JOINT INSTITUTE FOR NUCLEAR RESEARCH
Dzhelepov Laboratory of Nuclear Problems

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Development of a software for studying neutrino oscillations in a media with variable density

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Abstract

In this document I report on the main task that I was in charge of, during the Summer Student Program 2018 at JINR: the study of neutrino oscillations in vacuum and in a media with variable density by solving the time-dependent Schrödinger equation (TDSE) through the Magnus Expansion (ME) numerical method. ME turns out to be an important numerical method because it preserves the unitarity of the time-evolution operator such that the total probability of the possible outcomes of any measurement is conserved. The result is a code skeleton currently in process which will solve the TDSE for neutrino oscillations in a media with a given density, using the PYTHON framework.

1 Introduction

The idea of neutrino oscillations was introduced by Pontecorvo in 1957. The theory of neutrino mixing in vacuum was developed by Maki, Nakagawa and Sakata in 1962. A connection between neutrino mixing and neutrino mass was proposed by Nakagawa, Okonigi, Sakata and Toyoda in 1963. In 1968, Wolfenstein pointed out the matter effect due to neutrinos propagating through ordinary matter; and it was physically described later by Mikheyev and Smirnov in 1986. Finally, it was in 2015 when the results of SNO (Sudbury Neutrino Observatory) and Super-Kamiokande were recognized as a proof of neutrino oscillations. Since when and a few years before, a big number of experiments have been studying neutrino physics. Neutrino Physics is one of the most important frontiers of physics, with them lies a key component in our understanding of Modern Physics if we pretend to develop a Beyond Standard Model theory. Because of the above statements, there are two frequently used acronyms in neutrino oscillations:

- PMNS mixing matrix, after Pontecorvo-Maki-Nakagawa-Sakata for the neutrino/leptonic mixing matrix.
- MSW effect, after Mikheyev, Smirnov and Wolfenstein for the matter effect in neutrino oscillations [1].

Unlike vacuum neutrino oscillations, when we want to study neutrino oscillations in matter, things get complicated, and usually only numerical solutions can help us. The main purpose of this project is to develop a software to study neutrino oscillations in a media with specifically variable density.

The following is a review of the basic concepts to understand the so called Magnus Expansion and how we are planning to use it to solve neutrino oscillations in a media with variable density. The Magnus Expansion review is based on S Blanes et al. [2] and the implementation is based on F Casas et al. [3].

1.1 Neutrino Oscillations in vacuum

Neutrinos in vacuum can be modeled as free particles. In particle physics, these physical states or mass eigenstates, are stationary states of the free particle Hamiltonian, and satisfy

the Schrödinger equation:

$$\hat{H}\psi = i\frac{\partial\psi}{\partial t} = E\psi.$$

So, the time evolution of a mass eigenstate is given by:

$$\psi(\mathbf{x}, t) = \phi(\mathbf{x})e^{-iEt}.$$

The neutrino mass eigenstates are commonly labeled as ν_1, ν_2 and ν_3. Nevertheless, it is important to remember that the mass eigenstates don't have to correspond to the weak or flavor eigenstates ν_e, ν_μ and ν_τ. The flavour eigenstates are produced along with the respective lepton in the weak interaction such that any of the three mass eigenstates can be produced. Since there is no way to know which mass eigenstate was produced, the system has to be described by superposition of ν_1, ν_2 and ν_3 states. And the matrix that parametrizes this mismatch is precisely by a unitary matrix U:

$$|\nu_l\rangle = \sum_{i=1}^{3} U_{li}^{*}|\nu_i\rangle, \tag{1}$$

where U_{li}^{*} is precisely the lepton mixing or PMNS matrix, $l = e, \mu, \tau$ is the lepton flavor and ν_i are the mass eigenstates. And the inverse relation:

$$|\nu_i\rangle = \sum_{l} U_{li}|\nu_l\rangle. \tag{2}$$

The time evolution of $|\nu_l\rangle$ will be given by:

$$|\nu_l(t)\rangle = \sum_{i=1}^{3} U_{li}^{*}|\nu_i(t)\rangle. \tag{3}$$

where $|\nu_i(t)\rangle = e^{-iE_it}|\nu_i(0)\rangle$. Then we can easily obtain:

$$|\nu_l(t)\rangle = \sum_{i=1}^{n} U_{li}^{*}e^{-iE_it}|\nu_i(0)\rangle. \tag{4}$$

Now using (3) and the fact that U is unitary ($U^\dagger = U^{-1}$):

$$\begin{aligned} |\nu_l(t)\rangle &= \sum_{i=1}^{3} U_{li}^{*}e^{-iE_it}|\nu_i(0)\rangle \\ &= \sum_{i=1}^{3} U_{li}^{*}e^{-iE_it}\left(\sum_{l'} U_{l'i}|\nu_{l'}(0)\rangle\right) \\ &= \sum_{l'}\left(\sum_{i=1}^{3} U_{li}^{*}e^{-iE_it}U_{l'i}\right)|\nu_{l'}(0)\rangle. \end{aligned} \tag{5}$$

From this last expression we can now find the transition amplitude:

$$\langle \nu_{l'}(0)|\nu_l(t)\rangle = \langle \nu_{l'}(0)| \sum_{l''} \left(\sum_{i=1}^{3} U_{li}^* e^{-iE_i t} U_{l''i} \right) \rangle |\nu_{l''}(0)\rangle = \sum_{i=1}^{3} U_{li}^* e^{-iE_i t} U_{l'i}.$$

The probability for a neutrino transition from ν_α to ν_β is given by:

$$P_{\nu_\alpha \to \nu_\beta} = |\langle \nu_\beta | \nu_\alpha(t)\rangle|^2.$$

Using (5) in this definition and a few manipulations:

$$P_{\nu_\alpha \to \nu_\beta} = \sum_{i=1}^{3} |U_{\alpha i}|^2 |U_{\beta i}|^2 + \sum_{i \neq j}^{3} \mathcal{Q}^*_{\alpha\beta,ij} e^{-i(E_i - E_j)t}, \tag{6}$$

where $\mathcal{Q}^*_{\alpha\beta,ij} = U_{\alpha i} U^*_{\beta i} U^*_{\alpha j} U_{\beta j}$. Noting that $\mathcal{Q}_{\alpha\beta,ij} = \mathcal{Q}^*_{\alpha\beta,ij}$, the second term in (6) can be rewritten as:

$$P_{\nu_\alpha \to \nu_\beta} = \sum_{i=1}^{3} |U_{\alpha i}|^2 |U_{\beta i}|^2 + \sum_{i>j}^{3} 2\,\mathrm{Re}\left[\mathcal{Q}^*_{\alpha\beta,ij} e^{-i(E_i - E_j)t}\right]. \tag{7}$$

Now it is useful to consider two limit cases. The first one when the time is very small such that the phases $(E_i - E_j)t$ are negligible. Using the fact that $|\langle \nu_\beta | \nu_\alpha \rangle| = \delta_{\alpha\beta}$, we get:

$$\delta_{\alpha\beta} = \sum_{i=1}^{3} |U_{\alpha i}|^2 |U_{\beta i}|^2 + \sum_{i>j}^{3} 2\,\mathrm{Re}\left[\mathcal{Q}^*_{\alpha\beta,ij}\right]. \tag{8}$$

And the second limit is when time is very large and all the phases $(E_i - E_j)t \gg 1$. The average over time is considered:

$$< P_{\nu_\alpha \to \nu_\beta} >= \lim_{T\to\infty} \frac{1}{T} \int_0^T P_{\nu_\alpha \to \nu_\beta}(t) = \sum_{i=1}^{3} |U_{\alpha i}|^2 |U_{\beta i}|^2. \tag{9}$$

Using $\phi_{ij} = \frac{E_i - E_j}{2} t$ and the identity (8), we finally get the general expression:

$$P_{\nu_\alpha \to \nu_\beta} = \delta_{\alpha\beta} - \sum_{i>j} \left(4\,\mathrm{Re}[\mathcal{Q}_{\alpha\beta,ij}] \sin^2 \phi_{ij} + 2\,\mathrm{Im}[\mathcal{Q}_{\alpha\beta,ij}] \sin^2 \phi_{ij} \right). \tag{10}$$

$E_i = \sqrt{\mathbf{p}^2 + m^2}$ can be approximated as $E_i \approx E + \frac{m^2}{2E}$ with $E = |\mathbf{p}|$ for ultrarelativistic particles (which is the case we have). Then we can write $E_i - E_j \approx \frac{m_i^2 - m_j^2}{2E}$. Using $\Delta m^2_{ij} = m_i^2 - m_j^2$ and $t \approx L$ because $v \approx c$ leads us to a new $\phi_{ij} = \frac{\delta m^2_{ij} L}{4E}$. Finally, the aproximated transition probability for neutrinos in vacuum is:

$$P_{\nu_\alpha \to \nu_\beta} \approx \delta_{\alpha\beta} - 4 \sum_{i>j} \mathrm{Re}[\mathcal{Q}_{\alpha\beta,ij}] \sin^2 \left(\frac{\Delta m^2_{ij} L}{4E} \right) + 2 \sum_{i>j} \mathrm{Im}[\mathcal{Q}_{\alpha\beta,ij}] \sin^2 \left(\frac{\Delta m^2_{ij} L}{4E} \right). \tag{11}$$

1.2 Neutrino Oscillations in a media

Now that we want to describe neutrinos in a medium, we need an interaction potential due to the *coherent forward elastic scattering* with the particles in the medium. That is to say, neutrinos will collide with nucleons and it will produce scattering. This phenomena can be compared with an index of refraction.

We need to remember that we have two types of neutrino interactions with matter:

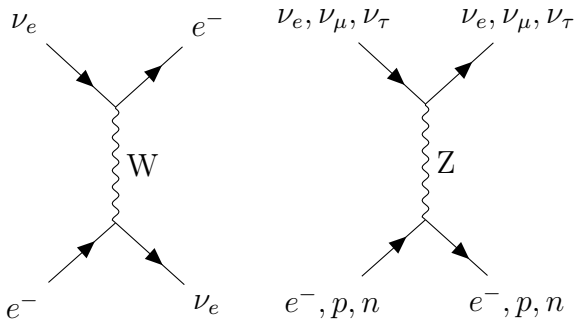

Figure 1: Elastic scattering processes that generate the *Charged Current CC* potential VCC through W exchange and the *Neutral Current NC* potential VNC through Z exchange.

Since there are no μ's or τ's in normal matter, our new potential will have effect only on electron neutrinos ν_e's.

$$V_{eff}^{CC} \equiv V = \sqrt{2} G_F N_e, \tag{12}$$

where G_F is the Fermi's constant and N_e the electron number density in the medium wich can be a constant or a time dependent function.

The time dependent Schrödinger equation (TDSE):

$$i\hbar \frac{d}{dt} \begin{bmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{bmatrix} = \mathbf{H} \begin{bmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{bmatrix}, \tag{13}$$

or

$$i\hbar \frac{d}{dt} \Psi(x,t) = \mathbf{H} \Psi(x,t), \tag{14}$$

where $\mathbf{H}$ is the flavor basis Hamiltonian for neutrinos in matter:

$$\mathbf{H} = U^\dagger \begin{bmatrix} m_1 & 0 & 0 \\ 0 & m_2 & 0 \\ 0 & 0 & m_3 \end{bmatrix} U + V \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{15}$$

where U is the PMNS matrix and $V = \pm\sqrt{2} G_F N_e$.

The solution to equation (14) takes the form:

$$\Psi(t) = e^{\Omega(t,t_0)} \Psi_0, \tag{16}$$

where $\Psi(t_0) = \Psi_0$ and is given by the initial conditions, and $e^{\Omega(t,t_0)}$ is the **evolution operator** and will play a main role in our problem. When the Hamiltonian is time independent, that is to say N_e is a constant, then $\Omega(t, t_0) = -\frac{i}{\hbar}(t - t_0)\mathbf{H}$. But in the general case, where N_e can be also time dependent, then the approximation to the solution is:

$$\Omega(t, t0) = \sum_{k=1}^{\infty} \Omega_k(t, t_0). \tag{17}$$

Now the problem is finding $\Omega_k(t, t_0)$ and the Magnus Expansion is going to help us.

1.2.1 Experimental results

The following figure illustrates the behavior of P_{ee} at the limiting regimes: when matter effects are negligible, when neutrinos propagate adiabatically and when neutrinos propagate in the extreme non-adiabatic limit [4].

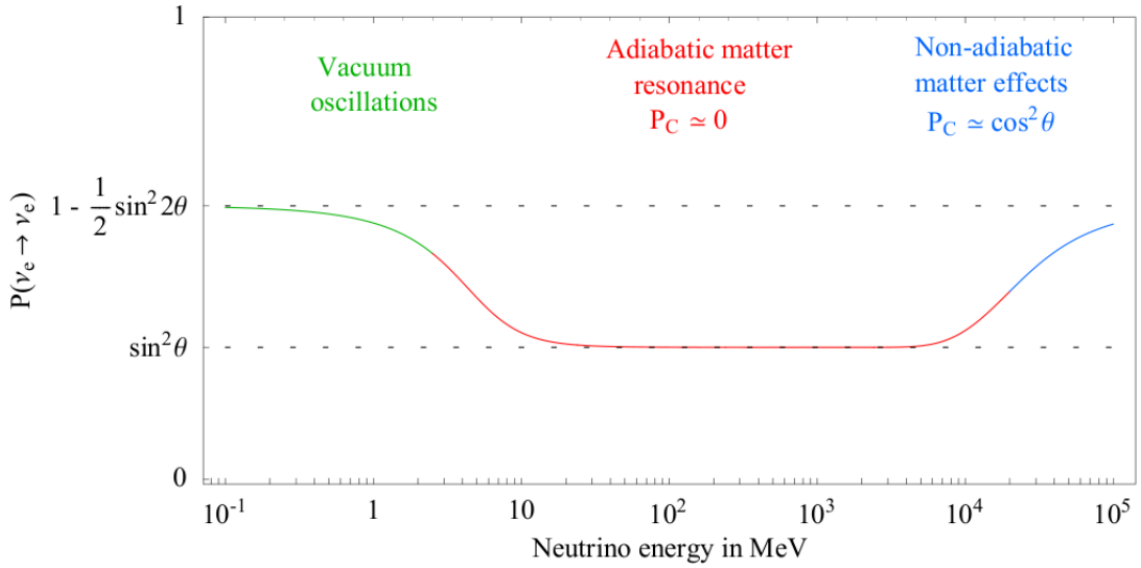

Figure 2: At lower energies, matter effects are negligible (green); at intermediate energies, matter effects are dominant and adiabatic (red); at higher energies, the MSW resonance is no longer adiabatic (blue). The numerical example corresponds to solar oscillations. Absorption is neglected [4].

The electron neutrinos that remain after the combination of matter enhanced effects in the Sun and neutrino oscillations through the vacuum of space as they reach Earth can be assigned a single survival probability P_{ee}. The discovery by the Homestake experiment that this value was less than 1.0 lead to the solar neutrino problem, a deficit of electron neutrinos from what the Standard Model predicts [5].

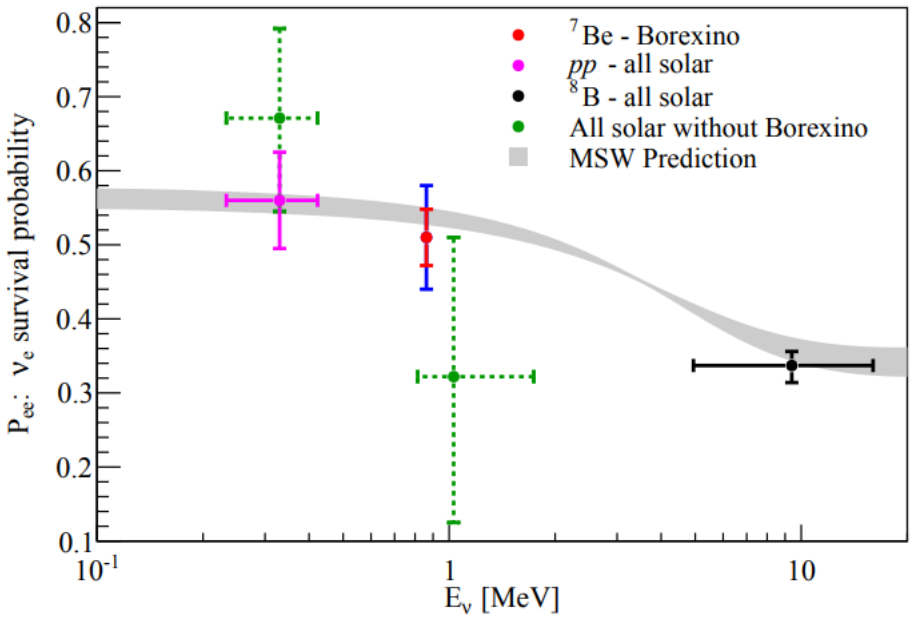

Figure 3: The global experimental constraints on the low energy solar electron neutrino survival probability (P_{ee}). For the 7Be point, the inner (red) error bars show the experimental uncertainty of Borexinos precision measurement, while the outer (blue) error bars show the total (experimental + SSM) uncertainty. The remaining points were obtained following the procedure where the survival probabilities of the low energy (pp), medium energy, and high energy (8B) solar neutrinos are obtained, with minimal model dependence, from a combined analysis of the results of all solar neutrino experiments. To illustrate Borexinos effect on the low energy P_{ee} measurements, the green (dashed) points are calculated without using Borexino data [5].

2 Magnus Expansion

Magnus expansion - also known as Exponential Perturbation Theory - provides unitarity to the approximate solutions to the Schrödinger equation (14). It means that the Magnus Expansion (ME) is a systematic way to build approximations to the time-dependent Schrödinger equation in such a way that, in any order, the **evolution operator** remains unitary [2].

The time evolution operator $U(t,t_0) = e^{\Omega(t,t_0)}$ evolves the wavefunction from time t_0 to t:

$$\psi(t) = U(t,t_0)\psi(t_0).$$

During the evolution, the norm of the wavefunction is kept constant. It ensures probability conservation. Mathematically, this means that U is a unitary operator.

$$U(t,t_0)U^\dagger(t,t_0) = U^\dagger(t,t_0)U(t,t_0) = \mathcal{I}.$$

It also satisfies the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = \lambda H(t)U(t,t_o), \tag{18}$$

with $U(t_0, t_0) = \mathcal{I}$, $H(t)$ the Hamiltonian of the system with possible dependence on time and λ a bookkeping parameter that will be taken as $\lambda = 1$.

Equation (18) is easily solved by iteration. This procedure is equivalent to the Time Dependent Perturbation Theory and gives the expansion:

$$U(t, t_0) = \mathcal{I} + \sum_{n=1}^{\infty} \lambda^n P_n(t, t_0), \tag{19}$$

where $P_n(t_0, t_0) = 0$. Substituting in (18) and comparing the terms of the same order in λ:

$$n = 1 \qquad i\hbar \frac{\partial}{\partial t} P_1(t, t_0) = H(t) \tag{20}$$

$$n = 2 \qquad i\hbar \frac{\partial}{\partial t} P_n(t, t_0) = H(t) P_{n-1}(t, t_0), \tag{21}$$

whence

$$P_n = P_n(t, t_0) \tag{22}$$

$$= \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n H_1 H_2 \cdots H_n, \tag{23}$$

with $H_i = H(t_i)$ When the Hamiltonian does not depend on time:

$$P_n = \frac{1}{n!} \left(-i(t - t_0)\frac{H}{\hbar}\right)^n. \tag{24}$$

And the sum in (19) gives:

$$U(t, t_0) = e^{-i(t-t_0)\lambda \frac{H}{\hbar}}, \tag{25}$$

Rewriting (25)

$$U(t, t_0) = e^{\left[-\frac{i}{\hbar}\int_{t_0}^{t} H dt'\right]}. \tag{26}$$

For the time-dependent case, neither (25) nor (26) are valid. Now it is customary to introduce the so called *Dyson Operator* τ:

$$\tau[H(t_1)H(t_2)] = \begin{cases} H(t_1)H(t_2) & t_1 > t_2 \\ H(t_2)H(t_1) & t_2 > t_1 \end{cases} \tag{27}$$

Now we can write $U(t, t_0)$ as:

$$U(t, t_0) = \tau\left(e^{(-\frac{i}{\hbar}\lambda \int_{t_0}^{t} H dt')}\right). \tag{28}$$

Despite its appearance, **it can not be represented as an exponential**. It means that it can't be written as the conventional series expansion of the exponential function.

The Magnus Expansion assumes that a true exponential solution for 18 does exist:

$$U(t,t_0) = e^{\Omega(t-t_0)} \tag{29}$$
$$= I + \sum_{n=1}^{\infty} \frac{1}{n!}\Omega^n,$$

with $\Omega(t_0,t_0) = 0$ and the next is to solve by series expansion an equation for $\Omega(t,t_0)$. Redefining the Hamiltonian:

$$\tilde{H}(t) = -\frac{i}{\hbar}H(t). \tag{30}$$

Now, the Schrödinger Equation (18) becomes:

$$\frac{\partial}{\partial t}U(t,t_0) = \lambda\tilde{H}(t)U(t,t_0), \tag{31}$$

with the initial condition $U(t_0,t_0) = \mathcal{I}$. Since H is hermitian, $\tilde{H}$ is antihermitian: $\tilde{H}^\dagger = -\tilde{H}$.

Recalling that any unitary matrix is the exponential of an anti-hermitian matrix, we can use it as our first condition for Ω: $\Omega(t,t_0)$ it has to be anti-hermitian to ensure that $U(t,t_0)$ is unitary.

We are now looking for the algorithm of $U(t,t_0)$. If H is time-independent, the equation is simple:

$$\Omega(t,t_0) = (t-t_0)\tilde{H}$$

To start with the difficulties when the Hamiltonian is time-dependent, we will consider the differential equation (31) (taking U and $\tilde{H}$ as ordinary scalar functions). We know that the solution is:

$$U(t,t_0) = e^{(\lambda\int_{t_0}^{t}\tilde{H}(t')dt')}. \tag{32}$$

The key point is that, if instead we deal with matrices, the familiar calculus rule:

$$\frac{d}{dt}e^{A(t)} = A'e^{A(t)} = e^{A(t)}A', \tag{33}$$

is not generally valid anymore.

The exponential in (32) is not a solution of 31 unless:

$$\left[\tilde{H}(t_1),\tilde{H}(t_2)\right] = 0,$$

for arbitrary t_1, t_2 or at least

$$\left[\int_{t_0}^{t}\tilde{H}(t'),\tilde{H}(t)\right] = 0.$$

But this is true only for time-independent H. So now the question is: if U obbeys (31), then, what is the differential equation for Ω? Since we are not allowerd to use the usual differentiation rules, we have to follow a different route. And the following two results will be helpful:

1. The intuitively "group property" of the time-evolution operator:

$$U(t_2, t_0) = U(t_2, t_1)U(t_1, t_0). \tag{34}$$

2. The Baker-Campbell-Hausdorff (BCH) formula for the product of two exponentials:

3. for any two, in general non-commuting operators X and Y, one has:

$$e^X e^Y = e^{(x+Y+\frac{1}{2}[X,Y]+\frac{1}{12}[X,[X,Y]]+\frac{1}{12}[Y,[Y,X]]+\cdots)}, \tag{35}$$

this is an infinite series of nested commutators of increasing order.

Despite of the BCH-series complexity, a compact formula exists, that gives the piece of the BCH-series to all orders in one operator, say Y and to first order in X:

$$e^X e^Y = \exp X + Y + \sum_{k=1}^{\infty}(-1)^k \frac{B_k}{k!}[Y, [\cdots [Y, X]] \cdots] + \mathcal{O}(X^2), \tag{36}$$

where the multiple nested commutators (k-times) are explicitly indicated. And B_k are the Bernoulli numbers.

To derive the equation satisfied by Ω, we consider a short time interval $\delta t \to 0$. Using (34) with $t_2 = t + \delta t$, $t_1 = t$, in exponential form:

$$e^{\Omega(t+\delta t),t_0} = e^{\Omega(t+\delta t),t}.e^{\Omega(t,t_0)}. \tag{37}$$

The crucial point now is that, during $[t, t + \delta t]$ the Hamiltonian can be assumed to take the constant value $\tilde{H}(t)$. And the Schrödinger equation can be solved in the exponential form: $e^{\Omega(t,t+\delta t)} \simeq e^{\lambda \tilde{H}(t)\delta t}$;

$$e^{\Omega(t+\delta t),t_0} \simeq e^{\lambda \tilde{H}(t)\delta t} e^{\Omega(t,t_0)}. \tag{38}$$

Applying (36) to (38) and keeping the first order in δt:

$$\Omega(t+\delta t, t_0) = \Omega(t, t_0) + \lambda \tilde{H} + \lambda \delta t \sum_{k=1}^{\infty}(-1)^k \frac{B_k}{k!}[\Omega(t, t_0), [\cdots, [\Omega(t, t_0), \tilde{H}]] \cdots] + O(\delta t^2), \tag{39}$$

in the limit when $\delta t \to 0$:

$$\frac{\partial}{\partial t}\Omega(t + \delta t, t_0) = \lambda \tilde{H} + \lambda \sum_{k=1}^{\infty}(-1)^k \frac{B_k}{k!}[\Omega(t, t_0), [\cdots, [\Omega(t, t_0), \tilde{H}]] \cdots] \tag{40}$$

with the condition

$$\Omega(t_0, t_0) = 0, \tag{41}$$

which is a highly non-linear differential equation for Ω.

Although it seems more difficult to find a solution for Ω now that we have such a complex differential equation, there is a gain with the exponential representation of the time evolution operator when Ω it expanded in a power series in λ. We finally call:

$$\Omega = \sum_{k=1}^{\infty} \lambda^k \Omega_k, \tag{42}$$

the ***Magnus Series***.
Using it in (41) and equating terms of the same order in λ, we break the previous differential equation into an infinite set of trivially differential equations for each Ω_k, where the first three terms are:

$$\begin{aligned}
\Omega_1(t,t_0) &= \int_{t_0}^{t} \tilde{H}(t_1)dt_1 \\
\Omega_2(t,t_0) &= \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2[\tilde{H}(t_1), \tilde{H}(t_2)] \\
\Omega_3(t,t_0) &= \frac{1}{6}\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \int_{t_0}^{t_2} dt_3 \left([\tilde{H}_1, [\tilde{H}_2, \tilde{H}_3]] + [\tilde{H}_3, [\tilde{H}_2, \tilde{H}_1]]\right).
\end{aligned} \tag{43}$$

where $\tilde{H}(t_i) = \tilde{H}_i$. Ω reproduces, after exponentiation, the result in (32). But now it is only part of the solution. The terms Ω_k with $k > 1$ are the successive corrections generated by the non-vanishing commutators, necessary to have an exponential solution for $U(t, t_0)$. We can say that, to obtain Ω_k, all we need is to commute and integrate:

- The important point is that by doing so to any order, the truncated sum of the series for Ω is always anti-hermitian, because of the arguments we said before.
- Consequently, its exponential furnishes a unitary approximation for $U(t, t_0)$.
- And that is precisely what we are looking for.

2.1 ME implementation

To finally use the ME as a numerical integrator it is necessary to define the so called integration step $h_n = \xi_{n+1} - \xi_n$. If we start our integration at ξ_0 with initial value $\Psi(\xi_0)$, the approximate solution at ξ_1 would be $\Psi(\xi_1 = \xi_0 + h_1)$. Then we can say that in a generic point ξ_n, the solution $\Psi(\xi_n)$ determines $\Psi(\xi_n + h_n)$ as:

$$\Psi(\xi_{n+1}) = exp\Omega^{[r]}(\xi_n; h_n)\}\Psi(\xi_n), \tag{44}$$

where

$$\Omega^{[r]}(\xi_n; h_n) = \sum_{k=1}^{p} \Omega_k(t_n; h_n), \tag{45}$$

which is the truncated Magnus Series (42) at an appropriate index. We were working with orders 2 and 4, and using the next definitions:

$$H = H_0 + v(\xi)W,$$

where H_0 is the vacuum Hamiltonian, $v(\xi)$ is the potential (14) and $W = U^T V U$ with U the PMNS matrix and $V = diag(1, 0, 0)$.

(i). **Order 2 formula: M2**

$$\Omega^{[2]}(\xi_n; h_n) = -iH(\bar{\xi})h_n = -i(H_0 + \bar{v}W)h_n, \tag{46}$$

where $\bar{\xi} = \xi_n + h_n/2$ and the quantity $\bar{v} = v(\bar{xi})$ must be re-evaluated at every step.

(ii). **Order 4 formula: M4**

$$\xi_\pm = \xi_n + (1 \pm \frac{1}{\sqrt{3}})\frac{h_n}{2}, \tag{47}$$

$$\Omega^{[4]}(\xi_n; h_n) = -i(H_0 + \frac{1}{2}(v_+ + v_-)W)h_n + \frac{\sqrt{3}}{12}(v_+ - v_-)[H_0, W]h_n^2, \tag{48}$$

where $v_\pm = v(\xi_\pm)$ [3].

(iii). **Variable step size**
It would be easy to use a constant step size by taking $h = (\xi_f - \xi_0)/$ such that $\xi_n = \xi_0 + nh$ but it would be inefficient because the solution $\Psi(\xi)$ can have whether rapid or slow changes along its evolution. This is why it is better to adjust h_n depending on the integration procedure. In the algorithm we used, we defined a tolerance `tol` and produced the numerical solutions according to M2 and M4.

$$\begin{aligned} \hat{\Psi}_{n+1} &= e^{\Omega^{[2]}(\xi_n; h_n)}\Psi_n \\ \Psi_{n+1} &= e^{\Omega^{[4]}(\xi_n; h_n)}\Psi_n. \end{aligned} \tag{49}$$

Then, we estimate the local error which is given by:

$$E_r = ||\hat{\Psi}_{n+1} - \Psi_{n+1 n+1}||. \tag{50}$$

- If $E_r <$ `tol` at ξ_{n+1}, the step from ξ_n to ξ_{n+1} is accepted and the approximation to the solution at ξ_{n+2} is computed.
- if $E_r >$ `tol`, the approximation at ξ_{n+1} is rejected and a smaller step is chosen to compute the solution at ξ_{n+1} again.
- In both cases, the new step is gien by:

$$h_{new} = s h_c \left(\frac{\texttt{tol}}{E_r}\right)^{1/3}, \tag{51}$$

where h_c is the current step size and s is a *safety factor*. We used $s = 0.8$ and `tol` $= 0.001$.

Each iteration will produce two approximate solutions: $\hat{\Psi}$ and Ψ and the higher order one is chosen: Ψ.
The most time-consuming part of ME is the direct evaluation of E_r using equation (50). We can do some math on this expression to avoid it and get the next approximation for E_r:

$$E_r = ||h_n^2 S_1 + h_n^3 S_2 + \frac{1}{2} h_n^4 S_1^2) \Psi_{n+1}|| + \mathcal{O}(h_n^5), \tag{52}$$

where:

$$\begin{aligned} S_1 &= -\frac{\sqrt{3}}{12}(v_+ - v_-)[H_0, W] \\ S_2 &= i\frac{\sqrt{3}}{24}(v_+ - v_-)\left([H_0,[H_0,W]] + \frac{1}{2}(v_+ + v_-)[W,[H_0,W]]\right). \end{aligned} \tag{53}$$

We can see that (52) only requires the evaluation of $v_\pm$ at each step and the nested commutators $[H_0,[H_0,W]]$, $[W,[H_0,W]]$ which are evaluated at the beginning of the integration. We used as initial step size $h_0 = \texttt{tol}/2$. But the computation of the matrix exponential in Ψ_{n+1} is still there and we use the *Putzer algorithm* to also avoid it and save some computation time.

2.2 Putzer algorithm

The Putzer Algorithm is an analytical method for evaluating matrix exponentials using the eigenvalues and components in the solution of a linear system. In our problem we have need to compute a unitary matrix like $\exp(itA)$, where t is a parameter. At first we need to make A a traceless matrix, by using the following: $\exp(itA) = \exp(itz\mathcal{I})\exp(itA_0)$, where $\mathcal{I}$ is the identity matrix, $z = Tr(A)/3$. Now we get our traceless matrix: $A_0 = A - z\mathcal{I}$. Is well known that the eigenvalues of the traceless matrix A_0 are real valued and given by the characteristic equation:

$$\lambda^3 - \frac{1}{3}Tr(A_0^2)\lambda + \det(A_0) = 0, \tag{54}$$

and the solutions from the so called Cardano's method, are:

$$\lambda_k = 2\sqrt{\frac{p}{3}}\cos\left(\frac{1}{3}\arccos\left(\frac{3q}{2p}\sqrt{\frac{3}{p}}\right) - \frac{2\pi k}{3}\right), \tag{55}$$

for $k = 0, 1, 2$, where $p = Tr(A_0^2)/2$ and $q = \det(A_0)$. By reordering the eigenvalues λ_k such that $\lambda_0 < \lambda_1 < \lambda_2$, we define now:

$$\begin{aligned} r_0 &= -\frac{1 - \exp(iat)}{a} \\ r_1 &= -\frac{1}{a-b}\left(\frac{1-\exp(iat)}{a} - \frac{1-\exp(ibt)}{b}\right) \end{aligned} \tag{56}$$

where $a = \lambda_1 - \lambda_0$, $b = \lambda_2 - \lambda_0$. Finally, using the Putzer algorithm, one gets:

$$\exp(itA_0) = \exp(i\lambda_0 t)[(1 - \lambda_0(r_0 - \lambda_1 r_1))\mathcal{I} + (r_0 + \lambda_2 r_1)A_0 + r_1 A_0^2]. \tag{57}$$

3 Results

The first stages of the project gave as result a set of small classes related to Neutrino Physics which are useful for the rest of the project. We called this module *Oscillation Base* and is conformed by:

- **PMNS**: produces the PMNS matrix given the PDG values for $sin^2(\theta_{ij})$ and δ_{cp}.
- **BigHam**: produces the Hamiltonian (15) given the PDG values for Δm_{ij}, the mass hierarchy, the neutrino energy, the PMNS matrix and the electron density N_e.
  - **ConstantDensity**: produces N_e constant.
  - **ExponentialDensity**: produces $N_e(t)$ with the shape of an exponential function.
- **Amplitude**: Computes the probability amplitude given an initial flavor/mass eigenstate and a Hamiltonian.
- **NaturalUnits**: it makes the conversion from SI to particle physics natural units (c=$\hbar$=1).
- **FlavorTransitions**: it makes the vector conversion from mass basis to flavor basis and viceversa.

The following figures were made using the tools mentioned above.

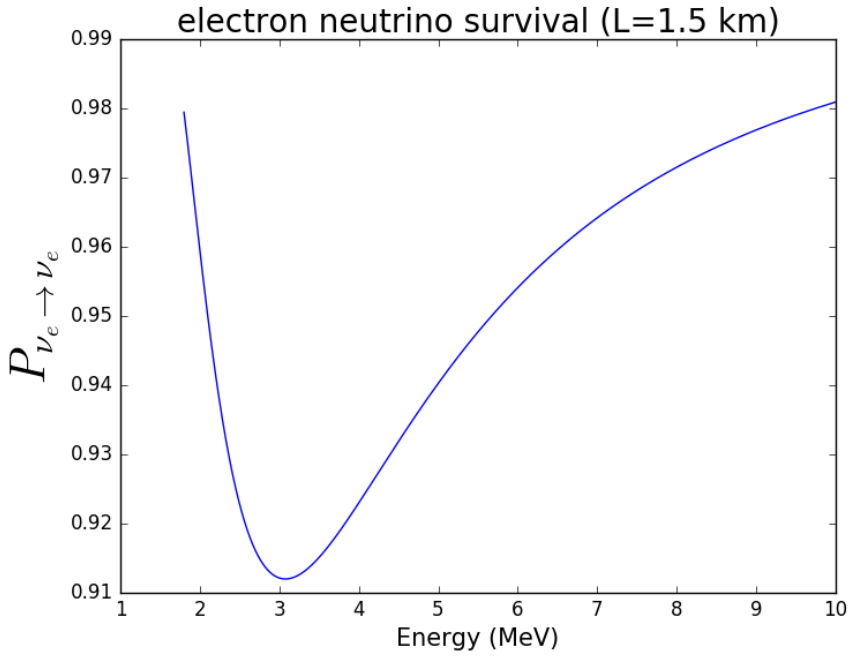

Figure 4: Electron neutrino survival $P_{nu_e \to \nu_e}$, with normal hierarchy and JUNO experiment conditions: E=0-10 MeV, L=1.5 km, N_e=0.

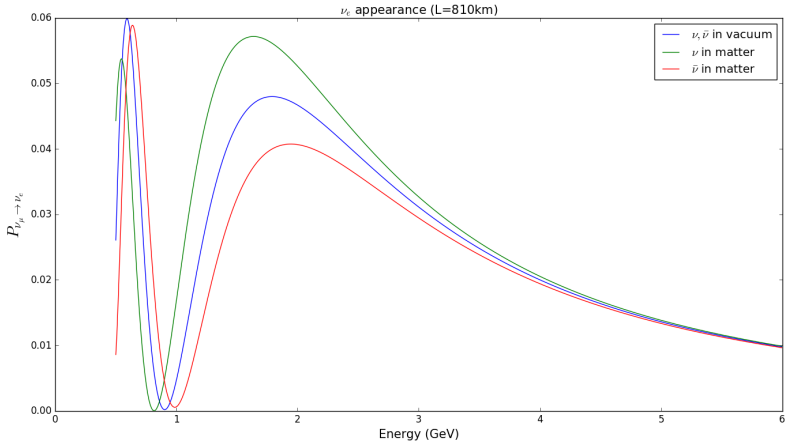

Figure 5: Electron neutrino appearance $P_{nu_\mu \to \nu_e}$, with normal hierarchy and NOvA experiment conditions: E=0-6 GeV, L=810 km, $N_e = 2.75 g/cm^3$

Finally, the main result of this project is a solver that implements the Magnus Expansion given the inputs:

- ν_i: the initial flavor state.
- H: the Hamiltonian, which depends on the neutrino density of the media and is built with **BigHam**, mentioned above.
- `tol`: tolerance
- h_0: initial step size
- s: safety factor
- final point/distance to the detector

and uses also the *Putzer algorithm* instead of the direct computation of the matrix exponential to reduce the computation time for the error estimation between **M2** and **M4**.

4 Conclusion

Oscillation Base is ready to be used for probability amplitude computations for neutrino oscillations in vacuum (see fig.4) and neutrino oscillations in a media with constant density (see fig.5).

The full Magnus Expansion implementation is currently in progress:

- The Putzer algorithm can be improved by also avoiding the computation of A_0^2 in (57).
- Gauss-Kronrod quadrature can be implemented in the algorithm for the step size problem.
- Medias with different electron density functions such as a supernova could be solved with ME.

ME is very promising because of its potential improvements regarding to precision and adaptability to different physical conditions.

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