COMPUTATIONAL METHODS IN SCIENCE AND TECHNOLOGY **11(1)**, 63-71 (2005)

CPT and effective Hamiltonians for neutral kaon and similar complexes*

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(Rec. 17 June 2005)

Abstract: This paper begins with a discussion of the general form and general CP- and CPT- transformation properties of the Lee-Oehme-Yang (LOY) effective Hamiltonian for the neutral kaon complex. Next, the properties of the exact effective Hamiltonian determined by the properties of the exact transition amplitudes for this complex are discussed. Using the Khalfin Theorem we show that contrary to the standard result of the LOY theory, the diagonal matrix elements of the effective Hamiltonian governing the time evolution in the subspace of states of an unstable particle and its antiparticle need not be equal at for $t > t_0$ (t_0 is the instant of creation of the pair) when the total system under consideration is CPT invariant but CP noninvariant. The unusual consequence of this result is that, contrary to the properties of stable particles, the masses of the unstable particle "1" and its antiparticle "2" need not be equal for $t \gg t_0$ in the case of preserved CPT and violated CP symmetries. We also show that there exists an approximation which is more accurate than the LOY, and which leads to an effective Hamiltonian whose diagonal matrix elements posses properties consistent with the conclusions for the exact effective Hamiltonian described above.

Key words: approximate methods, Weisskopf-Wigner approximation, CPT symmetry, neutral kaons

1. INTRODUCTION

The question under which symmetry transformations physical laws are invariant belongs to the class of fundamental and universal physical problems. Properties of physical systems determined by so-called discrete symmetries such as $\mathcal{P}$ (parity), $\mathcal{C}$ (charge conjugation), $\mathcal{T}$ (time reversal) and $\mathcal{CP}$, $\mathcal{CPT}$ transformations are considered as especially important. The problem of testing CPT-invariance experimentally has attracted the attention of physicist, practically since the discovery of antiparticles. CPT symmetry is a fundamental theorem of axiomatic quantum field theory which follows from locality, Lorentz invariance, and unitarity [1]. Many tests of CPT-invariance consist in searching for decay process of neutral kaons, that is K_0 and $\overline{K}_0$ mesons. The standard approach to searching for the properties of the K_0, $\overline{K}_0$ and similar, two particle, subsystems makes use of more or less accurate approximate methods to solve evolution equation for such subsystems. A typical example of such methods is Weisskopf-Wigner (WW) approximation [2]. All intermediate steps of WW approximation leading to the final formulae describing the time evolution of unstable particles are rather far from mathematical precision. What is more, attempts to confront the predicted properties of the considered systems, obtained within the use of such approximate methods, with those following from the analytical properties of the exact solutions of the quantum evolution equation are rather sporadic. These analytical properties can be extracted from properties of the transition amplitudes

$$A_{\alpha\beta}(t) = \langle \alpha | U(t) | \beta \rangle, \tag{1}$$

where $|\alpha\rangle, |\beta\rangle \in \mathcal{H}$, $\mathcal{H}$ is the Hilbert state space of the total system considered, and $U(t)$ is the total unitary evolution equation solving the Schrödinger equation

$$i\frac{\partial}{\partial t}U(t)|\phi\rangle = HU(t)|\phi\rangle, \qquad U(0) = I, \tag{2}$$

(we use $\hbar = c = 1$ units), I is the unit operator in $\mathcal{H}$, $|\phi\rangle \equiv |\phi; t_0 = 0\rangle \in \mathcal{H}$ is the initial state of the system, (in our case $|\phi; t\rangle = U(t)|\phi\rangle$), and H is the total (selfadjoint) Hamiltonian, acting in $\mathcal{H}$.

Amplitudes $A_{\alpha\beta}(t)$ can be expressed in terms of the energy (mass) densities $\rho_{\alpha\beta}(m)$ as follows

$$A_{\alpha\beta}(t) = \int_{\mathrm{Spec}(H)} \rho_{\alpha\beta}(m) e^{-imt} dm, \tag{3}$$

Assuming that the exact properties of real systems containing neutral kaons are described by the exact solutions of Eq. (2), properties of amplitudes $A_{\alpha\beta}(t)$ following, *eg*., from $\mathcal{CP}$ or $\mathcal{CPT}$ invariance of H, can be used to examine properties of some parameters describing the unstable particles considered and obtained by means of approximate methods of calculations [3, 4]. Moreover amplitudes $A_{\alpha\beta}(t)$ are convenient for numerical simulations of time evolution of the states considered: It is sufficient to assume the form of the densities

* The paper is based on the talk given at the Conference on *Irreversible Quantum Dynamics*, 29 July-2 August 2002, Abdus Salam International Centre for Theoretical Physics, Trieste, Italy; hep-ph/0208032.

$\rho_{\alpha\beta}(m)$ and then to use computer methods to find $A_{\alpha\beta}(t)$ as a function of time t.

All known CP- and hypothetically possible CPT-violation effects in the neutral kaon complex are described by solving the Schrödinger-like evolution equation [5-12]

$$i\frac{\partial}{\partial t}|\psi;t\rangle_{||} = H_{||}|\psi;t\rangle_{||} \tag{4}$$

for $|\psi;t\rangle_{||}$ belonging to the subspace $\mathcal{H}_{||} \subset \mathcal{H}$, *e.g.*, spanned by orthonormal neutral kaons states $|K_0\rangle$, $|\overline{K}_0\rangle \in \mathcal{H}$, and so on, (then states corresponding to the decay products belong to $\mathcal{H} \ominus \mathcal{H}_{||} \stackrel{\text{def}}{=} \mathcal{H}_{\perp}$), and nonhermitian effective Hamiltonian $H_{||}$ obtained usually by means of the Lee-Oehme-Yang (LOY) approach (within the WW approximation) [5-8, 12]:

$$H_{||} \equiv M - \frac{i}{2}\Gamma, \tag{5}$$

where

$$M = M^{+}, \quad \Gamma = \Gamma^{+}, \tag{6}$$

are (2×2) matrices.

The solutions of Eq. (4) can be written in matrix form and such a matrix defines the evolution operator (which is usually nonunitary) $U_{||}(t)$ acting in $\mathcal{H}_{||}$:

$$|\psi;t\rangle_{||} = U_{||}(t)|\psi;\ t_0 = 0\rangle_{||} \stackrel{\text{def}}{=} U_{||}(t)|\psi\rangle_{||}, \tag{7}$$

where,

$$|\psi\rangle_{||} \equiv q_1|\mathbf{1}\rangle + q_2|\mathbf{2}\rangle, \tag{8}$$

and $|\mathbf{1}\rangle$ | stands for the vectors of the $|K_0\rangle$, $|B_0\rangle$, type and $|\mathbf{2}\rangle$ denotes antiparticles of particle "1": $|\overline{K}_0\rangle, |\overline{B}_0\rangle$, $\langle \mathbf{j}|\mathbf{k}\rangle = \delta_{jk},\ j, k = 1, 2.$

In many papers it is assumed that the real parts, $\Re(.)$, of the diagonal matrix elements of $H_{||}$:

$$\Re(h_{jj}) \equiv M_{jj}, \quad (j = 1, 2) \tag{9}$$

where

$$h_{jk} = \langle \mathbf{j}|H_{||}|\mathbf{k}\rangle, \quad (j, k = 1, 2), \tag{10}$$

correspond to the masses of particle "1" and its antiparticle "2" respectively [5-12], (and such an interpretation of $\Re(h_{11})$ and $\Re(h_{22})$ will be used in this paper), whereas the imaginary parts, $\Im(.)$,

$$-2\Im(h_{jj}) \equiv \Gamma_{jj}, \quad (j = 1, 2), \tag{11}$$

are interpreted as the decay widths of these particles [5-12]. Such an interpretation seems to be consistent with the recent and the early experimental data for the neutral kaon and similar complexes [13].

Relations between matrix elements of $H_{||}$ implied by CP- and CPT-transformation properties of the Hamiltonian H of the total system, containing neutral kaon complex as a subsystem, are crucial to designing CPT-invariance and CP-violation tests and to proper interpretation of their results.

The aim of this paper was to show how the matrix elements of the exact $H_{||}$ can be calculated using amplitudes $A_{\alpha\beta}(t)$. Then to examine properties of these matrix elements of the exact $H_{||}$ generated by the CP- or CPT-symmetry of the total system and by analytical properties of $A_{\alpha\beta}(t)$. Note that expressing $H_{||}$ in terms of $A_{\alpha\beta}(t)$ also allows one to use the same numerical methods to simulate properties of $A_{\alpha\beta}(t)$ as well as matrix elements of $H_{||}$. The aim of the paper was also to propose and to discus a more accurate approximation than the LOY approximation. Starting from the exact evolution equation for a given n-dimensional subspace $\mathcal{H}_{||}$ of $\mathcal{H}$ it is shown how to obtain mathematically well defined formulae for $H_{||}$ by using this equation. This new approximation is more accurate than the WW and the LOY approximations and can be applied not only for the searching for properties of neutral mesons but also in the case of general multi-level (multi-particle) subsystems. In general the computational methods described are of universal character and might be used outside the elementary particles.

The paper is organized as follows. In Sec. 2 we review briefly the Lee-Oehme-Yang methods of description of the neutral K subsystem. Sec. 3 describes connections between the exact amplitudes $A_{\alpha\beta}(t)$ and matrix elements of the exact effective Hamiltonian $H_{||}$ and implications of the CPT-invariance of the total system for the properties of the diagonal matrix elements, $(h_{11} - h_{22})$, of the exact $H_{||}$. In Sec. 4 the new approximation mentioned above is discussed. Sec. 5 contains final remarks.

2. H_{LOY} AND CPT-SYMMETRY

Now, let us consider briefly some properties of the LOY model. In this case the initial condition for the Eq. (2) has the following form

$$|\phi\rangle \equiv |\psi\rangle_{||}. \tag{12}$$

Let P denote the projection operator onto the subspace $\mathcal{H}_{||}$:

$$P\mathcal{H} = \mathcal{H}_{||}, \quad P = P^2 = P^{+}, \tag{13}$$

then the subspace of decay products $\mathcal{H}_{\perp}$ equals

$$\mathcal{H}_{\perp} = (I - P)\mathcal{H} \stackrel{\text{def}}{=} Q\mathcal{H}, \quad Q \equiv I - P. \tag{14}$$

For the case of neutral kaons or neutral B-mesons, *etc.*, the projector P can be chosen as follows:

$$P \equiv |\mathbf{1}\rangle\langle\mathbf{1}| + |\mathbf{2}\rangle\langle\mathbf{2}|, \tag{15}$$

and the definition of $|K_0\rangle$ and $|\overline{K}_0\rangle$ is analogous to the one used in the LOY theory for corresponding vectors. In the LOY approach it is assumed that vectors $|\mathbf{1}\rangle$, $|\mathbf{2}\rangle$ considered above are eigenstates of $H^{(0)}$ for a 2-fold degenerate eigenvalue m_0:

$$H^{(0)}|\mathbf{j}\rangle = m_0|\mathbf{j}\rangle, \quad j = 1, 2, \tag{16}$$

where $H^{(0)}$ is the so called free Hamiltonian, $H^{(0)} \equiv H_{\text{strong}} = H - H_W$, and H_W denotes weak and other interactions which are responsible for transitions between the eigenvectors of $H^{(0)}$, *i.e.*, for the decay process. This means that

$$\left[P, H^{(0)}\right] = 0. \tag{17}$$

The condition guaranteeing the occurrence of transitions between subspaces $\mathcal{H}_{||}$ and $\mathcal{H}_{\perp}$, *i.e.*, the decay process of states in $\mathcal{H}_{||}$, can be written as follows

$$[P, H_W] \neq 0, \tag{18}$$

that is

$$[P, H] \neq 0. \tag{19}$$

Usually, in LOY and related approaches, it is assumed that

$$\Theta H^{(0)}\Theta^{-1} = H^{(0)^{+}} \equiv H^{(0)}, \tag{20}$$

where Θ is the antiunitary operator:

$$\Theta \stackrel{\text{def}}{=} \mathcal{CPT}. \tag{21}$$

The subspace of neutral kaons $\mathcal{H}_{||}$ is assumed to be invariant under Θ:

$$\Theta P\Theta^{-1} = P^{+} \equiv P. \tag{22}$$

In the kaon rest frame, the time evolution is governed by the Schrödinger equation (2), where the initial state of the system has the form (12), (8). Within assumptions (16)-(18) the Weisskopf-Wigner approach, which is the source of the LOY method, leads to the following formula for H_{LOY} (*e.g.*, see [5-7, 12]):

$$H_{\text{LOY}} = m_0 P - \Sigma(m_0) \equiv PHP - \Sigma(m_0), \tag{23}$$

$$= M_{\text{LOY}} - \frac{i}{2}\Gamma_{\text{LOY}} \tag{24}$$

where it has been assumed that $\langle\mathbf{1}|H_W|\mathbf{2}\rangle = \langle\mathbf{1}|H_W|\mathbf{2}\rangle^{*} = 0$ (see [5-12]),

$$\Sigma(\varepsilon) = PHQ\frac{1}{QHQ - \varepsilon - i0}QHP. \tag{25}$$

The matrix elements H_{jk}^{LOY} of H_{LOY} are

$$h_{jk}^{\text{LOY}} = H_{jk} - \Sigma_{jk}(m_0), \quad (j, k = 1, 2), \tag{26}$$

$$= M_{jk}^{\text{LOY}} - \frac{i}{2}\Gamma_{jk}^{\text{LOY}} \tag{27}$$

where, in this case,

$$H_{jk} = \langle\mathbf{j}|H|\mathbf{k}\rangle \equiv \langle\mathbf{j}|(H^{(0)} + H_W)|\mathbf{k}\rangle \equiv m_0\delta_{jk}\,\langle\mathbf{j}|H_W|\mathbf{k}\rangle, \tag{28}$$

and $\Sigma_{jk}(\varepsilon) = \langle\mathbf{j}|\Sigma(\varepsilon)|\mathbf{k}\rangle$.

Now, if $\Theta H_W\Theta^{-1} = H_W^{+} \equiv H_W$, that is if

$$[\Theta, H] = 0, \tag{29}$$

then using, *e.g.*, the following phase convention [6-12]

$$\Theta|\mathbf{1}\rangle \stackrel{\text{def}}{=} -|\mathbf{2}\rangle, \quad \Theta|\mathbf{2}\rangle \stackrel{\text{def}}{=} -|\mathbf{1}\rangle, \tag{30}$$

and taking into account that $\langle\psi|\varphi\rangle = \langle\Theta\varphi|\Theta\psi\rangle$, one easily finds from (23)-(28) that

$$h_{11}^{\text{LOY}^{\Theta}} - h_{22}^{\text{LOY}^{\Theta}} = 0, \tag{31}$$

and thus

$$M_{11}^{\text{LOY}} = M_{22}^{\text{LOY}}, \tag{32}$$

(where $h_{jk}^{\text{LOY}^{\Theta}}$ denotes the matrix elements of H_{LOY}^{Θ} – of the LOY effective Hamiltonian when the relation (29) holds), in the CPT-invariant system. This is the standard result of the LOY approach and this is the picture which one meets in the literature [5-11].

If it is assumed that the CPT-symmetry is not conserved in the physical system under consideration, *i.e.*, that

$$[\Theta, H] \neq 0, \tag{33}$$

then $h_{11}^{\text{LOY}} \neq h_{22}^{\text{LOY}}$.

It is convenient to express the difference between H_{LOY}^{Θ} and the effective Hamiltonian H_{LOY} appearing within the LOY approach in the case of nonconserved CPT-symmetry as follows

$$H_{\text{LOY}} \equiv H_{\text{LOY}}^{\Theta} + \delta H_{\text{LOY}} = \tag{34}$$

$$= \begin{pmatrix} \left(M_0 + \frac{1}{2}\delta M\right) - \frac{i}{2}\left(\Gamma_0 + \frac{1}{2}\delta\Gamma\right) & M_{12} - \frac{i}{2}\Gamma_{12} \\ M_{12}^{*} - \frac{i}{2}\Gamma_{12}^{*} & \left(M_0 - \frac{1}{2}\delta M\right) - \frac{i}{2}\left(\Gamma_0 - \frac{1}{2}\delta\Gamma\right) \end{pmatrix}.$$

In other words

$$h_{jk}^{\text{LOY}} = h_{jk}^{\text{LOY}^{\Theta}} + \Delta h_{jk}^{\text{LOY}}, \tag{35}$$

where

$$\Delta h_{jk}^{\text{LOY}} = (-1)^{j+1}\frac{1}{2}\left(\delta M - \frac{i}{2}\delta\Gamma\right)\delta_{jk}, \tag{36}$$

and j, k = 1, 2. Within this approach the δM and $\delta\Gamma$ terms violate the CPT-symmetry.

3. CPT AND THE EXACT EFFECTIVE HAMILTONIAN

The aim of this Section is to show that, contrary to the LOY conclusion (31), the diagonal matrix elements of the exact effective Hamiltonian $H_{\|}$ can not be equal when the total system under consideration is CPT invariant but CP noninvariant. This will be done by means of the method used in [14].

The universal properties of the (unstable) particle-antiparticle subsystem of the system described by the Hamiltonian H, for which the relation (29) holds, can be extracted from the matrix elements of the exact $U_{\|}(t)$ appearing in (7). Such $U_{\|}(t)$ has the following form

$$U_{\|}(t) = PU(t)P, \tag{37}$$

where P is defined by the relation (15), and $U(t)$ is the total unitary evolution operator $U(t)$, which solves the Schrödinger equation (2). Of course, $U_{\|}(t)$ has a nontrivial form only if (19) holds, and only then transitions of states from $\mathcal{H}_{\|}$ into $\mathcal{H}_{\perp}$ and vice versa, *i.e.*, decay and regeneration processes, are allowed.

Using the matrix representation one finds

$$U_{\|}(t) \equiv \begin{pmatrix} \mathbf{A}(t) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \tag{38}$$

where $\mathbf{0}$ denotes the suitable zero submatrices and a submatrix $\mathbf{A}(t)$ is the (2×2) matrix acting in $\mathcal{H}_{\|}$

$$\mathbf{A}(t) = \begin{pmatrix} A_{11}(t) & A_{12}(t) \\ A_{21}(t) & A_{22}(t) \end{pmatrix} \tag{39}$$

and $A_{jk}(t) = \langle \mathbf{j}|U_{\|}(t)|\mathbf{k}\rangle \equiv \langle \mathbf{j}|U(t)|\mathbf{k}\rangle$, $(j, k = 1, 2)$ (see (1)). In the case of n-dimensional $\mathcal{H}_{\|}$ the submatrix $\mathbf{A}(t)$ is the $(n \times n)$ matrix.

Now, assuming (29) and using the phase convention (30), [5-8], one easily finds that [10, 3, 15, 17]

$$A_{11}(t) = A_{22}(t). \tag{40}$$

Note that assumptions (29) and (30) give no relations between $A_{12}(t)$ and $A_{21}(t)$.

The important relation between amplitudes $A_{12}(t)$ and $A_{21}(t)$ follows from the famous Khalfin's Theorem [10, 15--17]. This Theorem states that in the case of unstable states, if amplitudes $A_{12}(t)$ and $A_{21}(t)$ have the same time dependence

$$r(t) \stackrel{\text{def}}{=} \frac{A_{12}(t)}{A_{21}(t)} = \text{const} \equiv r, \tag{41}$$

there must be $|r| = 1$.

For unstable particles relation (40) means that the decay laws

$$p_j(t) \stackrel{\text{def}}{=} |A_{jj}(t)|^2, \tag{42}$$

(where $j = 1, 2$), of the particle $|\mathbf{1}\rangle$ and its antiparticle $|\mathbf{2}\rangle$ are equal,

$$p_1(t) \equiv p_2(t). \tag{43}$$

The consequence of this last property is that the decay rates of the particle $|\mathbf{1}\rangle$ and its antiparticle $|\mathbf{2}\rangle$ must be equal too.

From (40) it does not follow that the masses of particle "1" and the antiparticle "2" should be equal.

More conclusions about the properties of the matrix elements of $H_{\|}$ one can infer analyzing the following identity [18-23]

$$H_{\|} \equiv H_{\|}(t) = i\frac{\partial U_{\|}(t)}{\partial t}\left[U_{\|}(t)\right]^{-1}, \tag{44}$$

where $[U_{\|}(t)]^{-1}$ is defined as follows

$$U_{\|}(t)\left[U_{\|}(t)\right]^{-1} = \left[U_{\|}(t)\right]^{-1}U_{\|}(t) = P. \tag{45}$$

(Note that the identity (44) holds, independent of whether $[P, H] \neq 0$ or $[P, H] = 0$). The expression (44) can be rewritten using the matrix $\mathbf{A}(t)$

$$H_{\|}(t) \equiv i\frac{\partial \mathbf{A}(t)}{\partial t}[\mathbf{A}(t)]^{-1}. \tag{46}$$

Relations (44), (46) must be fulfilled by the exact as well as by every approximate effective Hamiltonian governing the time evolution in every two dimensional subspace $\mathcal{H}_{\|}$ of states $\mathcal{H}$ [18-23].

It is easy to find from (46) the general formulae for the diagonal matrix elements, h_{jj}, of $H_{\|}(t)$, in which we are interested. We have

$$h_{11}(t) = \frac{i}{\det \mathbf{A}(t)}\left(\frac{\partial A_{11}(t)}{\partial t}A_{22}(t) - \frac{\partial A_{12}(t)}{\partial t}A_{21}(t)\right), \tag{47}$$

$$h_{22}(t) = \frac{i}{\det \mathbf{A}(t)}\left(-\frac{\partial A_{21}(t)}{\partial t}A_{12}(t) + \frac{\partial A_{22}(t)}{\partial t}A_{11}(t)\right). \tag{48}$$

Now, assuming (29) and using the consequence (40) of this assumption, one finds

$$h_{11}(t) - h_{22}(t) = \frac{i}{\det \mathbf{A}(t)}\left(\frac{\partial A_{21}(t)}{\partial t}A_{12}(t) - \frac{\partial A_{12}(t)}{\partial t}A_{21}(t)\right) \tag{49}$$

Next, after some algebra one obtains

$$h_{11}(t) - h_{22}(t) = -i\frac{A_{12}(t)A_{21}(t)}{\det \mathbf{A}(t)}\frac{\partial}{\partial t}\ln\left(\frac{A_{12}(t)}{A_{21}(t)}\right). \tag{50}$$

This result means that in the considered case for $t > 0$ the following Theorem holds:

$$h_{11}(t) - h_{22}(t) = 0 \iff \frac{A_{12}(t)}{A_{21}(t)} = \text{const.}, \quad (t > 0). \tag{51}$$

Thus for $t > 0$ the problem under study is reduced to the Khalfin's Theorem (see the relation (41)).

From (47) and (48) it is easy to see that at $t = 0$

$$h_{jj}(0) = \langle \mathbf{j} | H | \mathbf{j} \rangle, \quad (j = 1, 2), \tag{52}$$

which means that in a CPT invariant system (29) in the case of pairs of unstable particles, for which transformations of type (30) hold

$$M_{11}(0) = M_{22}(0) \equiv \langle \mathbf{1} | H | \mathbf{1} \rangle, \tag{53}$$

the unstable particles "1" and "2" are created at $t = t_0 \equiv 0$ as particles with equal masses.

Now let us go on to analyze the conclusions following from the Khalfin's Theorem. CP noninvariance requires that $|r| \neq 1$ [3, 10, 15, 17] (see also [5-7, 13]). This means that in such a case there must be $r \equiv r(t) \neq \text{const}$. So, if in the system considered the property (29) holds but

$$[\mathcal{CP}, H] \neq 0, \tag{54}$$

and the unstable states "1" and "2" are connected by a relation of type (30), then at $t > 0$ it must be $(h_{11}(t) - h_{22}(t)) \neq 0$ in this system. Assuming the LOY interpretation of $\Re(h_{jj}(t))$, $(j = 1, 2)$, one can conclude from the Khalfin's Theorem and from the property (51) that if $A_{12}(t)$, $A_{21}(t) \neq 0$ for $t > 0$ and if the total system considered is CPT-invariant, but CP-noninvariant, then $M_{11}(t) \neq M_{22}(t)$ for $t > 0$, that is, that contrary to the case of stable particles (the bound states), the masses of the simultaneously created unstable particle "1" and its antiparticle "2", which are connected by the relation (30), need not be equal for $t > t_0 = 0$. Of course, such a conclusion contradicts the standard LOY result (31), (32). However, one should remember that the LOY description of neutral K mesons and similar complexes is only an approximate one, and that the LOY approximation is not perfect. On the other hand the relation (51) and the Khalfin's Theorem follow from the basic principles of the quantum theory and are rigorous. Consequently, their implications should also be considered rigorous.

4. BEYOND THE WW AND LOY APPROXIMATIONS

The approximate formulae for $H_{||}(t)$ have been derived in [24, 25] using the Krolikowski-Rzewuski equation for the projection of a state vector [26], which results from the Schrödinger equation (2) for the total system under consideration, and, in the case of the initial conditions of the type (12), takes the following form

$$\left(i\frac{\partial}{\partial t} - PHP \right) U_{||}(t) |\psi\rangle_{||} = -i \int_0^\infty K(t-\tau)\, U_{||}(\tau) |\psi\rangle_{||}\, d\tau, \tag{55}$$

where $U_{||}(0) = P$,

$$K(t) = \Theta(t) PHQ \exp\left(-itQHQ\right) QHP, \tag{56}$$

and $\Theta(t) = \{1 \text{ for } t \geq 0,\ 0 \text{ for } t < 0\}$.

The integro-differential equation (55) can be replaced by the following differential one (see [19-26])

$$\left(i\frac{\partial}{\partial t} - PHP - V_{||}(t) \right) U_{||}(t) |\psi\rangle_{||} = 0, \tag{57}$$

where

$$PHP + V_{||}(t) \stackrel{\text{def}}{=} H_{||}(t). \tag{58}$$

Taking into account (55) and (57) or (4) one finds from (7) and (55)

$$V_{||}(t) U_{||}(t) = -i \int_0^\infty K\left(t-\tau\right) U_{||}(\tau) d\tau \stackrel{\text{def}}{=} -iK * U_{||}(t). \tag{59}$$

(Here the asterisk, $*$, denotes the convolution: $f * g(t) = \int_0^\infty f(t-\tau) g(\tau) d\tau$). Next, using this relation and a retarded Green's operator $G(t)$ for the equation ((55)

$$G(t) = -i\,\Theta(t)\, \exp(-iPHP)P, \tag{60}$$

one obtains [24, 25]

$$U_{||}(t) = \left[1_* + \sum_{n=1}^\infty (-i)^n L * \ldots * L \right] * U_{||}^{(0)}(t), \tag{61}$$

where L is convoluted n times, $1_* \equiv 1_*(t) \equiv \delta(t)$,

$$L(t) = G * K(t), \tag{62}$$

$$U_{||}^{(0)} = \exp(-itPHP)P \tag{63}$$

is a "free" solution of Eq. (55). Thus from (59)

$$V_{||}(t)\, U_{||}(t) = -iK * \left[1_* + \sum_{n=1}^\infty (-i)^n L * \ldots * L \right] * U_{||}^{(0)}(t), \tag{64}$$

Of course, the series (61), (64) are convergent if $\| L(t) \| < 1$. If for every $t \geq 0$

$$\| L(t) \| \ll 1, \tag{65}$$

then, to the lowest order of $L(t)$, one finds from (64) [24, 25]

$$V_{||}(t) \cong V_{||}^{(1)}(t) \stackrel{\text{def}}{=} -i \int_0^\infty K(t-\tau) \exp\left[i(t-\tau) PHP \right] d\tau. \tag{66}$$

Thus [21, 23-25]

$$H_{||}(0) \equiv PHP, \quad V_{||}(0) = 0, \quad V_{||}(t \to 0) \simeq -itPHQHP. \tag{67}$$

Now let us consider a general case of n-dimensional subspace $\mathcal{H}_{||}$. Vectors from such subspaces describe states of n-level (n-particle) subsystems. The only problem is to calculate $P \exp[itPHP]$ in (66) for the case of $\dim(\mathcal{H}_{||}) = n$. Note that it is convenient to consider such $\mathcal{H}_{||}$ as the subspace spanned by a set of orthonormal vectors $\{|\mathbf{e}_j\rangle\}_{j=1}^{n} \in \mathcal{H}$, $\langle \mathbf{e}_j | \mathbf{e}_k \rangle = \delta_{jk}$. Then the projection operator P defining this subspace (see (13)) can be expressed as follows

$$P = \sum_{j=1}^{n} \left| \mathbf{e}_j \right\rangle \left\langle \mathbf{e}_j \right|. \tag{68}$$

The operator PHP is selfadjoint, so the ($n \times n$) matrix representing PHP in the subspace $\mathcal{H}_{\|}$ is Hermitian matrix. Solving the eigenvalue problem for this matrix,

$$PHP \left| \lambda_j \right\rangle = \lambda_j \left| \lambda_j \right\rangle, \qquad (j = 1, 2, \dots n), \tag{69}$$

one obtains the eigenvalues $\lambda_j = \lambda_j^*$, and eigenvectors $\left|\lambda_j\right\rangle$, ($j$ = 1, 2, ..., n). Here for simplicity we assume that $\lambda_1 \neq \lambda_2 \neq \dots \neq \lambda_n \neq \lambda_1 \neq \dots$ *etc*. In other words it is assumed that all λ_j are nondegenerate and thus all $\left|\lambda_j\right\rangle$ must be orthogonal,

$$\left\langle \lambda_j \middle| \lambda_k \right\rangle = \left\langle \lambda_j \middle| \lambda_j \right\rangle \delta_{jk}, \qquad (j, k = 1, 2, \dots n), \tag{70}$$

By means of these eigenvectors one can define new projection operators,

$$P_j \overset{\text{def}}{=} \frac{1}{\left\langle \lambda_j \middle| \lambda_j \right\rangle} \left| \lambda_j \right\rangle \left\langle \lambda_j \right|, \qquad (j = 1, 2, \dots n). \tag{71}$$

The property (70) of the solution of the eigenvalue problem for PHP considered implies that

$$P_j P_k = P_j \delta_{jk}, \qquad (j = 1, 2, \dots n), \tag{72}$$

and that the completeness requirement for the subspace $\mathcal{H}_{\|}$

$$\sum_{j=1}^{n} P_j = P, \tag{73}$$

holds. Now, using the projectors P_j one can write

$$PHP = \sum_{j=1}^{n} \lambda_j P_j, \tag{74}$$

and

$$Pe^{+itPHP} = P \sum_{j=1}^{n} e^{+it\lambda_j} P_j. \tag{75}$$

This last relation is the solution for the problem of finding $P \exp[itPHP]$ in the considered case of nondegenerate λ_j and leads to the following formula for $V_{\|}(t)$,

$$V_{\|}(t) \simeq V_{\|}^{(1)}(t) = -i \sum_{j=1}^{n} \int_0^t PHQ\, e^{-i(t-\tau)(QHQ - \lambda_j)} QHP d\tau P_j. \tag{76}$$

A computation of the value of this integral can be easy performed and yields

$$V_{\|}^{(1)}(t) = -\sum_{j=1}^{n} PHQ \frac{e^{-it(QHQ - \lambda_j)} - 1}{QHQ - \lambda_j} QHP\, P_j, \tag{77}$$

which leads to $V_{\|} \overset{\text{def}}{=} \lim_{t \to \infty} V_{\|}^{(1)}(t)$,

$$V_{\|} = -\sum_{j=1}^{n} \Sigma(\lambda_j) P_j, \tag{78}$$

(where $\Sigma(\lambda)$ is defined by the formula (25). This solves the problem of finding the effective Hamiltonian

$$H_{\|} \equiv PHP + V_{\|}, \tag{79}$$

(where $V_{\|} = \lim_{t \to \infty} V_{\|}(t)$) governing the time evolution in the n-state subspace $\mathcal{H}_{\|}$ of the total state space $\mathcal{H}$.

The simplest case is when the operator PHP has n-fold degenerate eigenvalue λ_0, that is when $\lambda_1 = \lambda_2 = \dots = \lambda_n \overset{\text{def}}{=} = \lambda_0$. Then

$$V_{\|}^{(1)}(t) = -PHQ \frac{e^{-it(QHQ - \lambda_0)} - 1}{QHQ - \lambda_0} QHP, \tag{80}$$

which gives

$$V_{\|} = -\Sigma(\lambda_0). \tag{81}$$

The most interesting cases seem to be the cases when the eigenvalues λ_j of PHP are k-fold degenerate, where $k < n$. Then the form of $V_{\|}$ differs from (78) and (81).

So, let $\lambda_1, \lambda_2, \dots, \lambda_k$ be the nondegenerate eigenvalues for PHP and $\lambda_{k+1} = \lambda_{k+2} = \dots = \lambda_n \overset{\text{def}}{=} \lambda$. Then

$$PHP = \sum_{j=1}^{k} \lambda_j P_j + \lambda \left(P - \sum_{j=1}^{k} P_j \right), \tag{82}$$

(here P_j is given by the formula (71)) and

$$Pe^{+itPHP} = P \sum_{j=1}^{k} e^{+it\lambda_j} P_j + P \left(P - \sum_{j=1}^{k} P_j \right) e^{it\lambda}. \tag{83}$$

Using this last relation and the general formula (66) for $V_{\|}(t)$ and then taking $t \to \infty$ one finds

$$V_{\|} = -\sum_{j=1}^{k} \Sigma(\lambda_j) P_j - \Sigma(\lambda) \left(P - \sum_{j=1}^{k} P_j \right). \tag{84}$$

The other cases, *e.g.* of type $\lambda_1 = \lambda_2 \neq \lambda_3 = \lambda_4 \neq \lambda_5 \neq \lambda_6 \neq \dots \neq \lambda_n$, *etc*., will be discussed in future papers.

Now let us pass on to n =2 case, *i.e.* to the case of two-dimensional subspace $\mathcal{H}_{\|}$, which can be applied to the problems discussed in Sec. 2 and 3. So, if the projector P is defined as in (15) and H has the following property

$$PHP \equiv m_0 P, \tag{85}$$

that is for

$$H_{12} = H_{21} = 0, \tag{86}$$

the approximate formula (66) for $V_{\|}(t)$ leads to the following form of Pe^{itPHP},

$$Pe^{itPHP} = Pe^{itm_0}, \tag{87}$$

and thus to

$$V_{\|}^{(1)}(t) = -PHQ\frac{e^{-it(QHQ-m_0)}-1}{QHQ-m_0}QHP, \tag{88}$$

which leads to

$$V_{\|} = \lim_{t\to\infty} V_{\|}^{(t)} = -\Sigma(m_0). \tag{89}$$

This means that in the case (85)

$$H_{\|} = m_0 P - \Sigma(m_0), \tag{90}$$

and $H_{\|} = H_{\mathrm{LOY}}$.

On the other hand, in the case

$$H_{12} = H_{21}^{*} \neq 0, \tag{91}$$

the form of Pe^{itPHP} is more complicated. For example in the case of conserved CPT, formula (66) leads to the following form of $V_{\|} \stackrel{\text{def}}{=} \lim_{t\to\infty} V_{\|}^{(1)}(t)$ [12, 27].

$$\begin{aligned} V_{\|}^{\Theta} = &-\frac{1}{2}\Sigma\left(H_0+|H_{12}|\right)\left[\left(1-\frac{H_0}{|H_{12}|}\right)P+\frac{1}{|H_{12}|}PHP\right]+ \\ &-\frac{1}{2}\Sigma\left(H_0-|H_{12}|\right)\left[\left(1+\frac{H_0}{|H_{12}|}\right)P-\frac{1}{|H_{12}|}PHP\right], \end{aligned} \tag{92}$$

where

$$H_0 \stackrel{\text{def}}{=} \frac{1}{2}\left(H_{11}+H_{22}\right), \tag{93}$$

and $V_{\|}^{\Theta}$ denotes $V_{\|}$ when (29) occurs.

In the general case (91), when there are no assumptions on symmetries of the type CP-, T-, or CPT-symmetry for the total Hamiltonian H of the system considered, the form of $V_{\|} = V_{\|}(t\to\infty) \cong V_{\|}^{(1)}(\infty)$ is even more complicated. In such a case one finds the following expressions for the matrix elements $v_{jk}(t\to\infty) \stackrel{\text{def}}{=} v_{jk}$ of $V_{\|}$ [24, 25],

$$\begin{aligned} v_{j1} = &-\frac{1}{2}\left(1+\frac{H_z}{\kappa}\right)\Sigma_{j1}(H_0+\kappa)-\frac{1}{2}\left(1-\frac{H_z}{\kappa}\right)\Sigma_{j1}(H_0-\kappa)+ \\ &-\frac{H_{21}}{2\kappa}\Sigma_{j2}\left(H_0+\kappa\right)+\frac{H_{21}}{2\kappa}\Sigma_{j2}\left(H_0-\kappa\right), \end{aligned} \tag{94}$$

$$\begin{aligned} v_{j2} = &-\frac{1}{2}\left(1-\frac{H_z}{\kappa}\right)\Sigma_{j2}(H_0+\kappa)-\frac{1}{2}\left(1+\frac{H_z}{\kappa}\right)\Sigma_{j2}(H_0-\kappa)+ \\ &-\frac{H_{12}}{2\kappa}\Sigma_{j1}\left(H_0+\kappa\right)+\frac{H_{12}}{2\kappa}\Sigma_{j1}\left(H_0-\kappa\right), \end{aligned}$$

where $j, k = 1, 2$,

$$H_z = \frac{1}{2}\left(H_{11}-H_{22}\right), \tag{95}$$

and

$$\kappa = \left(|H_{12}|^2 + H_z^2\right)^{1/2}. \tag{96}$$

Hence, by (58)

$$h_{jk} = H_{jk} + v_{jk}. \tag{97}$$

It should be emphasized that all components of the expressions (94) are of the same order with respect to $\Sigma(\varepsilon)$.

In the case of preserved CPT-symmetry (29), one finds $H_{11} = H_{22}$ which implies that $\kappa \equiv |H_{12}|$, $H_z \equiv 0$ and $H_0 \equiv H_{11} \equiv H_{22}$, and [24, 25].

$$\Sigma_{11}\left(\varepsilon=\varepsilon^*\right) \equiv \Sigma_{22}\left(\varepsilon=\varepsilon^*\right) \stackrel{\text{def}}{=} \Sigma_0\left(\varepsilon=\varepsilon^*\right). \tag{98}$$

Therefore matrix elements v_{jk}^{Θ} of operator $V_{\|}^{\Theta}$ take the following form

$$\begin{aligned} v_{j1}^{\Theta} = -\frac{1}{2}\Bigg\{&\Sigma_{j1}\left(H_0+|H_{12}|\right)+\Sigma_{j1}\left(H_0-|H_{12}|\right)+ \\ &+\frac{H_{21}}{|H_{12}|}\Sigma_{j2}\left(H_0+|H_{12}|\right)-\frac{H_{21}}{|H_{12}|}\Sigma_{j2}\left(H_0-|H_{12}|\right)\Bigg\}, \end{aligned} \tag{99}$$

$$\begin{aligned} v_{j2}^{\Theta} = -\frac{1}{2}\Bigg\{&\Sigma_{j2}\left(H_0+|H_{12}|\right)+\left\{\Sigma_{j2}\left(H_0-|H_{12}|\right)+\right. \\ &+\frac{H_{12}}{|H_{12}|}\Sigma_{j1}\left(H_0+|H_{12}|\right)-\frac{H_{12}}{|H_{12}|}\Sigma_{j1}\left(H_0-|H_{12}|\right)\Bigg\}, \end{aligned}$$

Assuming

$$|H_{12}| \ll |H_0|, \tag{100}$$

we find

$$v_{j1}^{\Theta} \simeq -\Sigma_{j1}(H_0) - H_{21} \frac{\partial \Sigma_{j2}(x)}{\partial x}\bigg|_{x=H_0}, \tag{101}$$

$$v_{j2}^{\Theta} \simeq -\Sigma_{j2}(H_0) - H_{12} \frac{\partial \Sigma_{j1}(x)}{\partial x}\bigg|_{x=H_0}, \tag{102}$$

where j = 1, 2. One should stress that due to the presence of resonance terms, derivatives $\frac{\partial}{\partial x}\Sigma_{jk}(x)$ need not be small and the same is true about products $H_{jk}\frac{\partial}{\partial x}\Sigma_{jk}(x)$ in (101), (102). Finally, assuming that (100) holds and using relations (101), (102), (97) and the expression (26), we obtain for the CPT-invariant system [28, 29]

$$h_{j1}^{\Theta} \simeq h_{j1}^{\text{LOY}} - H_{21} \frac{\partial \Sigma_{j2}(x)}{\partial x}\bigg|_{x=H_0} \stackrel{\text{def}}{=} h_{j1}^{\text{LOY}} + \delta h_{j1}, \tag{103}$$

$$h_{j2}^{\Theta} \simeq h_{j2}^{\text{LOY}} - H_{12} \frac{\partial \Sigma_{j1}(x)}{\partial x}\bigg|_{x=H_0} \stackrel{\text{def}}{=} h_{j2}^{\text{LOY}} + \delta h_{j2}, \tag{104}$$

where j = 1, 2. From these formulae we conclude that, *e.g.*, the difference between the diagonal matrix elements of $H_{\|}^{\Theta}$ which plays an important role in designing CPT-invariance tests for the neutral kaons system, equals

$$\Delta h \stackrel{\text{def}}{=} h_{11} - h_{22} \simeq H_{12} \frac{\partial \Sigma_{21}(x)}{\partial x}\bigg|_{x=H_0} - H_{21} \frac{\partial \Sigma_{12}(x)}{\partial x}\bigg|_{x=H_0} \neq 0. \tag{105}$$

The conclusions following from this property are discussed in details in [29].

5. FINAL REMARKS

In the case of conserved CPT- and violated CP-symmetries there must be

$$h_{11}^{\Theta}(t) - h_{22}^{\Theta}(t) \neq 0 \qquad \text{for} \qquad t > t_0 = 0,$$

and, $h_{11}(0) = h_{22}(0) = \langle \mathbf{1}|H|\mathbf{1}\rangle$, for the exact $H_{\|}$.

Note that properties of the more accurate approximation described in Sec. 4 are consistent with the general properties and conclusions obtained in Sec. 3 for the exact effective Hamiltonian – compare (67) and (52) and relations (51) with (105).

From the result (105) it follows that Δh = 0 can be achieved only if $H_{12} = H_{21} = 0$. This means that if the first order $|\Delta S| = 2$ interactions are forbidden in the $K_0, \overline{K}_0$ complex then predictions following from the use of the mentioned more accurate approximation and from the LOY theory should lead to the same masses for K_0 and for $\overline{K}_0$. This does not contradict the results of Sec. 3 derived for the exact $H_{\|}$: the mass difference is very, very small and should arise at higher orders of the more accurate approximation.

On the other hand from (105) it follows that $\Delta h \neq 0$ if and only if $H_{12} \neq 0$. This means that if measurable deviations from the LOY predictions concerning the masses of, *e.g.* $K_0, \overline{K}_0$ mesons are ever detected, then the most plausible interpretation of this result will be the existence of first order $|\Delta S| = 2$ interactions in the system considered.

The formulae (78), (79), (81) and (84), and the like, can be used to searching for solutions of equations governing the time evolution of n-level (n-particle) complexes. It seems that the cases when some eigenvalues λ_j of *PHP* acting in n-dimensional $\mathcal{H}_{\|}$ are degenerate, can be especially interesting (these cases will be investigated in future papers). In general the Schrödinger like evolution equations of the type (4) with $H_{\|}$ given by (79) and (78), (81) or (84) can lead to more the accurate description of properties of n-level physical subsystems.

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