Exact neutrino oscillation probabilities: a fast general-purpose computation method for two and three neutrino flavors

Mauricio Bustamante

1 Niels Bohr International Academy & DARK, Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark

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In neutrino oscillations, a neutrino created with one flavor can be later detected with a different flavor, with some probability. In general, the probability is computed exactly by diagonalizing the Hamiltonian operator that describes the physical system and that drives the oscillations. Here we introduce an alternative, general-purpose method to compute exact oscillation probabilities, that bypasses diagonalization, and that produces concise and exact expressions for the probabilities. It can be applied to any closed system of two or three neutrino flavors, described by an arbitrary time-independent Hamiltonian. This includes, but is not limited to, oscillations in vacuum, in matter of constant density, with non-standard matter interactions, and in a Lorentz-violating background. We employ properties of SU(2) and SU(3) matrices in our derivation, but the final probability expressions are simple and transparent to these manipulations, and can be readily evaluated. To show this, we provide the user-friendly code NuOscProbExact that implements our method.

I. INTRODUCTION

Neutrinos are created and detected in weak interactions as flavor states — $\nu_e$, $\nu_\mu$, $\nu_\tau$ — but they propagate as superpositions of propagation states — in vacuum, these are the mass eigenstates $\nu_1$, $\nu_2$, $\nu_3$. Because the superposition evolves with time, a neutrino created with a certain flavor has a non-zero probability of being detected later with a different flavor [1–5]. The observation of oscillations in solar, atmospheric, reactor, and accelerator neutrinos has led to the momentous discovery of neutrino mass and of flavor mixing in leptons [6, 7].

Computing the probabilities of flavor transition is integral to studying oscillations. Computing them exactly involves diagonalizing the Hamiltonian operator that drives the time-evolution of neutrinos. But, because the expressions involved are often complex, it is notoriously hard to produce concise and exact analytical expressions for the probabilities that also provide physical insight. The case of oscillations in vacuum is an exception [8–10], beyond that, there is a large body of work dedicated to derivations with precisions that reach the per-cent level; see, e.g., Refs. [11–28]. Yet, though some of these expressions are superficially elegant, they are seldom used due to their underlying complexity, particularly in the case of oscillations amongst three neutrino flavors.

More often, carefully selected perturbative expansions and approximations are employed to cast the probabilities in forms that are amenable to physical interpretation. Many such approximate expressions exist in the literature [29–33], especially for oscillations in matter [37–41] with precisions that reach the per-cent level; they are regularly used to fit data from oscillation experiments. Unfortunately, there is no systematic way to produce these useful expressions, since they are tailored to specific Hamiltonians (however, see, Ref. [45]), their derivation is not trivial, or their application is limited to specific ranges of values of a perturbative parameter.

Thus, the safest course of action in cases where we seek high precision in the computation of probabilities in an arbitrary physical scenario — i.e., for an arbitrary Hamiltonian — is to compute the exact probabilities. For instance, this is the case when scanning a wide parameter space without knowing a priori our region of interest, or how to find approximate expressions of the probabilities that are valid inside that region. Traditionally, in cases like this we resort to diagonalizing the Hamiltonian.

We present an alternative method to compute concise and exact expressions of the flavor-transition probabilities in systems of two and three neutrino flavors. The method relies on expanding the quantum operators responsible for the time-evolution of neutrinos in terms of SU(2) and SU(3) matrices, and using convenient properties of them. It has two assumptions:

1. The system must be closed, i.e., it must conserve the total number of participating neutrinos summed over all flavors; and

2. The Hamiltonian must be time-independent (but solutions with a time- or position-dependent Hamiltonian exist in some cases; see Section V A 2).

Both conditions are satisfied in many physical scenarios studied in the literature, e.g., oscillations in vacuum and matter of constant density, non-standard oscillations in matter, and diverse new-physics scenarios. The method does not apply to scenarios where neutrinos “leak out” of the system, e.g., 3+1 systems of sterile neutrinos [46–50], with neutrino decays into invisible products [51–56], or open systems, like those with decoherence [57–61].

Our objective is to provide a useful, simple, and fast calculation tool of exact probabilities for arbitrary time-independent Hamiltonians, rather than to obtain analytic expressions in particular oscillation scenarios. Thus, we
provide an implementation of our method, in the form of the user-friendly code NuOscProbExact [62].

In Section II, we set the scope, context, and approach of the paper. In Section III, we recap the basics of neutrino oscillations and establish the concrete goal of our computation. In Sections IV and V we develop the method for systems of two and three flavors. In Section VI we conclude.

II. SCOPE, CONTEXT, AND APPROACH

When introducing the method below, we show that a crucial step is to write the Hamiltonian as a linear combination of $2 \times 2$ Pauli matrices — in the case of two neutrino flavors — or of $3 \times 3$ Gell-Mann matrices — in the case of three flavors. Appendix A shows these matrices. When studying neutrino oscillations, these expansions are sometimes performed, though not on the Hamiltonian, but on the associated density matrix. The procedure is typically tailored to a handful of oscillation scenarios. It is particularly useful to describe oscillations in the early Universe [63–68] and in supernovae [69–76].

Choosing instead to expand the Hamiltonian leads to the alternative way to compute exact oscillation probabilities that we present. We follow the expansion of the Hamiltonian itself by the expansion of its associated time-evolution operator, i.e., of $e^{-iHt}$, which we introduce below. For the latter, we use the well-known exponential expansion of Pauli matrices — in the two-neutrino case — and the lesser-known, but handy, exponential expansion of Gell-Mann matrices [77–79] — in the three-neutrino case. The expansions allow us to express the time-evolution operators in a practical form, and to bypass the explicit diagonalization of the Hamiltonian that would otherwise be needed to compute the probabilities.

While the ingredients of the method are not novel, some of them have not yet been used to compute neutrino oscillations and might be relatively obscure — notably, the SU(3) exponential expansion. The novelty stems from their use in computing probabilities for arbitrary Hamiltonians. Accordingly, our approach is expository: we provide sufficient detail to facilitate implementation.

III. NEUTRINO OSCILLATION RECAP

Let $\nu$ represent the flavor state of a neutrino. The state evolves according to the Schrödinger equation

$$i \frac{d\nu}{dt} = H\nu,$$  \hspace{1cm} (1)

where $t$ is the time elapsed since the creation of the neutrino and $H$ is the Hamiltonian operator written in flavor space. Here and below we use units where $c = \hbar = 1$. By definition, $H$ is Hermitian. In a system of $n$ neutrinos, we represent $H$ by a $n \times n$ matrix and $\nu$ by a column vector with $n$ entries. Below, we consider the cases $n = 2$, for two-neutrino oscillations, and $n = 3$, for three-neutrino oscillations.

We restrict the discussion to time-independent Hamiltonians, so that the corresponding time-evolution operator is $U(t) = e^{-iHt}$. Hamiltonians of this type describe, for instance, neutrino propagation in vacuum and in matter of constant density. Because neutrinos are relativistic, we approximate the propagated distance $L \approx t$. Thus, the evolved state of a neutrino born as $\nu_\alpha (\alpha = e, \mu, \tau)$ is

$$\nu_\alpha (L) = U(L)\nu_\alpha = e^{-iHL}\nu_\alpha. \hspace{1cm} (2)$$

Since $H$ is Hermitian, the evolution operator $U$ is unitary.

Because the Hamiltonian in flavor space is non-diagonal, i.e., because it mixes flavor states, after propagating for a distance $L$, the neutrino of initial flavor $\nu_\alpha$ becomes a superposition of neutrinos of all flavors, each with a different probability amplitude, $\nu_\beta (L) \approx \nu_\beta (L) \approx \nu_\beta (L)$. The probability of detecting the neutrino with flavor $\beta$ is $P_{\nu_\alpha \rightarrow \nu_\beta} (L) = |\nu_\beta (L)|^2$.

In Eq. (2), to compute the action of the evolution operator, $\nu_\alpha$ must be an eigenstate of $H$. Yet, because $H$ is non-diagonal, this is normally not the case. Thus, the usual procedure to compute the evolved state is to diagonalize the Hamiltonian in Eq. (2), compute the evolved state in the space spanned by the eigenvectors of the Hamiltonian, and rotate back to flavor space to obtain $\nu_\alpha (L)$. These steps are often carried out numerically, especially in the three-neutrino case, because the equations involved quickly become unmanageable.

Our goal below is to find concise, exact expressions of the probabilities, for arbitrary time-independent Hamiltonians, that also lend themselves to straightforward numerical calculation. We achieve this by adopting the alternative approach that we alluded to in Section II.

IV. TWO-NEUTRINO OSCILLATIONS

We consider first oscillations between only two neutrino flavors; later, we consider three flavors. This is a good approximation when describing reactor, accelerator, and atmospheric neutrinos. We represent the two-neutrino Hamiltonian operator by a $2 \times 2$ matrix $\mathbb{H}_2$. The three traceless, Hermitian Pauli matrices $\sigma^k \ (k = 1, 2, 3)$ — the generators of the SU(2) algebra — plus the identity matrix $1$ make up the orthogonal basis of $2 \times 2$ matrices. Thus, we expand the Hamiltonian as

$$\mathbb{H}_2 = h_0 \mathbb{1} + h_k \sigma^k,$$  \hspace{1cm} (3)

where, here and below, we assume the Einstein convention of summing over repeated indices. The coefficients $h_0$ and the $h_k$ are functions of the components of the Hamiltonian; we show their explicit expressions in Table I. In the two-neutrino case, the neutrino state at any time is $\nu(L) = \nu_\alpha (L) + \nu_\beta (L)$. Here and below, $f_\alpha$ and $f_\beta$ are, respectively, the probability amplitudes of measuring the state to be a $\nu_\alpha$ or a $\nu_\beta$ (with $\alpha \neq \beta$). We represent the
neutrino state as a two-component column vector; the
pure states are $\nu_\alpha = (1 \ 0)^T$ and $\nu_\beta = (0 \ 1)^T$.

The evolution operator is $U_2(L) = e^{-i(h_0 + h_1 \sigma^k)L}$. We factorize3 this into $e^{-i(\frac{1}{2}[(\hat{T}_2)_{11} + (\hat{T}_2)_{22}])L}$. The operator that is proportional to the identity matrix introduces a
global phase that does not affect the probability, i.e., $e^{-i\hat{h}_0L} = e^{-ih_0L}$. After discarding it, we are left with $U_2(L) = e^{-i\hat{h}_k\sigma^kL}$.

To compute the action of $U_2$, we use the well-known
density of Pauli matrices,

$$ e^{\pm i\hat{h}_k\sigma^k} = \cos((|a|) \pm i\hat{a}_k\sigma^k \sin(|a|), \quad (4) $$

where $\hat{a}$ is a unit vector in the direction of the vector $a = (a_1, a_2, a_3)$ and $|a|$ is its modulus. Equation (4) is a generalization of Euler’s formula. So we can write the evolution operator as

$$ U_2(L) = \cos((|h|L) \pm i \frac{\sin(|h|L)}{|h|})\hat{h}_k\sigma^k, \quad (5) $$

where $|h|^2 \equiv |h|^2 + |h_2|^2 + |h_3|^2$.

The evolved state $\nu_\alpha(L)$ of a neutrino that was produced with flavor $\alpha$, i.e., with $f_\alpha(0) = 1$ and $f_\beta(0) = 0$, is $\nu_\alpha(L) = U_2(L)\nu_\alpha$. After some manipulation, the flavor-transition probability $P_{\nu_\alpha \rightarrow \nu_\beta}(L) = |\nu_\alpha^\dagger U_2(L)\nu_\alpha|^2$ is

$$ P_{\nu_\alpha \rightarrow \nu_\beta}(L) = |\hat{h}_1|^2 + |\hat{h}_2|^2 + |\hat{h}_3|^2 \sin^2((|h|L) \quad (\alpha \neq \beta), \quad (6) $$

where $|h_1|^2 + |h_2|^2 = |(\hat{T}_2)_{12}|^2$ and $|h|^2 = |(\hat{T}_2)_{12}|^2 + |(\hat{T}_2)_{11} - (\hat{T}_2)_{22}|^2/4$. Because of the conservation of probability, $P_{\nu_\alpha \rightarrow \nu_\alpha}(L) = 1 - P_{\nu_\alpha \rightarrow \nu_\beta}(L)$. Appendix D contains the derivation of Eq. (6). Equation (6) is our final result in the two-neutrino case.

The key to the calculation of Eq. (6) was to expand the time-evolution operator via the Pauli-matrix identity, Eq. (4). Later, in the three-neutrino case, we use an analogous identity for the Gell-Mann matrices.

A. Oscillations in vacuum

As an example and cross-check, we consider oscillations in vacuum. These are driven by the mass-squared difference between two mass eigenstates $\nu_1$ and $\nu_2$, with masses $m_1$ and $m_2$, out of which the flavor states $\nu_\alpha$ and $\nu_\beta$ are constructed (or $\nu_\mu$ and $\nu_\tau$ if we are studying atmospheric neutrinos). The spaces of flavor and mass states are connected by a unitary rotation that is parametrized by a mixing angle $\theta$, i.e.,

$$ P_{\nu_\alpha \rightarrow \nu_\beta}\nu_\nu(E) = \frac{1}{2E\nu}P_{\nu_\alpha \rightarrow \nu_\beta}\nu_\nu, \quad (8) $$

where $|h|^2 \equiv \text{diag}(\Delta m^2/2, -\Delta m^2/2)$ is the mass matrix, and $\Delta m^2 \equiv m_2^2 - m_1^2$. Using Table I we identify

$$ |\hat{h}_1|^2 = \frac{\Delta m^2}{2E} \sin^2(2\theta), \ |\hat{h}_3|^2 = \frac{\Delta m^2}{2E} \cos^2(2\theta), \ |\hat{h}_2|^2 = 0, \text{ so that } |\hat{h}_1|^2/|\hat{h}_2|^2 = \sin^2(2\theta). \quad \text{From Eq. (6), the probability is} $$

$$ P_{\nu_\nu}(E, L) = \sin^2(2\theta) \sin^2\left(\frac{\Delta m^2}{4E}L\right), \quad (9) $$

which is the standard expression for two-neutrino oscillations in vacuum; see, e.g., Refs. [9, 10].

B. Oscillations in other scenarios

We leave the discussion of oscillations in other scenarios to the case of three neutrino flavors, which we present next. Appendix C shows the two-neutrino counterparts of the example three-neutrino scenarios presented below. We provide implementations of these two-neutrino scenarios as part of NuOscProbExact [22].

V. THREE-NEUTRINO OSCILLATIONS

We mimic the recipe used in the two-neutrino case as closely as possible. We represent the three-neutrino Hamiltonian by a $3 \times 3$ matrix $H_3$. The eight traceless, Hermitian Gell-Mann matrices $\lambda^k$ ($k = 1, \ldots, 8$) — with $\lambda^k/2$ the generators of the SU(3) algebra — plus the identity matrix $\mathbb{1}$ make up the orthogonal basis of $3 \times 3$ matrices. Thus, we expand the Hamiltonian as

$$ H_3 = h_0\mathbb{1} + h_k\lambda^k, \quad (10) $$

where $h_0$ and the $h_k$ are now functions of the components of $H_3$; we show their explicit expressions in Table
The neutrino state at any time is \( \nu(L) = f_\alpha(L)\nu_\alpha + f_\mu(L)\nu_\mu + f_\tau(L)\nu_\tau \), where \( f_\alpha, f_\mu, \) and \( f_\tau \) are, respectively, the probability amplitudes of measuring the state to be a \( \nu_\alpha, \nu_\mu, \) or \( \nu_\tau \). We represent the neutrino state as a three-component column vector; the pure states are \( \nu_\alpha = (1 \ 0 \ 0)^T, \nu_\mu = (0 \ 1 \ 0)^T, \) and \( \nu_\tau = (0 \ 0 \ 1)^T. \)

The evolution operator is \( U_3(L) = e^{-i(h_{\alpha\lambda} + h_\lambda \lambda^k)L} = e^{-i\hbar L} L e^{-i h \lambda^k \L}. \) Again, the first exponential introduces a global phase; after discarding it, we are left with \( U_3(L) = e^{-i h \lambda^k \L}. \)

Next we compute the action of \( U_3 \) on a neutrino state. We wish to expand \( U_3 \) using an identity for the Gell-Mann matrices that is similar to the identity for the Pauli matrices, Eq. (4), and that allows us to write

\[
U_3(L) = u_0 \mathbb{1} + i u_k \lambda^k, 
\]

where the complex coefficients \( u_0 \) and \( u_k \) are functions of \( L \) and the \( h_k \). Reference [77] introduced and demonstrated such an identity; below, we make use of their results, leaving most of the proofs to the reference. See also Refs. [78–83] for further details.

The coefficients in Eq. (11) can be trivially written as \( u_0 = \frac{1}{3} \text{Tr} U_3 \) and \( u_k = -\frac{1}{3} \text{Tr}(\lambda^k U_3). \) An application of Sylvester’s formula [84] to \( 3 \times 3 \) matrices allows us to express the coefficients in terms of the SU(3) invariants

\[
L^2 |h|^2 = L^2 h_k^2 k^2, 
\]

\[
L^3 \langle h \rangle = -L^3 d_{ijk} h_i^* h_j^* h_k^*.
\]

The tensor \( d_{ijk} = \frac{1}{3} \text{Tr} (\langle \lambda_i, \lambda_j \rangle \lambda_k) \), where the brackets represent the anticommutator. It appears in the product law of Gell-Mann matrices and its components are the structure constants of the SU(3) algebra. Table II shows all non-zero components.

Next, we solve the characteristic equation of \( -h_k \lambda^k L \), i.e., \( \phi^3 - (L^2 |h|^2) \phi - \frac{5}{2} (L^3 \langle h \rangle) = 0. \) The equation follows from the Cayley-Hamilton theorem, written conveniently in terms of the invariants [77] [78]. Its three latent roots \( \phi_m \) \((m = 1, 2, 3)\), i.e., the eigenvalues, are

\[
\phi_m = L \langle h \rangle = L \sqrt{\frac{2}{3}} \cos \left( \frac{1}{3} \chi + 2 \pi m \right),
\]

where \( \cos (\chi) = -\sqrt{3} |h| / |h|^3. \) The step above is key: writing the eigenvalues in terms of the SU(3) invariants allows us to bypass an explicit diagonalization [78].

With this, the coefficients in Eq. (11) are

\[
 u_0 = \frac{1}{3} \sum_{m=1}^{3} e^{iL \psi_m}, 
\]

\[
 u_k = \sum_{m=1}^{3} e^{iL \psi_m} \left( \psi_m h_k^* - (h \cdot \h k) \right), 
\]

where \( (h \cdot \h k) \equiv d_{ijk} h^j \h^k. \) Appendix D contains the derivation of Eq. (14). Using Eqs. (12), (13), and (14), we write the evolution operator concisely as

\[
U_3(L) = \sum_{m=1}^{3} e^{iL \psi_m} \left[ \mathbb{1} + \psi_m h_k^* (h \cdot \h k) \lambda^k \right].
\]

For a numerical implementation it is convenient to calculate the coefficients \( u_0 \) and \( u_k \) with Eqs. (15), and use them to directly expand \( U_3 \) in Eq. (11). This is the strategy that we adopt in NuScProbExact [62]. Reference [85] presented an expression similar to Eq. (15), though applied exclusively to oscillations when traversing multiple slabs of matter with different densities; we treat this case in Section [62].

The evolved state of a neutrino created as \( \nu_\alpha \) is \( \nu_\alpha(L) = U_3(L) \nu_\alpha \). Therefore, the flavor-transition probability is \( P_{\nu_\alpha \rightarrow \nu_\beta} = |v_\alpha^* U_3(L) v_\beta|^2. \) Table IV shows the expressions for the probabilities in terms of the coefficients \( u_0 \) and \( u_k \). These are our final results in the three-neutrino case.

Because the algebra of Gell-Mann matrices is more complicated than that of Pauli matrices, the identity that expands the exponential of Gell-Mann matrices in Eq. (11) is notoriously more complicated than the identity that expands the exponential of Pauli matrices,

| Coefficient | Expression |
|-------------|------------|
| \( h_0 \) | \( \frac{1}{3} \left( (\hat{\beta} 1)_{11} + (\hat{\beta} 1)_{22} + (\hat{\beta} 3)_{33} \right) \) |
| \( h_1 \) | \( \text{Re} \left( (\hat{\beta} 1)_{12} \right) \) |
| \( h_2 \) | \( -\text{Im} \left( (\hat{\beta} 1)_{12} \right) \) |
| \( h_3 \) | \( \frac{1}{3} \left( (\hat{\beta} 1)_{11} - (\hat{\beta} 1)_{22} \right) \) |
| \( h_4 \) | \( \text{Re} \left( (\hat{\beta} 3)_{33} \right) \) |
| \( h_5 \) | \( -\text{Im} \left( (\hat{\beta} 3)_{13} \right) \) |
| \( h_6 \) | \( \text{Re} \left( (\hat{\beta} 3)_{23} \right) \) |
| \( h_7 \) | \( -\text{Im} \left( (\hat{\beta} 3)_{23} \right) \) |
| \( h_8 \) | \( \frac{\sqrt{3}}{3} \left( (\hat{\beta} 3)_{11} + (\hat{\beta} 1)_{22} - 2 (\hat{\beta} 3)_{33} \right) \) |

**Table II.** Coefficients in the expansion of the three-neutrino Hamiltonian \( \hat{H}_3 \) in Eq. (10). The coefficient \( h_0 \) does not take part in the calculation of the flavor-transition probability; we include it here for completeness.

| Tensor component | Value |
|-----------------|-------|
| \( d_{118} \) | \( \frac{1}{3} \) |
| \( d_{146} \) | \( \frac{1}{3} \) |
| \( d_{247} \) | \( -\frac{1}{3} \) |
| \( d_{448} \) | \( -\frac{1}{3} \) |
| \( d_{888} \) | \( -\frac{1}{3} \) |

**Table III.** All of the non-zero components of the tensor \( d_{ijk}, \) defined in the main text. The tensor is completely symmetric in its indices. Here, \( i, j, \) and \( k \) can each take integer values between 1 and 8. The notation \( (ijk) \) represents all permutations of the indices in parentheses. A component vanishes if the number of indices in the set \{2, 5, 7\} is odd.
A. Applications to oscillations in different scenarios

Below, we apply the method to the computation of three-neutrino probabilities in four representative scenarios: oscillations in vacuum, oscillations in matter of constant density, with non-standard matter interactions, and in a Lorentz-violating background. We introduce each scenario briefly; our focus is not on exploring the phenomenology, for which we provide references. Following our tenet, we do not derive analytic expression for the probabilities, since they do not necessarily provide physical insight compared to approximate expressions but instead numerically evaluate them.

Figure 1 shows the probabilities $P_{\nu_e \rightarrow \nu_e}$ (top), $P_{\nu_e \rightarrow \nu_\mu}$ (center), and $P_{\nu_e \rightarrow \nu_\tau}$ (bottom), computed using the method presented here, via NuOscProbExact [62]. The scenarios shown are propagation in vacuum, in matter of constant density, with non-standard interactions in matter of constant density (NSI), and propagation in a CPT-odd Lorentz-violating background (LIV). In all cases, the baseline is $L = 1300$ km. See the main text for details.

1. Oscillations in vacuum

In analogy to the two-neutrino case, the Hamiltonian that drives oscillations in vacuum is

$$H_{3\text{vac}}(E) = \frac{1}{2E} \left( R_{3,0} \mathbf{m}^2 R_{3,0}^\dagger \right).$$

Now $\mathbf{m}^2 \equiv \text{diag}(0, \Delta m^2_{21}, \Delta m^2_{31})$ is the mass matrix, with $\Delta m^2_{21} \equiv m_2^2 - m_1^2$ and $\Delta m^2_{31} \equiv m_3^2 - m_1^2$, and the $3 \times 3$ complex rotation matrix $R_{3,0}$ is the Pontecorvo-Maki-Nakagawa-Sakata (PMNS) mixing matrix. We express it

\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
Three-neutrino probability & Expression \\
\hline
$P_{\nu_e \rightarrow \nu_e}$ & $|u_0 + i u_3 + \frac{\sqrt{3} i}{\sqrt{2}}|^{-2}$ \\
$P_{\nu_e \rightarrow \nu_\mu}$ & $|i u_1 - u_2|^2$ \\
$P_{\nu_e \rightarrow \nu_\tau}$ & $|i u_4 - u_5|^2$ \\
$P_{\nu_\mu \rightarrow \nu_e}$ & $|i u_1 + u_2|^2$ \\
$P_{\nu_\mu \rightarrow \nu_\mu}$ & $|u_0 - i u_3 + \frac{\sqrt{3} i}{\sqrt{2}}|^2$ \\
$P_{\nu_\mu \rightarrow \nu_\tau}$ & $|i u_6 - u_7|^2$ \\
$P_{\nu_\tau \rightarrow \nu_e}$ & $|i u_4 + u_5|^2$ \\
$P_{\nu_\tau \rightarrow \nu_\mu}$ & $|i u_6 + u_7|^2$ \\
$P_{\nu_\tau \rightarrow \nu_\tau}$ & $|u_0 - i \frac{2 \sqrt{3} i}{\sqrt{2}}|^2$ \\
\hline
\end{tabular}
\caption{Exact three-neutrino oscillation probabilities, for an arbitrary time-independent Hamiltonian. The complex coefficients $u_0$ and $u_k$ are computed in Eqs. (13) and (14).}
\end{table}
in terms of three mixing angles, $\theta_{13}$, $\theta_{12}$, $\theta_{23}$, and one CP-violation phase, $\delta_{CP}$ [10].

To compute the probabilities in Fig. [1] we fix the mixing parameters to their best-fit values provided by the recent NuFit 4.0 global fit to oscillation data [87, 88], assuming normal mass hierarchy, and including Super-Kamiokande atmospheric neutrino data: $\theta_{12} = 33.82^\circ$, $\theta_{23} = 49.7^\circ$, $\theta_{13} = 8.61^\circ$, $\delta_{CP} = 217^\circ$.

2. Oscillations in matter of constant density

When neutrinos propagate in matter, $\nu_e$ and $\bar{\nu}_e$ scatter on electrons via charged-current interactions. The interactions introduce potentials that shift the energies of the neutrinos. As a result, the values of the mass-squared differences and mixing angles in matter differ from their values in vacuum, and depend on the number density of electrons [89–93]. Computing oscillation probabilities in constant matter is integral to long-baseline experiments, where neutrinos traverse hundreds of kilometers in the crust of the Earth to reach the detectors [94, 95].

The Hamiltonian that drives oscillations in matter is

$$H_m^\text{matt}(E) = H_3^\text{vac}(E) + A_3 .$$

The term $A_3 \equiv \text{diag}(V_{CC}, 0, 0)$ is due to interactions with matter, where $V_{CC} = \sqrt{2}G_F n_e$ is the charged-current potential and $n_e$ is the number density of electrons.

To compute the probabilities for oscillations in matter (and also with non-standard interactions) in Fig. [1] we consider a constant matter density of $\rho = 3$ g cm$^{-3}$, the average density of the crust of the Earth [96]. The number density of electrons is $n_e = Y_e \rho / [(m_p + m_n)/2]$, where $m_p$ and $m_n$ are the masses of the proton and neutron, respectively, and $Y_e = 0.5$ is the average electron fraction in the crust, which is electrically neutral.

It is possible to extend the method presented above to compute oscillation probabilities when traversing multiple slabs of matter, each of constant, but different density. See Ref. [88] for an example. This is relevant to long-baseline neutrino experiments, where the traversed matter density profile might not be uniform [97–101]. The probability amplitudes obtained after traversing each slab need to be stitched together [9]. If a neutrino created as $\nu_\alpha$ traverses $N_{\text{slabs}}$ slabs of constant-density matter, each of width $L_j$, then the evolved state is

$$\nu_\alpha(L_j) = \sum_{j=1}^{N_{\text{slabs}}} \frac{\mu^{(j)}}{3} (L_j) \nu_\alpha,$$

where $\mu^{(j)}$ is the evolution operator, Eq. (15), computed using the matter Hamiltonian, Eq. (17), evaluated with the matter density of the $j$-th slab. The final oscillation probability is $P_{\nu_\alpha \rightarrow \nu_\beta}(L_j) = |\mu^{(j)} \nu_\alpha(L_j)|^2$.

3. Oscillations in matter with non-standard interactions

Oscillations in matter might receive sub-leading contributions due to new neutrino interactions with the fermions of the medium that they propagate in. These are known as non-standard interactions (NSI); see Refs. [102–105] for reviews.

In this case, the Hamiltonian is

$$H_3^\text{NSI}(E) = H_3^\text{vac}(E) + A_3 + V_3,$$

where $V_3 \equiv V_{CC}<3$ is the matter potential due to NSI and $\epsilon_3$ is the matrix of NSI strength parameters, i.e.,

$$\epsilon_3 = \begin{pmatrix} \epsilon_{ee} & \epsilon_{e\mu} & \epsilon_{e\tau} \\ \epsilon_{\mu e} & \epsilon_{\mu\mu} & \epsilon_{\mu\tau} \\ \epsilon_{\tau e} & \epsilon_{\tau\mu} & \epsilon_{\tau\tau} \end{pmatrix}. \quad (19)$$

The parameters $\epsilon_{\alpha\beta}$ represent the total strength of the NSI between leptons of flavors $\alpha$ and $\beta$ interacting with the electrons, $\nu$ quarks, and $d$ quarks that make up standard matter. Following Ref. [109], we write $\epsilon_{\alpha\beta} = \epsilon_{\alpha\beta}^{\nu} + (2 + Y_e) \epsilon_{\alpha\beta}^{\nu<3} + (1 + 2 Y_e) \epsilon_{\alpha\beta}^{\nu<3}$, with the ratio of the number densities of neutrons to electrons $Y_e = n_n/n_e \approx 1$ in the Earth. In our simplified treatment, we do not consider separately interactions with each fermion type or each chiral projection of the fermion [102–103].

To compute the probabilities for NSI in Fig. [1] we again consider propagation in the constant-density crust of the Earth, with $V_{CC}$ evaluated as in Section V A 2. Because NSI have not been observed, we choose arbitrary values for the strength parameters that are allowed at the 2$\sigma$ level by a recent global fit to oscillation (LMA solution) plus COHERENT data [105] (see also Refs. [106, 109]): $\epsilon_{ee}^{\nu} = -\epsilon_{e\mu}^{\nu} = 0.01$, $\epsilon_{\mu\mu}^{\nu} = 0.2$, $\epsilon_{e\tau}^{\nu} = \epsilon_{\mu\tau}^{\nu} = \epsilon_{\tau\tau}^{\nu} = 0$, and the same for $d$ quarks. Like in Ref. [105], we set all $\epsilon_{\alpha\beta}^{\nu<3} = 0$. Thus, for Fig. [1] the NSI parameters in Eq. (19) are $\epsilon_{ee} = -\epsilon_{e\mu} = 0.06$, $\epsilon_{\mu\mu} = 1.2$, and $\epsilon_{e\tau} = \epsilon_{\mu\tau} = \epsilon_{\tau\tau} = 0$. (20)

4. Oscillations in a Lorentz-violating background

Lorentz invariance is one of the linchpins of the Standard Model (SM), but is violated in proposed extensions, some related to quantum gravity; see Refs. [110–113] for reviews. There is no experimental evidence for Lorentz-invariance violation (LIV), but there are stringent constraints on it [20, 114, 115]. The effects of LIV are numerous, e.g., changes in the properties and rates of processes of particles versus their anti-particles, introduction of anisotropies in particle angular distributions, and, in the case of neutrinos, changes to the effective mixing parameters and, thus, to the oscillation probabilities.

To study LIV, we adopt the framework of the Standard Model Extension (SME) [117], an effective field theory that augments the SM by adding LIV parameters to all sectors, including neutrinos [118–120]. In the SME, LIV is suppressed by a high energy scale $\Lambda$, still undetermined. We focus on CPT-odd LIV, where the CPT symmetry is also broken. This is realized by means of a new vector coupling of neutrinos to a new LIV background field. Unlike the other oscillation cases presented
above, the contribution of CPT-odd LIV to the Hamiltonian grows with neutrino energy. This makes high-energy atmospheric and astrophysical energies ideal for testing LIV. \[ \text{The second term on the right-hand side is the effective Hamiltonian that introduces LIV. Here, } B(\text{diag}(b_1, b_2, b_3), \text{where } b_i (i = 1, 2, 3) \text{ are the eigenvalues of the LIV operator } B_3, \text{ and } R_{3,\xi} \text{ is the } 3 \times 3 \text{ mixing matrix that rotates it into the flavor basis. It has the same structure as the PMNS matrix, but different values of the mixing angles and phase. In general, there is a relative phase between } R_{3,\xi} \text{ and } R_{3,0} \text{ that cannot be rotated away} \]

Because LIV has not been observed, the values of the eigenvalues \( b_i \) and of the LIV mixing parameters \( \xi \) are undetermined. Current upper limits \[ \text{set using high-energy atmospheric neutrinos imply that } b_i/\Lambda < 10^{-28} \text{ (this is } \xi^{(4,21)} \text{ in the notation of Ref. [116]). The LIV energy scale is believed to be at least } \Lambda = 1 \text{ TeV. However, to compute the probabilities for LIV in Fig. 1 such that they exhibit features at the lower energies used in the plot, we set artificially high values: } b_1/\Lambda = b_3/\Lambda = 10^{-21} \text{ and } b_3/\Lambda = 5 \times 10^{-21}. \text{ For simplicity, we set all mixing angles to zero, so that } R_{3,0} = 1. \]

VI. CONCLUSIONS

We have provided a general procedure to compute exact two-neutrino and three-neutrino oscillation probabilities for arbitrary time-independent Hamiltonians in systems that conserve the total number of neutrinos of all flavors. This includes many physical scenarios that are often studied in the literature, including oscillations in vacuum, in constant matter density, non-standard neutrino interactions, and new-physics scenarios, like Lorentz-invariance violation.

Our goal has been to provide a method to compute probabilities that is exact, concise, and that can be easily implemented numerically. This is especially useful in the case of three-neutrino oscillations, where the derivation of analytic expressions of the probabilities is a challenging task that has been the subject of abundant work. To derive our results, we have used exponential expansions of SU(2) and SU(3) matrices that allow us to bypass the more commonly used diagonalization of the Hamiltonian.

We have demonstrated our method for representative oscillation scenarios for two-neutrino and three-neutrino oscillations, numerically, using the publicly available code NuDiscProbExact \[ \text{that we provide. While it is possible to extend the method to systems of } n > 3 \text{ neutrino flavors, the expansions in } \text{SU}(n) \text{ quickly become complicated} [79, 83]. \text{ Exploring these generalizations is beyond the scope of this paper.} \]

The method that we have presented is particularly suitable for efficiently exploring wide parameter spaces of standard and non-standard oscillation scenarios. We provide it with this application in mind.

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The three Pauli matrices $\sigma^k$ are:

$$
\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
$$

The eight Gell-Mann matrices $\lambda^k$ are:

$$
\lambda_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},
$$

$$
\lambda_3 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & i \\ -i & i & 0 \end{pmatrix}, \quad \lambda_4 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},
$$

$$
\lambda_5 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},
$$

$$
\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.
$$

**Appendix B: Derivation of Eq. (6)**

We proceed by computing the survival probability $P_{\nu_\alpha \to \nu_\alpha} = |\nu_\alpha^\dagger U_2(L) \nu_\alpha|^2$. We start by operating on $\nu_\alpha$ with the linear combination $h_k \sigma^k$ that appears in the expansion of the time-evolution operator $U_2(L)$, Eq. (5), i.e., $(h_k \sigma^k) \nu_\alpha$. In matrix form, with $\nu_\alpha = (1 \ 0 \ 0)^T$, this is

$$
\begin{pmatrix} h_3 \\ h_1 + ih_2 \\ -h_3 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} h_3 \\ h_1 + ih_2 \end{pmatrix}.
$$

So, using Eq. (5) for $U_2(L)$, the survival probability amplitude is

$$
|\nu_\alpha^\dagger U_2(L) \nu_\alpha| = \cos(|h|L) - \frac{h_3}{|h|} \sin(|h|L),
$$

where the coefficient $h_3 = [\langle H_2 \rangle_{11} - \langle H_2 \rangle_{22}] / 2$: see Table 1. Since $H_2$ is Hermitian, its diagonal elements are real, and, hence, $h_3$ is real. Because of this, we can write the survival probability $|\nu_\alpha^\dagger U_2(L) \nu_\alpha|^2$ as

$$
P_{\nu_\alpha \to \nu_\alpha}(L) = \cos^2(|h|L) + \frac{|h_3|^2}{|h|^2} \sin^2(|h|L).
$$

Now, because $|h_3|^2 = |h|^2 - |h_1|^2 - |h_2|^2$, this becomes

$$
P_{\nu_\alpha \to \nu_\beta}(L) = 1 - \frac{|h_1|^2 + |h_2|^2}{|h|^2} \sin^2(|h|L).
$$

Because of the conservation of probability, $P_{\nu_\alpha \to \nu_\beta} = 1 - P_{\nu_\alpha \to \nu_\alpha}$, with $\alpha \neq \beta$, which gives Eq. (6).

**Appendix C: Sample two-neutrino Hamiltonians**

Here we present the two-neutrino Hamiltonians included as examples in NuOscProbExact. These are the

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**Appendix A: Pauli and Gell-Mann matrices**

For completeness, and to avoid any ambiguity in the method presented in the main text, we show here explicitly all the Pauli and Gell-Mann matrices.
For oscillations in matter, we use
\[ P_{2\nu}^{\text{matt}}(E) = P_{2\nu}^{\text{vac}}(E) + \delta_2, \]
where \( \delta_2 \equiv \text{diag}(V_{CC}, 0) \) and \( V_{CC} \) is defined as before. In Fig. 2, we set \( \rho = 3 \text{ g cm}^{-3} \).

For oscillations in matter with non-standard interactions, we use \[ P_{2\nu}^{\text{NSI}}(E) = P_{2\nu}^{\text{vac}}(E) + \delta_2 + \nu_2, \]
where \( \nu_2 \equiv V_{CC}c_2 \) and the matrix of NSI strength parameters is
\[ \epsilon = \begin{pmatrix} \epsilon_{ee} & \epsilon_{e\mu} \\ \epsilon_{e\mu} & \epsilon_{\mu\mu} \end{pmatrix}. \]

In Fig. 2, we set \( \epsilon_{ee} = -\epsilon_{em} = 0.06 \) and \( \epsilon_{\mu\mu} = 1.2. \)

For oscillations in a CPT-odd Lorentz-violating background, we use \[ P_{2\nu}^{\text{LIV}}(E) = P_{2\nu}^{\text{vac}}(E) + \frac{E}{\Lambda} R_{2,\xi} \mathbb{E}_{2,\xi}^\dagger, \]
where \( U_{2,\xi} \) is a \( 2 \times 2 \) rotation matrix, like Eq. (7), but evaluated at a different mixing angle \( \xi \). In Fig. 2, we set \( R_{2,\xi} = \mathbb{I}, b_1/\Lambda = 10^{-21} \), and \( b_2/\Lambda = 5 \cdot 10^{-21}. \)

\[ \text{Appendix D: Derivation of Eq. (14)} \]

First, we write
\[ u_k = -\frac{1}{2} \sum_{m=1}^{3} \epsilon_{\phi m} \frac{\partial \phi_m}{\partial (-h_k L)} \]
where
\[ \frac{\partial \phi_m}{\partial (-h_k L)} = 2 \left[ \phi_m (-h_k L) + d_{ijk} (-h^i L) (-h^j L) \right]. \]

This can be expanded as
\[ u_k = -\frac{1}{2} \text{Tr} \frac{\partial}{\partial (-h_k L)} \frac{\partial}{\partial (-h_k L)} \]
\[ = -\frac{1}{2} \text{Tr} \frac{\partial}{\partial (-h_k L)} \mathbb{U}_3 \]
\[ = -\frac{1}{2} \sum_{m=1}^{3} \epsilon_{\phi m} \frac{\partial \phi_m}{\partial (-h_k L)}. \]

Thus, the coefficients \( u_k \) can be written as
\[ u_k = -Lx_h_k + L_y (h \ast h) \]
\[ \text{Eq. (D1)} \]

where
\[ x = -\frac{1}{2} \sum_{m=1}^{3} \frac{\psi_m e^{iL\psi_m}}{3 \hbar^2 \psi_m^2 - |h|^2} \]
\[ \text{Eq. (D2)} \]
\[ y = -\frac{1}{2} \sum_{m=1}^{3} \frac{\psi_m e^{iL\psi_m}}{3 \hbar^2 \psi_m^2 - |h|^2} \]
\[ \text{Eq. (D3)} \]

Inserting Eqs. (D2) and (D3) into Eq. (D1) results in Eq. (14) in the main text.

\[ \text{FIG. 2. Two-neutrino oscillation probabilities } P_{\nu_e \rightarrow \nu_e} \text{ (top), } P_{\nu_\mu \rightarrow \nu_e} \text{ (center), and } P_{\nu_\mu \rightarrow \nu_\mu} \text{ (bottom), computed using the method presented here, via NuOscProbExact [62]. This figure is the two-neutrino counterpart of Fig. 1. See the main text and Appendix C for details.} \]