Oscillation probabilities for a $\mathcal{PT}$-symmetric non-Hermitian two-state system

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There is growing interest in viable quantum theories with $\mathcal{PT}$-symmetric non-Hermitian Hamiltonians, but a formulation of transition matrix elements consistent with positivity and perturbative unitarity has so far proved elusive. This Letter provides such a formulation, which relies crucially on the ability to span the state space in such a way that the interaction and energy eigenstates are orthonormal with respect to the same positive-definite inner product. We mention possible applications to the oscillations of mesons and neutrinos.

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Non-Hermitian quantum field theories [1] offer the possibility of constructing viable extensions of the Standard Model of particle physics, and there has been significant progress in understanding them, including the formulation of spontaneous symmetry breaking, the Goldstone theorem and the Englert-Brout-Higgs mechanism [2–4]. However, a satisfactory description of the oscillations between states that can arise when the diagonal bases of the interaction terms and mass terms of a quantum field theory are misaligned, which has applications to quark and neutrino flavour physics, has so far proved elusive. In a misaligned situation, an interaction eigenstate can be decomposed in terms of a superposition of energy eigenstates. Since each of the energy eigenstates evolves with a different phase, the interaction eigenstate is not stationary, and there is a non-zero probability of measuring a different interaction eigenstate at some later time. The dynamics of such oscillations are well studied for Hermitian quantum theories, and have been applied with great success to the phenomena of flavour oscillations in particle physics, such as meson mixing and neutrino oscillations (see, e.g., Ref. [5]).

However, studies of oscillation phenomena in non-Hermitian quantum theories remain unsatisfactory, despite the fact that the viability of non-Hermitian quantum theories is well established in the presence of some antilinear symmetry of the Hamiltonian $\hat{H}$. Examples include $\mathcal{PT}$ (parity-time-reversal)-symmetric quantum theories [1], wherein $[\hat{H}, \mathcal{PT}] = 0$, and the more general class of pseudo-Hermitian quantum theories [6]. The problem lies in the following observation: Whilst unitarity is guaranteed in, e.g., $\mathcal{PT}$-symmetric theories, due to the existence of an additional discrete symmetry of the Hamiltonian [7], existing analyses have arrived at individual transition probabilities that can be negative or larger than unity [8, 9].

Motivated by the desire to construct viable non-Hermitian extensions of the Standard Model, we consider here a simple and well-studied quantum field-theoretic model comprising two complex scalar fields ϕ_1 and ϕ_2 (introduced in Ref. [10]) that can be arranged in a complex doublet $\Phi = (\phi_1, \phi_2)$, which mix via a non-Hermitian mass matrix $M \neq M^\dagger$. However, our analysis holds for any two-state system with a non-Hermitian but $\mathcal{PT}$-symmetric Hamiltonian, as considered, e.g., in Refs. [9].

The Lagrangian density for the scalar field theory is

$$\mathcal{L} \;=\; \partial_\alpha \tilde{\Phi}^\dagger \partial^\alpha \Phi - \tilde{\Phi}^\dagger M^2 \Phi \,, \tag{1}$$

where ∂_α is a spacetime derivative and the squared mass matrix is

$$M^2 \;=\; \begin{bmatrix} m_1^2 & \mu^2 \\ -\mu^2 & m_2^2 \end{bmatrix} \;\neq\; (M^2)^\dagger \,. \tag{2}$$

The formulation in Eq. (1) of the dynamics in terms of the tilde-conjugate doublet $\tilde{\Phi}^\dagger \neq \Phi^\dagger$ (where $\dagger$ denotes Hermitian conjugation), first introduced in Ref. [8], is necessary for the mutual consistency of the Euler-Lagrange equations obtained directly by varying this Lagrangian.

The squared mass eigenvalues

$$m_\pm^2 = \frac{1}{2}(m_1^2 + m_2^2) \pm \frac{1}{2}\sqrt{(m_1^2 - m_2^2)^2 - 4\mu^4} \tag{3}$$

are real, so long as the argument of the square root is positive, and the corresponding eigenvectors are

$$\mathbf{e}_+ = N \begin{bmatrix} \eta \\ -1+\sqrt{1-\eta^2} \end{bmatrix} , \tag{4a}$$

$$\mathbf{e}_- = N \begin{bmatrix} -1+\sqrt{1-\eta^2} \\ \eta \end{bmatrix} , \tag{4b}$$

where the normalisation factor N is defined below and

$$\eta \ \equiv \ \frac{2\mu^2}{|m_1^2 - m_2^2|} \, . \tag{5}$$

The parameter η must be less than or equal to unity for the eigenvalues to be real. At $\eta = 1$, the eigenvalues merge, corresponding to an exceptional point at which the mass matrix becomes defective. Such exceptional points are novel features of non-Hermitian quantum theories and we will see that, in the context of flavour oscillations, the exceptional point is that at which the transition probabilities saturate for finite values of the Lagrangian parameters, in stark contrast to the Hermitian case.

Since the squared mass matrix is not Hermitian, it is diagonalised by a similarity (rather than orthogonal) transformation, and its eigenvectors are not orthogonal with respect to the usual Hermitian scalar product (the Dirac inner product). Nevertheless, there exists in the regime where the eigenvalues are real an orthogonal inner product, which has been described at length in the existing literature, both in the case of non-Hermitian quantum mechanics (see, e.g, Refs. [1, 6, 7, 11]) and non-Hermitian quantum field theory (see Ref. [8] for the present scalar theory and Ref. [12] for a related Dirac fermion theory). Positive norms are obtained with respect to the so-called $\mathcal{C}'\mathcal{PT}$ inner product, where the transformation $\mathcal{C}'$ (not to be confused with charge conjugation in the case of quantum field theory, see Ref. [8]) is an additional discrete symmetry of the Hamiltonian, i.e., $[\hat{H}, \mathcal{C}'] = 0$, and this symmetry ensures unitarity [7].

The eigenvectors $\mathbf{e}_+$ and $\mathbf{e}_-$ are orthogonal with respect to the $\mathcal{PT}$ inner product

$$\mathbf{e}_\pm^\ddagger \mathbf{e}_\pm \ = \ \mathbf{e}_\pm^\dagger P \mathbf{e}_\pm = \pm 1 \, , \qquad \mathbf{e}_\pm^\ddagger \mathbf{e}_\mp \ = \ 0 \, , \tag{6}$$

where $\ddagger \equiv \mathcal{PT} \circ \mathsf{T}$, with T denoting matrix transposition, and we have fixed the normalisation [8]

$$N \ = \ \left[2 \left(\eta^2 - 1 + \sqrt{1-\eta^2} \right) \right]^{-1/2} \, . \tag{7}$$

This normalisation diverges in the Hermitian limit $\eta \to 0$, but the normalised eigenvectors themselves remain well defined. In addition, we have introduced the parity matrix

$$P \ = \ \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} , \qquad P^2 \ = \ \mathbb{I} , \tag{8}$$

which satisfies $PM^2P = (M^2)^\dagger$. The eigenvector $\mathbf{e}_-$ has negative $\mathcal{PT}$ norm, but its $\mathcal{C}'\mathcal{PT}$ norm is positive:

$$\mathbf{e}_\pm^\S \mathbf{e}_\pm \ = \ \mathbf{e}_\pm^\dagger C' P \mathbf{e}_\pm = 1 \, , \qquad \mathbf{e}_\pm^\S \mathbf{e}_\mp \ = \ 0 \, , \tag{9}$$

where $\S \equiv \mathcal{C}'\mathcal{PT} \circ \mathsf{T}$ and

$$C' \ = \ \frac{1}{\sqrt{1-\eta^2}} \begin{bmatrix} 1 & -\eta \\ \eta & -1 \end{bmatrix} \qquad (C')^2 \ = \ \mathbb{I} \, , \tag{10}$$

and we have used $(C' \cdot P)^\mathsf{T} = C' \cdot P$ (see Ref. [8]).

In order to calculate the transition and survival probabilities of the flavour states, we introduce a two-dimensional state space spanned by the eigenvectors $\mathbf{e}_+$ and $\mathbf{e}_-$. These are related to the flavour kets $|\phi_{i,\vec{p}}(t,\vec{x})\rangle$ by the similarity transformation that diagonalises the squared mass matrix, and we obtain

$$|\phi_{1,\vec{p}}(x)\rangle = \cosh(\theta)\, \xi_{+,\vec{p}}(x)\, \mathbf{e}_+ + \sinh(\theta)\, \xi_{-,\vec{p}}(x)\, \mathbf{e}_- \, , \tag{11a}$$

$$|\phi_{2,\vec{p}}(x)\rangle = \cosh(\theta)\, \xi_{-,\vec{p}}(x)\, \mathbf{e}_- + \sinh(\theta)\, \xi_{+,\vec{p}}(x)\, \mathbf{e}_+ \, , \tag{11b}$$

where $\theta = \frac{1}{2}\mathrm{arctanh}(\eta)$, such that

$$\cosh(\theta) = \frac{1}{\sqrt{2}} \left(1 + \frac{1}{\sqrt{1-\eta^2}} \right)^{1/2} , \tag{12a}$$

$$\sinh(\theta) = \frac{1}{\sqrt{2}} \frac{\eta}{\sqrt{1-\eta^2}} \left(1 + \frac{1}{\sqrt{1-\eta^2}} \right)^{-1/2} . \tag{12b}$$

The eigenfunctions $\xi_{\pm,\vec{p}}(x)$ satisfy the classical equations of motion $(\Box + m_\pm^2)\xi_\pm = 0$ ($\Box \equiv \partial_\alpha \partial^\alpha$), with solutions

$$\xi_{\pm,\vec{p}}(x) = \exp(i\omega_\pm t + i\vec{p}\cdot\vec{x}) \, , \tag{13}$$

where $\omega_\pm = \sqrt{\vec{p}^{\,2} + m_\pm^2}$. Hereafter, for simplicity, we will consider only the zero-momentum modes with $\vec{p} = \vec{0}$. At $t = 0$, the flavour states then reduce to

$$|\phi_1(0)\rangle \ = \ \begin{bmatrix} 1 \\ 0 \end{bmatrix} , \qquad |\phi_2(0)\rangle \ = \ \begin{bmatrix} 0 \\ 1 \end{bmatrix} , \tag{14}$$

as we would expect.

The flavour-conjugate states (see Ref. [8]) can be expressed in the form

$$\langle \tilde{\phi}_1(t)| = \cosh(\theta)\, \xi_+^*(t)\, \mathbf{e}_+^\S - \sinh(\theta)\, \xi_-^*(t)\, \mathbf{e}_-^\S \, , \tag{15a}$$

$$\langle \tilde{\phi}_2(t)| = \cosh(\theta)\, \xi_-^*(t)\, \mathbf{e}_-^\S - \sinh(\theta)\, \xi_+^*(t)\, \mathbf{e}_+^\S \, . \tag{15b}$$

We emphasise the change of sign $\sinh(\theta) \to -\sinh(\theta)$ relative to the states in Eq. (11). These states satisfy

$$\langle \tilde{\phi}_i(t)|\phi_j(t)\rangle \ = \ \delta_{ij} \, , \tag{16}$$

and, at $t = 0$, the conjugate states reduce to

$$\langle \tilde{\phi}_1(0)| \ = \ \begin{bmatrix} 1 & 0 \end{bmatrix} , \qquad \langle \tilde{\phi}_2(0)| \ = \ \begin{bmatrix} 0 & 1 \end{bmatrix} . \tag{17}$$

The latter are, in fact, the Hermitian-conjugate flavour states, as identified in Ref. [8] [see Eq. (50) therein]. Thus, the flavour states are orthogonal with respect to the Dirac inner product (constructed via Hermitian conjugation) at $t = 0$, but cease to be so for any $t \neq 0$. As a result (see the Appendix), attempts to construct transition probabilities using the Dirac inner product necessarily lead to the violation of time-translation invariance.

An important observation is that the conjugate states in Eq. (15) do not coincide with the $\mathcal{C}'\mathcal{PT}$-conjugates of the flavour states, which are instead given by

$$\langle\phi_1^{\mathcal{C}'\mathcal{PT}}(t)| = \cosh(\theta)\,\xi_+^*(t)\,\mathbf{e}_+^{\S} + \sinh(\theta)\,\xi_-^*(t)\,\mathbf{e}_-^{\S}\,, \tag{18a}$$

$$\langle\phi_2^{\mathcal{C}'\mathcal{PT}}(t)| = \cosh(\theta)\,\xi_-^*(t)\,\mathbf{e}_-^{\S} + \sinh(\theta)\,\xi_+^*(t)\,\mathbf{e}_+^{\S}\,. \tag{18b}$$

These do not, however, provide an orthogonal basis with respect to $\mathcal{C}'\mathcal{PT}$:

$$\langle\phi_i^{\mathcal{C}'\mathcal{PT}}(t)|\phi_j(t)\rangle \;=\; \begin{cases}\cosh(2\theta), & i \;=\; j\\ \sinh(2\theta), & i \;\neq\; j.\end{cases} \tag{19}$$

At $t = 0$, the states in Eq. (18) reduce to

$$\langle\phi_1^{\mathcal{C}'\mathcal{PT}}(0)| = \frac{1}{\sqrt{1-\eta^2}}\begin{bmatrix}1 & \eta\end{bmatrix}\,, \tag{20a}$$

$$\langle\phi_2^{\mathcal{C}'\mathcal{PT}}(0)| = \frac{1}{\sqrt{1-\eta^2}}\begin{bmatrix}\eta & 1\end{bmatrix}\,, \tag{20b}$$

and we see that the $\mathcal{C}'\mathcal{PT}$-conjugates of the flavour states do not have a direct interpretation as flavour states.

However, the choice of basis $\{|\phi_1\rangle\,, |\phi_2\rangle\}$ is not unique. Since the Hamiltonian is $\mathcal{C}'$-symmetric (i.e., $C'^{\mathsf{T}}M^2C'^{\mathsf{T}} = M^2$), we can also span the state space with $\{|\phi_1\rangle\,, |\phi_2^{\mathcal{C}'}\rangle\}$ (or, equivalently, $\{|\phi_1^{\mathcal{C}'}\rangle\,, |\phi_2\rangle\}$). Remarkably, this choice allows us to construct an orthonormal flavour basis with respect to $\mathcal{C}'\mathcal{PT}$, with

$$\langle\phi_1^{\mathcal{C}'\mathcal{PT}}(t)|\phi_1(t)\rangle \;=\; 1\,, \quad \langle\phi_2^{\mathcal{PT}}(t)|\phi_2^{\mathcal{C}'}(t)\rangle \;=\; 1\,, \tag{21a}$$

$$\langle\phi_1^{\mathcal{C}'\mathcal{PT}}(t)|\phi_2^{\mathcal{C}'}(t)\rangle \;=\; 0\,, \quad \langle\phi_2^{\mathcal{PT}}(t)|\phi_1(t)\rangle \;=\; 0, \tag{21b}$$

where we have adjusted the normalisations of all of the flavour states by a factor of $\sqrt{\mathrm{sech}(2\theta)}$. Crucially, with this choice of basis, the flavour and mass eigenstates are orthonormal with respect to the same positive-definite inner product. Notice that the norms of the flavour states are with respect to $\mathcal{C}'\mathcal{PT}$, but the inner product between different flavour states is, in fact, the $\mathcal{PT}$ inner product, since, e.g., $\langle\phi_2^{\mathcal{PT}}(t)|\phi_1(t)\rangle = (|\phi_2^{\mathcal{C}'}(t)\rangle)^{\S}\,|\phi_1(t)\rangle$.

Spanning the state space in this way, our initial density operators are

$$\hat{\rho}_1(t_0) = |\phi_1(t_0)\rangle\,\langle\phi_1^{\mathcal{C}'\mathcal{PT}}(t_0)|\,, \tag{22a}$$

$$\hat{\rho}_2(t_0) = |\phi_2^{\mathcal{C}'}(t_0)\rangle\,\langle\phi_2^{\mathcal{PT}}(t_0)|\,, \tag{22b}$$

and the final-state projection operators are

$$\hat{\pi}_1(t) = |\phi_1(t)\rangle\,\langle\phi_1^{\mathcal{C}'\mathcal{PT}}(t)|\,, \tag{23a}$$

$$\hat{\pi}_2(t) = |\phi_2^{\mathcal{C}'}(t)\rangle\,\langle\phi_2^{\mathcal{PT}}(t)|\,. \tag{23b}$$

The transition and survival probabilities are calculated as $\mathbb{P}_{i\to j}(t,t_0) = \mathrm{tr}\hat{\rho}_i(t_0)\hat{\pi}_j(t)$, and we obtain

$$\mathbb{P}_{1(2)\to 1(2)}(t,t_0) = 1 - \eta^2\sin^2\left[\Delta\omega\Delta t/2\right]\,, \tag{24a}$$

$$\mathbb{P}_{1(2)\to 2(1)}(t,t_0) = \eta^2\sin^2\left[\Delta\omega\Delta t/2\right]\,, \tag{24b}$$

where $\Delta\omega \equiv \omega_1 - \omega_2$ and $\Delta t \equiv t - t_0$. These probabilities are consistent with positivity, unitarity, perturbative unitarity (in that they are finite for all $\eta \in [0,1]$) and respect time-translation invariance (cf. the Appendix).

We note, however, that these are not the analytic continuations via $\mu^4 \to -\mu^4$ of the corresponding probabilities for the model with Hermitian mass mixing given by taking

$$M^2 \;\to\; M^2_{\mathrm{Herm}} \;=\; \begin{bmatrix}m_1^2 & \mu^2\\ \mu^2 & m_2^2\end{bmatrix}\,, \qquad \tilde{\Phi}^\dagger \;\to\; \Phi^\dagger\,, \tag{25}$$

in Eq. (1). The transition probabilities for this Hermitian model are given by

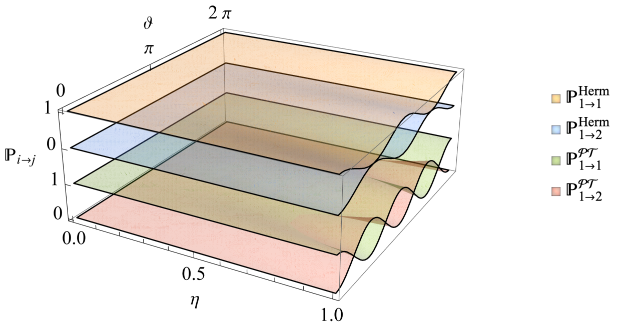
$$\mathbb{P}^{\mathrm{Herm}}_{1(2)\to 2(1)}(t,t_0) \;=\; \frac{\eta^2}{1+\eta^2}\sin^2\left[\Delta\omega\Delta t/2\right]\,. \tag{26}$$

Whereas the Hermitian case saturates for $\eta \to \pm\infty$, the non-Hermitian probabilities saturate at the exceptional point $\eta \to \pm 1$ ($\mu^2 = \pm(m_1^2 - m_2^2)/2$) (see Fig. 1a). Moreover, the masses become degenerate at this exceptional point, but they diverge in the Hermitian case, with the lower squared mass becoming negative for sufficiently large mixing, signalling a tachyonic instability (see Fig. 1b). Note that the analytic continuation $\mu^4 \to -\mu^4$ of the Hermitian result in Eq. (26) (as reported in Ref. [8]) would be negative, with a modulus exceeding unity for $\eta > 1/\sqrt{2}$.

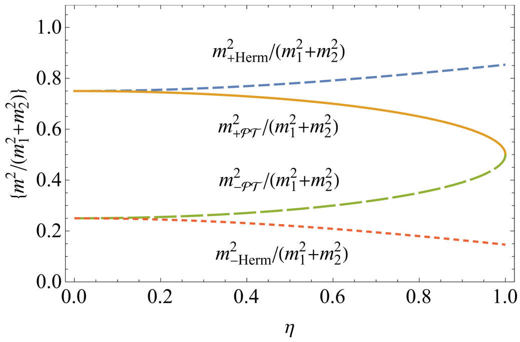
All our key results are illustrated in Fig. 1, where in the upper panel we see explicitly that the survival and transition probabilities have very different dependences on η and the phase $\vartheta = \Delta\omega\Delta t/2$ in the Hermitian and non-Hermitian models, and in the lower panel we see differences in the mass eigenstates as functions of η for $(m_1^2 - m_2^2)/(m_1^2 + m_2^2) = 0.5$. These results are in principle directly applicable to the analysis of meson mixing, specifically in the $K^0 - \bar{K}^0$, $D^0 - \bar{D}^0$ and $B^0_{d,s} - \bar{B}^0_{d,s}$ systems (see, e.g., Ref. [5]). However, phenomenological studies of these systems lie beyond the scope of this Letter.

The potential relevance of $\mathcal{PT}$-symmetric extensions of the Dirac Lagrangian to neutrino oscillations was first identified in Ref. [13] (see also the later works [14–16]). We expect the results of this Letter to carry over to the case of fermion mixing, but leave this to future work, together with the generalisation to the three-flavour case.

In summary, the results of this Letter place the treatment of non-Hermitian flavour mixing matrices on



(a) Oscillation probabilities for the Hermitian (topmost two planes, $\mathbb{P}^{\rm Herm}_{i\to j}$) and non-Hermitian (bottommost two planes, $\mathbb{P}^{\mathcal{PT}}_{i\to j}$) models as a function of η and the phase $\vartheta \equiv \Delta\omega\Delta t/2$. The legend is ordered from topmost to bottommost planes.



(b) Squared eigenmasses of the Hermitian ($m^2_{\pm\rm Herm}$) and non-Hermitian ($m^2_{\pm\mathcal{PT}}$) models divided by $m_1^2+m_2^2$ versus η for $(m_1^2-m_2^2)/(m_1^2+m_2^2)=0.5$.

FIG. 1. Comparison of the transition and survival probabilities (a) and squared eigenmasses (b) for the Hermitian and non-Hermitian models as a function of the parameter η. For the Hermitian case, the mass eigenvalues diverge for large η, with the lower eigenvalue crossing zero and becoming negative at a value of $\eta^2 = (m_1^2+m_2^2)^2/(m_1^2-m_2^2)^2-1$. This occurs before the transition and survival probabilities saturate. For the non-Hermitian case, the mass eigenvalues merge at the exceptional point $\eta = 1$, at which the probabilities saturate.

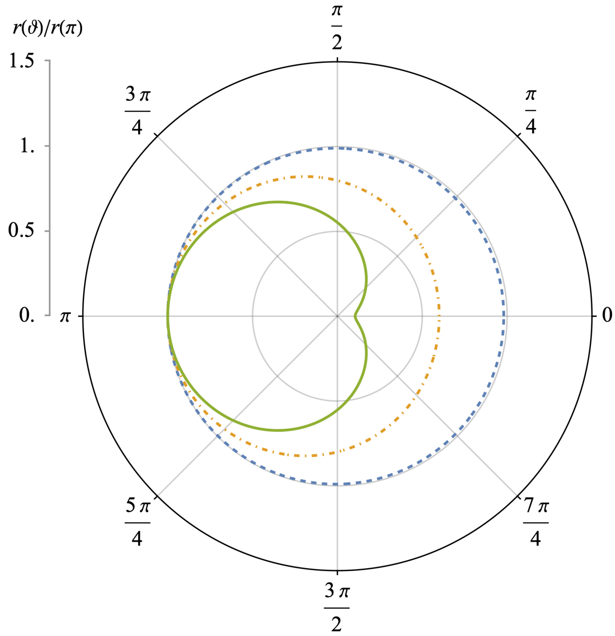


FIG. 2. Polar plot of the Dirac norm $r(\vartheta)/r(\pi)$ for different values of the parameter η: that for $\eta = 0.1$ (dashed, blue) is close to a unit circle, centered on the origin; that for $\eta = 0.5$ (dot-dashed, yellow) clearly deviates from the unit circle; and that for $\eta = 0.9$ (solid, green) has a distinctive cardioid shape.

a firm footing, laying the foundation for a consistent treatment of flavour oscillations and CP violation in non-Hermitian extensions of the quark and lepton sectors of the Standard Model of particle physics. We re-emphasise that the construction of transition probabilities for the two-state, $\mathcal{PT}$-symmetric model described here, with results that are distinct from those in Hermitian theories in their dependences on the model parameters, is in principle experimentally testable.

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DATA ACCESS STATEMENT

No data were created or analysed in this study

APPENDIX

We briefly illustrate in this Appendix the violation of time-translation invariance that results if one attempts to construct transition probabilities with respect to the

Dirac inner product. The Dirac-conjugate states

$$\langle\phi_1(t)| = \cosh(\theta)\,\xi_+^*(t)\,\mathbf{e}_+^\dagger + \sinh(\theta)\,\xi_-^*(t)\,\mathbf{e}_-^\dagger\,, \tag{27a}$$

$$\langle\phi_2(t)| = \cosh(\theta)\,\xi_-^*(t)\,\mathbf{e}_-^\dagger + \sinh(\theta)\,\xi_+^*(t)\,\mathbf{e}_+^\dagger\,, \tag{27b}$$

lead to time-dependent norms

$$\langle\phi_1(t)|\phi_1(t)\rangle \;=\; \langle\phi_2(t)|\phi_2(t)\rangle \;=\; \frac{1-\eta^2\cos(\Delta\omega t)}{1-\eta^2}\,. \tag{28}$$

The Dirac norm traces out a cardioid as shown in Fig. 2, wherein we have defined $r(\vartheta) = [1-\eta^2\cos(\vartheta)]/(1-\eta^2)$. The flavour states are orthogonal with respect to the Dirac inner product only at $t = 0$:

$$\langle\phi_1(t)|\phi_2(t)\rangle \;=\; \langle\phi_2(t)|\phi_1(t)\rangle^* \;=\; \frac{\eta}{1-\eta^2} \times\Big[1-\cos(\Delta\omega t) - i\sqrt{1-\eta^2}\sin(\Delta\omega t)\Big]\,, \tag{29}$$

and the violation of time-translation invariance is made manifest by any adjustment of the normalisation of the states, e.g., by defining $|\bar{\phi}_i(t)\rangle \equiv |\phi_i(t)\rangle\,/\sqrt{\langle\phi_i(t)|\phi_i(t)\rangle}$.

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