtual double GammaScalar(unsigned int ix, unsigned int iscalar, double t) const;}\]

  It returns the Boltzmann attenuation term (first term) for the scalar function Eq.\((26)\) at the \(\text{ix}\) node for the scalar function \(\text{iscalar}\) at time \(t\).

  This function is used only if \texttt{Set\_GammaScalarTerms} has been called with a \texttt{true} argument.

- Other scalar interactions \(G_K\).
  
  \[\text{virtual double InteractionsScalar(unsigned int ix, unsigned int iscalar, double t) const;}\]

  Returns any necessary second term on the right hand side of Eq.\((26)\) at the \(\text{ix}\) node for the scalar function \(\text{iscalar}\) at time \(t\). This may include terms that depend on the other scalars and density matrices.

  This function is used only if \texttt{Set\_OtherScalarTerms} has been called with a \texttt{true} argument.
• Pre-Derivative Function.

    virtual void PreDerive(double t);

This function is called every time before computing the derivatives at time \( t \), i.e. before evaluating the virtual functions described above, and can be used to pre-calculate variables that will be used in the derivative or time evolve projectors in order to more easily and efficiently compute the preceding functions. In general, any update of the parameters in the preceding functions can be included. For example, in the case of neutrino oscillations, this can include the evolution of the flavor projectors that can be then used to define the \( H_{1J} \) Hamiltonian.

| Set Function                | Description                      |
|-----------------------------|----------------------------------|
| Set\_CoherentRhoTerms      | activate the use of HI           |
| Set\_NonCoherentRhoTerms   | activate the use of GammaRho     |
| Set\_OtherRhoTerms         | activate the use of InteractionsRho |
| Set\_GammaScalarTerms      | activate the use of GammaScalar  |
| Set\_OtherScalarTerms      | activate the use of InteractionsScalar |

Table 4: Set functions that control the use of virtual functions.

5.3.4. Set functions
The set functions configure different parameters in the SQUIDS object.

• Set GSL stepper function.

    void Set\_GSL\_set(const gsl_odeiv2\_step\_type * opt);

Sets the GSL stepper function for the differential numerical algorithm, see Table (5). Note that this is a subset of the methods supported by GSL and only includes those that do not require second derivative. By default \( \text{gsl}_\text{odeiv2\_step\_rkf45} \) is set. For more details see the GSL website [5].

• Set absolute error

    void Set\_abs\_error(double error);

Sets the GSL algorithm absolute error to \( \text{error} \).

• Set relative error

    void Set\_rel\_error(double error);

Sets the GSL algorithm relative error to \( \text{error} \).
Available GSL stepper functions

| Function                          |
|----------------------------------|
| gsl_odeiv2_step_rk2               |
| gsl_odeiv2_step_rk4               |
| gsl_odeiv2_step_rkf45             |
| gsl_odeiv2_step_rkck              |
| gsl_odeiv2_step_rk8pd             |
| gsl_odeiv2_step_msadams           |

Table 5: Available GSL stepper functions.

- Set initial step
  ```c
  void Set_h(double h);
  ```
  Sets the GSL algorithm initial step to \( h \).

- Set minimum step
  ```c
  void Set_h_min(double h);
  ```
  Sets the GSL algorithm minimum step to \( h \).

- Set maximum step
  ```c
  void Set_h_max(double h);
  ```
  Sets the GSL algorithm maximum step to \( h \).

- Switch adaptive stepping
  ```c
  void Set_AdaptiveStep(bool opt);
  ```
  If \( opt \) is \texttt{true} adaptive stepping will be used, otherwise a fixed step size will be used.
  In the fixed step case the number of steps can be set by \texttt{Set_NumSteps}.

- Set number of steps (for fixed stepping)
  ```c
  void Set_NumSteps(int steps);
  ```
  Sets the number of steps used when not using adaptive stepping.

- Switch Coherent Interactions
  ```c
  void Set_CoherentRhoTerms(bool opt);
  ```
  If \( opt \) is \texttt{true} the implemented HI will be used, otherwise it will be ignored and treated as zero.

- Switch Non Coherent Interactions
  ```c
  void Set_NonCoherentRhoTerms(bool opt);
  ```
If `opt` is `true` the implemented `GammaRho` will be used, otherwise it will be ignored and treated as zero.

- Switch extra $\rho$ Interactions
  
  ```cpp
  void Set_OtherRhoTerms(bool opt);
  ```

  If `opt` is `true` the implemented `InteractionsRho` will be used, otherwise it will be ignored and treated as zero.

- Switch Scalar Attenuation.

  ```cpp
  void Set_GammaScalarTerms(bool opt);
  ```

  If `opt` is `true` the implemented `GammaScalar` will be used, otherwise it will be ignored and treated as zero.

- Switch Scalar Interactions

  ```cpp
  void Set_OtherScalarTerms(bool opt);
  ```

  If `opt` is `true` the implemented `InteractionsScalar` will be used, otherwise it will be ignored and treated as zero.

5.3.5. Protected members

In this section we describe some useful protected member of the SQUIDS derive which derive classes may want to use.

- Const object
  
  ```cpp
  Const params;
  ```

  `Const` object that contains useful units and angles that define the transformation between basis.

- State of a node

  ```cpp
  struct SU_state {
  std::unique_ptr<SU_vector[]> rho;
  double* scalar;
  };
  ```

  Contains the state of a node consisting of density matrices contained in `rho` and scalar functions in `scalar`.

- System state

  ```cpp
  std::unique_ptr<SU_state[]> state;
  ```

  Contains the state of the system at the current time, namely the density matrices and scalars at all nodes.
- Number of nodes
  
  \texttt{unsigned int nx;}

  Number of nodes in the system.

- Number of scalars
  
  \texttt{unsigned int nscalars;}

  Number of scalar functions per node.

- Number of density matrices.
  
  \texttt{unsigned int nrhos;}

  Number of density matrices per node.

- Hilbert space dimension
  
  \texttt{unsigned int nsun;}

  Dimension of the Hilbert space of the density matrices.

6. Included examples

6.1. Vacuum neutrino oscillations

This is a basic example in which vacuum neutrino oscillations are implemented. In this case, the code does not use any numerical integration, just the analytic solutions given by the \texttt{SU\_vector} class.

The evolution is defined by $H_0$, which in the mass basis has the following form

\begin{equation}
H_0 = \frac{1}{2E} \begin{pmatrix}
0 & 0 & 0 \\
0 & \Delta m_{21}^2 & 0 \\
0 & 0 & \Delta m_{31}^2
\end{pmatrix},
\end{equation}

where the mixing matrix Eq.(6), which relates the mass and flavor bases, depends on three mixing angles and one complex phase: $\{\theta_{12}, \theta_{23}, \theta_{13}, \delta\}$.

In the following, we describe the derived class and the functions that implement this example.

6.1.1. Derived Class (\texttt{vacuum})

This class is defined in \texttt{SQuIDS/examples/VacuumNeutrinoOscillations/vacuum.h} and implemented in \texttt{SQuIDS/examples/VacuumNeutrinoOscillations/vacuum.cpp}.

The \texttt{vacuum} class constructor has the following signature

\begin{verbatim}
vacuum(unsigned int nbins, unsigned int nflavor, double Eini, double Efin);
\end{verbatim}
where \(nbins\) is the number of energy bins in a logarithm scale from a minimum \(E_{\text{ini}}\) to a maximum \(E_{\text{fin}}\) and \(nflavor\) is the number of neutrino flavors. On the constructor it calls the SQUIDS ini function in the following way

\[\text{ini}(nbins,nflavor,1,0,0.);\]

which initializes \(nbins\) \(x\) nodes, which refer to the neutrino energy, with one \texttt{SU} vector of dimension \(nflavor\) and no scalar functions. The final parameter sets the initial time of the system to zero. Furthermore, in the constructor, it is useful to define the projectors in the flavor and mass basis given by Eq.\((3)\), since \(H_0\) is a linear combination of the mass projectors and the flavor projectors are needed to evaluate flavor expectation values. The projectors are stored in the following arrays

\[
\text{std::unique_ptr<\texttt{SU} vector[]> b0\_proj;}
\]
\[
\text{std::unique_ptr<\texttt{SU} vector[]> b1\_proj;}
\]

where the \(b0\) label corresponds to the mass basis and the \(b1\) to the flavor basis. In order to define the transformation between the mass and flavor basis we use \texttt{params.Set\_Mixing\_Angle}.

\[
\text{params.SetMixingAngle}(0,1,33.48*\texttt{params.\_degree}); //theta 1,2}
\]
\[
\text{params.SetMixingAngle}(0,2,8.55*\texttt{params.\_degree}); //theta 1,3}
\]
\[
\text{params.SetMixingAngle}(1,2,42.3*\texttt{params.\_degree}); //theta 2,3}
\]

Next we construct the \texttt{SU} vector \(\text{DM2}\) that represent the matrix in equation Eq.\((28)\).

\[
\text{const double ev2=\texttt{params.eV*params.eV};}
\]
\[
\text{params.SetEnergyDifference}(1,7.5e-5*ev2); //delta m^2 2,1}
\]
\[
\text{params.SetEnergyDifference}(2,2.45e-3*ev2); //delta m^2 3,1}
\]
\[
\text{for(int i = 1; i < nsun; i++)}
\]
\[
\text{DM2 += (b0\_proj[i])*\texttt{params.GetEnergyDifference}(i);}
\]

Finally, we set the initial state of system to the first flavor \((\nu_e)\) by means of the flavor projectors

\[
\text{for(int ei = 0; ei < nx; ei++)}
\]
\[
\text{state[ei].rho[0]=b1\_proj[0];}
\]

The next member function is

\[
\text{SU} \text{ vector } H_0(\texttt{double E, unsigned int irho}) \texttt{ const;}
\]

which returns the value of the time independent Hamiltonian \(H_0\). The last member function is defined to get the flux of a given flavor

\[
\texttt{double Get\_flux(unsigned int flavor, double enu);}\]

where \texttt{flavor} specifies the neutrino flavor and \texttt{enu} the neutrino energy.

### 6.1.2. Main file

The main file declares the object and propagates the three standard neutrino states in a 1000km baseline. The final flavor content is saved in the file \texttt{oscillations.dat}. The output is shown in Fig.6.1.
int main(){
    Const units;

    // Number of energy bins
    unsigned int Nenergy=1000;
    // Number of flavors
    unsigned int Nflavor=3;
    // Energy Range
    double Emin=10*units.MeV, Emax=10*units.GeV;
    // Declaration of the object
    vacuum V0(Nenergy,Nflavor,Emin,Emax);

    V0.Evolve(1000*units.km);

    std::ofstream file("oscillations.dat");

    const int nu_e=0, nu_mu=1, nu_tur=2;
    for(double lE=log(Emin); lE<log(Emax); lE+=0.0001){
        double E=exp(lE);
        file << E/units.GeV << " \text{\,GeV} " << V0.Get_flux(nu_e,E) << " \text{\,keV} " << V0.Get_flux(nu_mu,E) << " \text{\,keV} " << V0.Get_flux(nu_tur,E) << std::endl;
    }

    std::cout << std::endl << "Done!" << std::endl << "Do you want to run the gnuplot script? yes/no" << std::endl;
    std::string plt;
    std::cin >> plt;
    if(plt="yes" || plt="y"){
        return system("./plot.plt");
    }
}

6.2. Rabi oscillations

This example illustrates the numerical time dependent Hamiltonian solution. The code solves for the population of a two level system as a function of time under the influence of an external oscillating potential (e.g. a laser).

We consider two cases: in the first the frequency of the laser is resonant with the energy difference of the two level system, and in the second the laser has a small de-tuning.

The evolution of the Rabi system is driven by the Hamiltonian
Figure 6.1: Probability for a neutrino to interact as a particular flavor as a function of energy after propagating 1000 km, starting from a pure $\nu_e$ flux.

$$H(t) = H_0 + H_1(t) = \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix} + \begin{pmatrix} 0 & d \\ d & 0 \end{pmatrix} \xi(t),$$  \hspace{1cm} (29)

where $\epsilon_i$ is the energy of the $i$-state, $d$ is the dipole expected value, and the function $\xi(t)$ plays the role of an external laser acting on the system, which is given by

$$\xi(t) = A \cos(\omega t).$$  \hspace{1cm} (30)

In terms of the $H_0$ eigenstates projectors, $\Pi_i$, the full Hamiltonian has the form

$$H(t) = \Pi_2(\epsilon_2 - \epsilon_1) + (U^\dagger(\pi/4)\Pi_1 U(\pi/4) - U^\dagger(\pi/4)\Pi_2 U(\pi/4))\xi(t),$$  \hspace{1cm} (31)

where the dipole operator is constructed by a linear combination of rotated projectors.

6.2.1. Derived class ($\texttt{rabi}$)

The class is declared in SQuIDS/examples/RabiOscillations/rabi.h and implemented in SQuIDS/examples/RabiOscillations/rabi.cpp.

As in section 6.1 the projectors are included, where $\texttt{b0}$ and $\texttt{b1}$ label the projectors to the $H_0$ and dipole eigenstates respectively.

```cpp
std::unique_ptr<SU_vector[]> b0_proj;
std::unique_ptr<SU_vector[]> b1_proj;
```
It is also useful to define

```c
SU_vector suH0;
SU_vector d0;
SU_vector d;
```

where \(d0\) is the dipole operator, \(d\) is the time evolved dipole operator, and \(suH0\) is the time independent Hamiltonian.

The initialization and constructor depend on the energy difference of the two levels, \(D_E\), the frequency of the external potential, \(w_i\), and the amplitude of the external interaction, \(A_m\).

```c
rabi(double D_E, double wi, double Am);
void init(double D_E, double wi, double Am);
```

First we initialize the base SQUIDS object for this problem

```c
ini(1/*nodes*/, 2/*SU(2)*/, 1/*density matrices*/, 0/*scalars*/);
```

Next, we set the physical parameters of the problem: We use `SetEnergyDifference` to set the levels' energy difference and `SetMixingAngle` to construct the transformation between the two bases, which is \(U\) in Eq. (31).

```c
params.SetEnergyDifference(1, D_E);
params.SetMixingAngle(0, 1, params.pi/4);
```

We turn on the treatment of coherent terms (HI):

```c
Set_CoherentRhoTerms(true);
```

We construct the time independent hamiltonian using energy difference, the first term in Eq. (31):

```c
suH0 = b0_proj[1]*params.GetEnergyDifference(1);
```

We construct the dipole operators: \(d0\) is the initial dipole operator and \(d\) the time evolved one, which are defined initially to be

```c
d0=(b1_proj[0]-b1_proj[1]);
d=d0;
```

Finally, the system is initialized to the ground state.

We also defined the `PreDerive` function

```c
void rabi::PreDerive(double t){
    d=d0.Evolve(suH0, t-Get_t_initial());
}
```

which evolves the dipole operator to the necessary time. In this problem, \(H_0\) is just defined to return the constant `SU_vector` \(suH0\) which was computed at initialization. Finally, HI is returns the second term in equation Eq.(31)

```c
SU_vector rabi::HI(unsigned int ix,
                   unsigned int irho, double t) const{
    return (A*cos(w*t))*d;
}
```
6.2.2. Main file

The main file declares two rabi objects R0 and R1, the first with two matching frequencies and the second with two frequencies de-tuned by the value given by the user.

```c++
int main(){
    // Declaration of the objects
    rabi R0,Rd;
    // de-tuning
    double del;

    // delta time for the prints
    double dt=0.01;
    // Final time
    double tf=120;

    // Tuned Rabi system
    R0.init(10,10,0.1);

    // Setting the errors
    R0.Set_rel_error(1e-5);  
    R0.Set_abs_error(1e-5);

    std::cout << "Rabi system with frequency of 10 initialized." << std::endl;
    std::cout << "give the value for the detuning:" << std::endl;
    std::cin >> del;

    // un-tuned Rabi system
    Rd.init(10,10+del,0.1);

    // Setting the errors
    Rd.Set_rel_error(1e-5);  
    Rd.Set_abs_error(1e-5);

    std::cout << "Computing rabi" << std::endl;
    std::ofstream file("rabi.dat");

    // Evolve and save the evolution
    for(double t=0;t<tf;t+=dt){
        progressbar(100*t/tf);
        R0.Evolve(dt);
        file << t << "\t" << R0.GetExpectationValue(R0.d0,0,0) << "\t" << R0.GetExpectationValue(R0.b0_proj[0],0,0) << "\t" << R0.GetExpectationValue(R0.b0_proj[1],0,0) << std::endl;
    }
    file.close();
    file.open("rabi_detuned.dat");
}
```
```cpp
std::cout << std::endl << "Computing detuned rabi" << std::endl;
for(double t=0; t<tf; t+=dt){
    progressbar(100*t/tf);
    Rd.Evolve(dt);
    file << t << \"\t\" << Rd.GetExpectationValue(Rd.d0,0,0) << \" \" \\
    << Rd.GetExpectationValue(Rd.b0_proj[0],0,0) << \" \" \\
    << Rd.GetExpectationValue(Rd.b0_proj[1],0,0) << std::endl;
}
file.close();

//Ask whether to run the gnuplot script
std::string plt;
std::cout << std::endl << "Done!\n" << std::endl << "Do you want to run the gnuplot script? yes/no" << std::endl;
std::cin >> plt;
if(plt==\"yes\" || plt==\"y\")
    return system(\"./plot.plt\");
return 0;
```

As before a gnuplot script is added in order to plot the result Fig.6.2. This result is comparable to the one obtained in [15].

![Figure 6.2: Time dependence of the expected value of the dipole and occupation number for the ground-state (GS) and exited state (ES) for exact tuning (upper panel) and a system with a frequency de-tuned by 0.01 (lower panel).](image-url)
6.3. Collective Neutrino Oscillation

In this example we implement a simple version of the collective neutrino oscillation phenomena. We will follow the notation given in [16].

For a two level system and in the absence of non-coherent interactions, the operators can be interpreted as a vectors in a three dimensional space, in particular the state of the system is

\[ \rho_w = P^i_w \lambda_i, \] (32)

and the time independent Hamiltonian is

\[ H_0 = B^i_w \lambda_i \] (33)

where \( i \in \{1, 2, 3\} \) and \( w = T/E \), with \( T \) being the temperature and \( E \) the energy of the state.

The evolution of the system is given by the density matrix equation

\[ \dot{\rho}_w = i[H_0 + \mu \rho, \rho_w], \] (34)

where \( \rho = \int \rho_w dw \) and \( \mu = \sqrt{2} G_F n_\nu \).

In order to get a geometrical description is useful to use the vector notation: In the vector notation the commutator of the operators is equivalent to the cross product of the vectors. Using this the equation for a system with self interacting terms is given by

\[ \dot{P}_w = (wB + \mu P) \times P_w, \] (35)

where

\[ P = \int P_w dw, \] (36)

and \( \mu = \sqrt{2} G_F n_\nu \) is the self-interaction strength, and \( B \) is the vacuum Hamiltonian.

The problem we solve is the evolution of the density matrix for the case where the parameter \( \mu \) is varying until it reaches 0 at some time \( T \). As the initial condition we set all the vectors \( P_w \) aligned together, with a small angle \( \theta \) from \( B \).

6.3.1. Derived object (collective)

The object is declared in SQuIDS/examples/CollectiveNeutrinoOscillations/collective.h and implemented in SQuIDS/examples/CollectiveNeutrinoOscillations/collective.cpp.

In this example, working in the interaction picture does not bring any advantage for the case of having a large number of \( w \) nodes. Therefore, we do not need to define the evolved projectors. Instead, and following the analogy of the vectors in three dimensional space, we define the \( SU(2) \) generators, which are equivalent the unit vectors in the three perpendicular directions.

```cpp
SU_vector ex, ey, ez;
ex = SU_vector::Generator(nsun, 1);
ey = SU_vector::Generator(nsun, 2);
ez = SU_vector::Generator(nsun, 3);
```
The constructor sets up the value of $\mu$ ($\mu$), the angle between $B$ and $P$ ($\theta$), the range for $w$ ($w_{\text{min}}$ to $w_{\text{max}}$) and the number of $w$-bins ($N_{\text{bins}}$).

```cpp
collective(double mu, double th, double wmin, double wmax, int Nbins);
void init(double mu, double th, double wmin, double wmax, int Nbins);
```

Next we define

```cpp
void collective::PreDerive(double t){
  if (bar)
    progressbar(100*t/period, mu);
  // compute the sum of 'polarizations' of all nodes
  P = state[0].rho[0];
  for (int ei = 1; ei < nx; ei++)
    P += state[ei].rho[0];
  // update the strength of self-interactions
  mu = mu_f + (mu_i - mu_f) * (1.0 - t/period);
}
```

in which we implement Eq. (36) and update the value of $\mu$.

We write $\text{HI}$ to implement Eq. (35):

```cpp
SU_vector collective::HI(unsigned int ix,
unsigned int irho, double t) const{
  // the following is equivalent to
  // return Get_x(ix)*B+P*(mu*(w_max-w_min)/(double)nx);

  // make temporary vectors which use the preallocated buffers
  SU_vector t1(nsun, buf1.get());
  SU_vector t2(nsun, buf2.get());

  // evaluate the subexpressions into the temporaries
  t1 = Get_x(ix)*B;
  t2 = P*(mu*(w_max-w_min)/(double)nx);

  // return the sum of the temporaries, noting that t1 is no
  // longer needed so its storage may be overwritten
  return (std::move(t1)+t2);
}
```

Note that in the commented line we directly write Eq. (35), but for efficiency reasons we write equivalent code in a somewhat more verbose manner. Instead of using unnamed temporary vectors we create temporary vectors using preallocated memory buffers. This avoids the need to allocate memory on each call to $\text{HI}$, although it comes at the cost that the function is neither reentrant nor thread-safe. In particular, to use this style one must ensure that no caller of $\text{HI}$ ever keeps the result across a second call as it would be overwritten when the buffer is reused.

The main function in the collective object is

```cpp
void Adiabatic_mu(double mu_i, double mu_f, double period, bool bar);
```
This function evolves the system, changing the parameter $\mu$ from $\mu_i$ to $\mu_f$ linearly during the period of time given by `period`. The parameter `bar` controls whether the progress bar for the evolution is shown.

### 6.3.2. Main file

The main file declares two collective objects: one in order to do the time evolution and the other as a reference.

```cpp
int main(){
  // Parameters
  double mu=10.0;
  double mu2=10;
  double wmin=-2;
  double wmax=2;
  double th=0.01;
  double th2=0.01;
  int Nbins=200;

  collective ColNus(mu,th,wmin,wmax,Nbins);
  collective ColNus_notevolved(mu2,th2,wmin,wmax,Nbins);

  // Evolution from mu=10 to mu=0 in a time period of 100
  ColNus.Adiabatic_mu(10,0,100,true);

  SU_vector o=ColNus.ez;
  double max=0;
  // find the maximum of the initial spectrum
  for(int w=0;w<Nbins;w++){  
    if(max<ColNus_notevolved.GetExpectationValue(o,0,w))  
      max=ColNus_notevolved.GetExpectationValue(o,0,w);
  }

  // write the output in the file
  // col 1 value of w
  // col 2 expectation value of ez for the evolved system normalized to the maximum
  // col 3 expectation value of ez for the non evolved system normalized to the maximum
  std::ofstream file("collective.dat");
  for(int w=0;w<Nbins;w++){  
    file << std::scientific << ColNus.Get_x(w) << "\t"  
      << ColNus.GetExpectationValue(o,0,w)/max "\t" <<  
      ColNus_notevolved.GetExpectationValue(o,0,w)/max "\n";
  }
}
```
After declaring the objects we evolve ConNus from $\mu = 10$ to $\mu = 0$ in a time period of 100 time units. As before a gnuplot script is added in order to plot the result, which is shown in Figure 6.3.

![Graph](image_url)

**Figure 6.3**: Swap factor (solid line) of the system after going from $\mu = 10$ to $\mu = 0$ in a time period of 100 time units. The dotted line shows the initial spectra.

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