HYPER VERSION

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On the modular invariance of mass eigenstates and CP violation

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Abstract: We investigate the modular transformation properties of observable (light) fields in heterotic orbifolds, in the light of recent calculations of CP-violating quantities. Measurable quantities must be modular invariant functions of string moduli, even if the light fields are not invariant. We show that physical invariance may arise by patching smooth functions that are separately noninvariant. CP violation for $\langle T \rangle$ on the unit circle, which requires light and heavy states to mix under transformation, is allowed in principle, although the Jarlskog parameter $J_{\mathrm{CP}}(T)$ must be amended relative to previous results. However, a toy model of modular invariant mass terms indicates that the assumption underlying these results is unrealistic. In general the mass eigenstate basis is manifestly modular invariant and coupling constants are smooth invariant functions of T, thus CP is unbroken on the unit circle. We also discuss the status of CP-odd quantities when CP is a discrete gauge symmetry, and point out a link with baryogenesis.

Keywords: Discrete and Finite Symmetries, Compactification and String Models, CP violation.

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1. Introduction

Recently, contradictory claims have appeared [1, 2] concerning the invariance of physical quantities under T-duality transformation in heterotic orbifolds, particularly for CP-violating quantities such as the Jarlskog parameter, and the consequences for phenomenology. In the (somewhat simplified) models under discussion CP is assumed to be spontaneously broken by a T (Kähler) modulus of compactification, which has the CP transformation $T \mapsto T^*$.[1] Low-energy quantities such as Yukawa couplings and soft terms are functions of T and inherit complex phases from its v.e.v.. The perturbative theory has a duality symmetry (properly, $\mathrm{SL}(2,\mathbb{Z})$ modular symmetry) [8] to all orders, generated by

$$\mathcal{T}\!: T \longmapsto T + i\,, \qquad \mathcal{S}\!: T \longmapsto \frac{1}{T}\,, \tag{1.1}$$

where the second generator $\mathcal{S}$, which exchanges large and small radii, is loosely referred to as T-duality. The action of the symmetry on orbifold twisted sectors [9, 10] is unitary and intrinsically nonabelian: the generators cannot be simultaneously made diagonal by any constant change of basis. In the "twist" basis usually found convenient, the shift $\mathcal{T}\!: T \mapsto T + i$ is diagonalised.

[1] The imaginary part of T is dual to the antisymmetric tensor field in the compact directions; thus its sign flips under orientation reversal of the compact space (equivalently, conjugation of the complex planes of the orbifold), which can be shown to be an appropriate CP transformation [4]–[7].

Then we showed in [2] that given a unitary modular transformation of observable matter fields, CP was unbroken for modulus v.e.v.'s satisfying either $1/T = T^*$ or $T + i = T^*$, that is those for which the CP transformation is a modular transformation. In particular, if either $\text{Im}\, T = \pm 1/2$ or $|T| = 1$, this condition is satisfied and no CP violation is expected. In contrast, it was recently claimed in a calculation based on a $\mathbb{Z}_6$ orbifold model [1] that the Jarlskog parameter $J_{\text{CP}}(T)$ does not vanish on the unit circle, and explicit numerical results were presented. Here, the result for $J_{\text{CP}}(T)$ changes sign on taking $T \mapsto T^*$, as naïvely expected for a CP-odd quantity. This claim raises an important question, whether observable quantities can depend on which one of two or more vacua related by $\text{SL}(2,\mathbb{Z})$ we live in. Since the theory is modular invariant, physics should be the same in vacua that are related by the modular group — here, by $T \mapsto 1/T$. In fact, since CP can be shown to be part of the gauge symmetry of the heterotic string [5, 6], one also expects CP-conjugate vacua to give the same value (rather than values differing by a sign) for any measurable quantity, by the same argument: vacua differing only by a constant element of the symmetry group are not physically distinguishable.

The calculation of [1] was based on an important assumption which allows the previous result [2] to be evaded. In this paper we examine this and other assumptions about modular invariance and low-energy physics, and reach a possibly unexpected conclusion, based on a careful definition of physical observables: modular invariance may be restored by patching smooth, non-invariant functions together, in a manner determined by which states are light at any particular point in moduli space. In principle, the result of [1] may be correct for some modulus values, but must be amended for others to restore its modular invariance and physical significance.

In the second part of the paper we use a formally modular invariant toy model to test the conjecture that light and heavy matter can mix under modular transformation. Applying the assumption of [1] to the model one obtains a somewhat unnatural result, requiring some mass matrix elements to vanish exactly at the physical value of $\langle T \rangle$. This condition is not maintained after modular transformation, and also results in an undesirable degenerate matter spectrum when $\langle T \rangle$ lies on the unit circle. In the more general case where all elements are non-zero, the rotation to the mass eigenstate basis and the nonabelian modular transformations combine in a complicated fashion.

Without plumbing the full algebraic depths of the situation, we show by an appropriate choice of initial basis that our earlier guess [2], that the mass eigenstates are invariant (up to unobservable phases) under the combined transformation of the modulus and the twisted states, was correct. Then since the action is invariant, all T-dependent coupling constants (or rephasing-invariant combinations thereof) written in the mass basis are also modular invariant. Any non-invariant couplings in the theory basis are "killed" by the *modulus-dependent* change to the mass basis. This result should hold also in more complex models, thus any observable property of the light matter fields should be a unique, smooth, invariant function of T, and CP is unbroken for T on the unit circle.

We also reconcile the status of CP as a gauge symmetry with the existence of "CP-odd" observables, using some elementary thought experiments.

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2. Nonunitary quark transformations

The technical point in [1] that allowed the Jarlskog parameter $J_{\rm CP}(T)$ as usually defined (as a function of quark mass matrices) not to be invariant under $T \mapsto 1/T$, is the transformation of the three generations of light quark fields.[2] The orbifold twisted sector in which the quarks live has many more states than required in the Standard Model. In general the states are labelled by the twists under which they are invariant and by the fixed points at which they are localized (see e.g. [11]). Then in a given twisted sector the states mix unitarily under duality, as already stated. But if, as assumed in [1] one picks a subset of these to represent the light quarks, the transformation of this subset will generally not be unitary and involve other states (assumed to be much heavier) in the twisted sector. After duality, the transformed Yukawa couplings or mass matrices are not related unitarily to the original couplings of only the light fields.

We have, schematically,

$$\mathcal{S}\colon q_A \longmapsto \tilde{q}_A \equiv \mathbf{S}_{AB} q_B\,, \qquad A,B = 1,\ldots,N_g \tag{2.1}$$

for the light and heavy generations together. The left-handed doublets and right-handed up- and down-type fields may each transform with a different $\mathbf{S}$, but to simplify the discussion (and also since transformations of the right-handed quarks cancel in the expression for $J_{\rm CP}$) we consider a single matrix. Then for the light quarks q_i

$$q_i \longmapsto \mathbf{S}_{ij} q_j + \mathbf{S}_{ia} q_a\,, \qquad i = 1,2,3\,, \qquad a = 1,\ldots,N_g - 3 \tag{2.2}$$

and $\mathbf{S}_{ij}$ will not in general be unitary (given that some $\mathbf{S}_{ia}$ are non-vanishing). Since the mass terms are invariant we have

$$\mathcal{S}\colon M^{u,d}_{AB}(T) \longmapsto \tilde{M}^{u,d}_{AB}(T) \equiv M^{u,d}_{AB}(\tilde{T}) = (\mathbf{S} M^{u,d}(T) \mathbf{S}^\dagger)_{AB} \tag{2.3}$$

and for the entries with the light state q_i labels

$$\begin{aligned} M^{u,d}_{ij} \longmapsto \tilde{M}^{u,d}_{ij} &= \mathbf{S}_{iA} M^{u,d}_{AB}(T) \mathbf{S}^\dagger_{Bi} \\ &= \mathbf{S}_{ik} M^{u,d}_{km}(T) \mathbf{S}^\dagger_{mj} + (\text{terms proportional to } M^{u,d}_{ab}(T)) \end{aligned} \tag{2.4}$$

which again is generically not a unitary transformation and involves the mass matrix of the heavy states q_a.

Now the $J_{\rm CP}$ parameter defined by

$$\begin{aligned} \det[M^u_{ij} M^{u\dagger}_{jk}, M^d_{mn} M^{d\dagger}_{np}] &= J_{\rm CP} (m_t^2 - m_c^2)(m_c^2 - m_u^2)(m_t^2 - m_u^2) \times \\ &\quad \times (m_b^2 - m_s^2)(m_s^2 - m_d^2)(m_b^2 - m_d^2) \end{aligned} \tag{2.5}$$

or by

$$J_{\rm CP} = \operatorname{Im}\, V_{11} V_{12}^* V_{22} V_{21}^* \tag{2.6}$$

[2] Light meaning compared to the GUT or Planck scales.

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is invariant precisely under unitary changes of basis for the three quark generations [3], which appear in the expression (2.5) as unitary transformations of the quark mass matrices. Thus with a nonunitary modular transformation of quarks $J_{\rm CP}(T)$, as defined on the mass matrix of the original states $M^{u,d}_{ij}$, may change in value. The corollary of this is that this value $J_{\rm CP}(\tilde{T})$ represents some function of the couplings of, in general, a linear combination of light and unobservably heavy fields.

In order to calculate the physically observed $J_{\rm CP}$ in the modular transformed vacuum, the complete mass matrix of twisted fields must be block-diagonalised to find the three new light eigenstates, and the relevant Yukawa couplings extracted, resulting in a possibly different function $J'_{\rm CP}(T)$; nevertheless, $J'_{\rm CP}(\tilde{T})$ must have the same numerical value as $J_{\rm CP}(T)$, since it is a physical observable dependent only on the modulus v.e.v., which cannot change under modular transformation of T if modular invariance is really a symmetry of the theory.[3]

It was already assumed that the q_i were the light states for the original v.e.v., which we denote as $\langle T\rangle = T_0$: thus the mass matrices $M^{u,d}_{AB}(T_0)$ are block-diagonal in the i, a basis. The light states in the transformed vacuum $\langle T\rangle = \tilde{T}_0$ result from diagonalising the mass term

$$\bar{q}_A M^{u,d}_{AB}(\tilde{T}_0) q_B = \bar{q}_A (\mathbf{S} M^{u,d}(T_0)\mathbf{S}^\dagger)_{AB} q_B \tag{2.7}$$

thus they are just $\psi_i = \mathbf{S}^\dagger_{iA} q_A$. Then, trivially, the mass matrices from which $J'_{\rm CP}$ is to be calculated are identical in value to the light quark mass matrices $M^{u,d}_{ij}$ in the original vacuum and we find (for any T)

$$J'_{\rm CP}(\tilde{T}) = J_{\rm CP}(T)\,.$$

Note that $J_{\rm CP}(\tilde{T}_0)$ may in general be different from $J_{\rm CP}(T_0)$: we have

$$J_{\rm CP}(\tilde{T}_0) \propto \det\left[\tilde{M}^u_{ij}\tilde{M}^{u\dagger}_{jk}, \tilde{M}^d_{mn}\tilde{M}^{d\dagger}_{np}\right] \tag{2.8}$$

and the off-diagonal (light-heavy) transformations $\mathbf{S}_{iA}$ of (2.4) do not cancel in the determinant. If one were to use the old function $J_{\rm CP}$ at $\langle T\rangle = \tilde{T}_0$, as a function of the transformed mass matrices in the q_i basis, such a result would apply to the linear superpositions $q_i = \mathbf{S}_{iA}\psi_A$, where the ψ_A are both light and heavy fields, so the calculation is not physically meaningful.

Let us apply this to the model in which $J_{\rm CP}(T)$ is claimed not to be invariant under the duality $T \mapsto 1/T$. On the unit circle the duality becomes $T \mapsto T^*$ and the lack of invariance allows a non-zero value of $J_{\rm CP}$ (see [1, figure 2]). In the calculation, certain twisted sector states are identified with the light quarks and others are assumed to be heavy. With this *ansatz* the Yukawas and mass matrices are found, resulting in a smooth, non-modular-invariant function $J_{\rm CP}(T)$ over the complex T plane. Then the result may be correct over

[3] Similarly, in a GUT where some matter decouples (e.g. E_6), a physical measure of CP violation (or of anything else!) cannot change on exchanging one set of Higgs v.e.v.'s for a gauge-equivalent set; the full theory is not invariant under the transformation of the Higgses without also transforming the matter fields, but given the gauge-transformed Higgs v.e.v.'s one is forced to use gauge-transformed matter fields, because they turn out to be the light fields.

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some of the unit circle (say, the part with Im $T > 0$) but, since a nonunitary transformation of the kind discussed must be happening precisely between this line segment and its image under duality, the derived function $J_{\rm CP}(T)$ cannot represent the physical quantity it is claimed to over the rest of the domain. It might seem *a priori* unlikely that a specific mechanism would make precisely those states light which are picked out in this calculation: given a specific mass matrix for the whole twisted sector, the light states would most probably be mixtures of the states in the fixed point basis. But granted the assumptions of [1], some light states must mix with heavy ones under modular transformation in order for $J_{\rm CP}(T)$ to be non zero on the unit circle, so the derived function $J_{\rm CP}(T)$ does not remain physical after modular transformation.

Instead we need a new function $J'_{\rm CP}(T)$ valid over the rest of the domain as described above. Since the duality is $\mathbb{Z}_2$, we have $J'_{\rm CP}(T) \equiv J_{\rm CP}(\tilde{T})$ and $J'_{\rm CP}(\tilde{T}) \equiv J_{\rm CP}(T)$, and realising that the original function $J_{\rm CP}(T)$ is odd under complex conjugation we find that $J'_{\rm CP}(T) = -J_{\rm CP}(T)$ must hold on the unit circle. Thus the physical Jarlskog parameter is given by $\pm J_{\rm CP}(T)$, the sign depending on which domain $\langle T \rangle$ lies in. In particular, there will be a "join" along which the two prescriptions collide, and the physical result will not in general be differentiable at that point. We know we are using the "right" prescription precisely when the couplings that appear in the calculation are just those of the light fields. In the $\mathbb{Z}_6$ orbifold model, one should find the explicit mechanism that makes the heavy fields decouple: the expectation is that different (linear combinations of) fields will be the light ones over different regions of moduli space. The manifestly modular invariant result on the unit circle will take the form $J_{\rm CP}^{\rm (phys)} = \pm|J_{\rm CP}(T)|$, the overall sign depending on which way the prescription turns out (see figure 1 below).

There is a further sign ambiguity in this (and any theoretical) result for a CP-violating quantity, connected with the definition of matter and antimatter; we return to this at the end of the paper.

The result of [1] is already invariant under the axionic shift generator $T \mapsto T + i$, and one might ask why this should be, since in a generic basis of states (such as the basis of light and heavy eigenstates will likely be) both generators will be off-diagonal. The reason is simply that the basis of light and heavy states was assumed to be exactly that in which $T \mapsto T + i$ did act as a diagonal matrix, thus the argument of [2] applies to this symmetry and CP symmetry is unbroken at Im $T = \pm 1/2$.

We briefly return to the result of [2] and ask, what went wrong with our reasoning for the $T \mapsto 1/T$ transformation? Unitary quark transformations were not strictly necessary for our result, but we required that a CP transformation acting on observable fields, followed by the action of a modular transformation on those fields, remained a physically reasonable CP transformation. But if there is mixing of light and heavy matter fields under duality, the resulting "general CP transformation" cannot correspond to anything testable in the laboratory: light particles have to remain light under CP.[4] However, if we imagine performing experiments with the heavy twisted states and their antiparticles, some kind of unbroken CP symmetry may reappear for $\langle T \rangle$ lying on the unit circle.

[4]Within the latitude implied by the CKM mixing, which allows us to mix, for example, bottom with down.

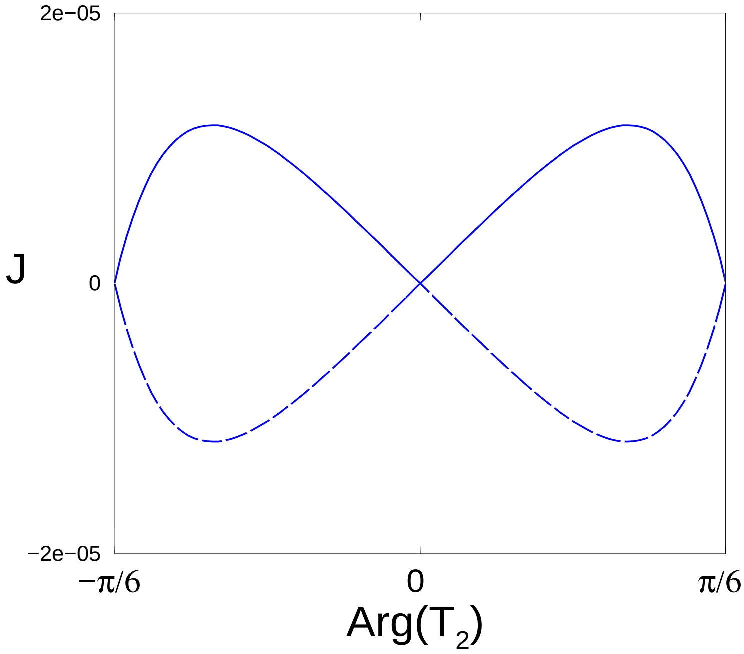

Figure 1: Amended version of [1, figure 2]: the physical $J_{\rm CP}$ parameter, invariant under duality and CP transformations of the modulus, is given by either the positive (solid) or the negative (dashed) value, depending on the correct identification of the light quark fields and of matter vs. antimatter.

3. A simple illustration

Since the nonabelian and nonunitary transformations involved in the system under consideration are rather complicated, we illustrate the general principle with a simple gedanken-experiment. Suppose we have deduced the correct value of the string scale M_s indirectly, and suspect that we live in a "large-radius" compactification (that is, with some radii differing significantly from M_s^{-1}). Given T-duality, we could equally well call it a "small-radius" compactification. Then imagine an accelerator experiment that could probe the energy of the lowest K-K or winding mode (but not the string scale itself). Clearly we cannot say that the mass of the mode that we hope to measure is given unambiguously in string units by $1/R$ (for a K-K mode) or R (winding mode). But there is a rather trivial and manifestly duality invariant expression for this mass, namely

$$m_{\rm detected} = \min\left(R, \frac{1}{R}\right) \tag{3.1}$$

in other words two noninvariant, continuous functions over moduli space, with a prescription for choosing between them. The prescription has a clear physical interpretation, namely that the lighter mode will be found at the experiment. The result is nonanalytic and not differentiable at $R = 1$, just as the prescription for $J_{\rm CP}^{\rm (phys)}(T)$ is at the real axis. Conversely, extending the smooth function $J_{\rm CP}(T)$ calculated in [1] over a region containing both T_0 and $\tilde{T}_0$ would correspond to assuming that one function, say $m_{\rm detected} = R$, holds for all values of R.

Of course, considering also the string excited states with mass scale 1 in our units, the real behaviour is likely to be more complicated near $T = 1$, but in the approximation that only the "geometric" (winding/KK) modes contribute our prescription appears reasonable.

4. The fundamental domain

One strategy to deal with the problem of degenerate vacua in a modular invariant theory is to restrict the value of T to the fundamental domain $\mathcal{F}$, usually defined as the region satisfying $-1/2 < \mathrm{Im}\, T \leq 1/2$, $|T| \geq 1$. The procedure is analogous to gauge-fixing. Any value in the half-plane $\mathrm{Re}\, T > 0$ can be reached by a modular transformation from exactly one point in $\mathcal{F}$ — no new physics occurs when we go outside. If we are interested in values on the unit circle then one half of the line segment $\mathcal{P}$ between $e^{-i\pi/6}$ and $e^{i\pi/6}$ must be excluded: let us keep the half with $\mathrm{Im}\, T \geq 0$. Then if we want to find the value of J_{CP} for T lying on the excluded part of $\mathcal{P}$, we just calculate it at the modular-equivalent value $T^* = 1/T$ lying in $\mathcal{F}$. On this basis, at first glance there is no objection to the result of [1, figure 2], as long as half of the graph is ignored as being outside $\mathcal{F}$, and replaced by the mirror reflection of the other half in $\phi = 0$ (figure 1). But this replacement creates trouble for the rest of $\mathcal{F}$ away from $|T| = 1$: since the original, noninvariant function $J_{\mathrm{CP}}(T)$ was continuous over the half-plane, the change of sign would create a discontinuity akin to a branch cut along the excluded part of $\mathcal{P}$. Clearly the replacement along $\mathcal{P}$ is not enough, since a discontinuity is definitely unphysical.

Thus the smooth function $J_{\mathrm{CP}}(T)$ must be amended over a whole region of $\mathcal{F}$. In fact, taking modular invariance in conjunction with the exact CP symmetry of the underlying theory (discussed in section 6), we find that the physical value of J_{CP} must be invariant under complex conjugation of T. Thus the most likely possibility is that the "kink" where the two prescriptions join is on the real axis, in which case half of the fundamental domain of $\mathrm{SL}(2,\mathbb{Z})$ needs replacement, and our previous answer $J_{\mathrm{CP}}^{(\mathrm{phys})} = \pm|J_{\mathrm{CP}}(T)|$ is extended to the whole of $\mathcal{F}$. Given that CP is also an exact symmetry acting on T, it makes sense to define a fundamental domain $\mathcal{F}'$ for the group $\mathrm{SL}(2,\mathbb{Z}) \otimes \mathrm{CP}$, which can be taken to be the half of $\mathcal{F}$ with $\mathrm{Im}\, T \geq 0$: then any value of T is physically equivalent to precisely one point in $\mathcal{F}'$. If we only consider T inside $\mathcal{F}'$ then there is no need to patch non-invariant functions.

What happens near $T = 1$? If, as required for nonunitary transformation of the light quarks, light and heavy states mix under duality, and mass matrix entries are continuous functions on the moduli space, something odd happens on passing through the self-dual point: light and heavy states cross over. We show in the next section that if the original basis was the mass basis, implying that off-diagonal entries vanish in the mass matrix, the self-duality condition which holds at $T = 1$ leads to an unacceptable degenerate mass spectrum. Thus the theory near this point bears no relation to the Standard Model and no value of J_{CP} can be meaningful. This may not count significantly against the assumptions of the model, since there is anyway no CP violation at $T = 1$. However, a similar argument also applies for values of T approaching the unit circle: the combination of $T \mapsto 1/T$ and CP transformation brings us to a physically equivalent v.e.v. just on the other side of the circle, but also (by assumption) mixes the light and heavy states. Thus a degenerate spectrum

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also occurs on the “CP self-dual” line $|T| = 1$. If, however, the mass matrix has off-diagonal elements in the original basis, the spectrum need not be degenerate at these values of T; but then we find that the modular transformation of the resulting mass eigenstates is trivial.

It is of course also possible in this class of theories that the light quarks *do* transform unitarily among themselves, in other words that there are no (light-heavy) off-diagonal elements in the representation of the modular group. In this case $J_{\rm CP}(T)$ is a unique modular invariant smooth function odd under $T \mapsto T^*$, which must vanish on the boundary of $\mathcal{F}$, and no prescriptions are needed to maintain modular invariance. But considerations of CP symmetry, discussed above and in more detail in section 6, may even in this case force us to adjust the result.

5. Modular invariance and mass eigenstates: a toy model

In order to see in more detail what happens at a self-dual point and what behaviour of light and heavy matter fields is consistent with a modular invariant theory, we consider a 2-by-2 mass matrix for complex scalars. This is to be our toy model for the $N_g - 3$ heavy and 3 light states that are supposed to result from a more realistic orbifold-based construction. We consider a nonabelian duality group with two generators, and formally write the modular invariant mass term as

$$\mathbf{M} = \begin{pmatrix} a & b \\ b^* & d \end{pmatrix}, \tag{5.1}$$

where a, b, d are functions of the modulus, with transformations under the duality group to be determined. We take a group action similar to the representation of $\mathrm{SL}(2,\mathbb{Z})$ on the twist fields σ_i, $i = 1,2,3$, of the two-dimensional orbifold $\mathbb{T}^2/\mathbb{Z}_3$, for which

$$\mathcal{S} = -\frac{i}{\sqrt{3}} \begin{pmatrix} 1 & 1 & 1 \\ 1 & \alpha & \alpha^2 \\ 1 & \alpha^2 & \alpha \end{pmatrix}, \qquad \mathcal{T} = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{5.2}$$

where $\alpha = e^{2\pi i/3}$ [10].[5] This representation is reducible into a singlet $\tau_0 = \sqrt{2}^{-1}(\sigma_2 - \sigma_3)$ and a doublet

$$\tau_1 \equiv \sigma_1\,, \qquad \tau_2 \equiv \frac{1}{\sqrt{2}}(\sigma_2 + \sigma_3) \tag{5.3}$$

for which

$$\mathcal{S}^{(\tau)} = -\frac{i}{\sqrt{3}} \begin{pmatrix} 1 & \sqrt{2} \\ \sqrt{2} & -1 \end{pmatrix}, \qquad \mathcal{T}^{(\tau)} = \begin{pmatrix} \alpha & 0 \\ 0 & 1 \end{pmatrix}. \tag{5.4}$$

We can generalise the representation slightly without complicating the system by taking

$$\mathcal{S}^{(\tau)} = -i \begin{pmatrix} \cos\theta_S & \sin\theta_S \\ \sin\theta_S & -\cos\theta_S \end{pmatrix}, \qquad \mathcal{T}^{(\tau)} = \begin{pmatrix} \alpha & 0 \\ 0 & 1 \end{pmatrix}. \tag{5.5}$$

The modular invariance conditions for the mass matrix analogous to (2.3) are

$$\mathcal{S}\colon \mathbf{M} \longmapsto \tilde{\mathbf{M}} = \begin{pmatrix} \tilde{a} & \tilde{b} \\ \tilde{b}^* & \tilde{d} \end{pmatrix}, \qquad \mathcal{T}\colon \mathbf{M} \longmapsto \bar{\mathbf{M}} = \begin{pmatrix} a & \bar{b} \\ \bar{b}^* & d \end{pmatrix},$$

[5] There is a sign error in the $\mathcal{S}$ generator in the first reference of [10].

where

$$\begin{aligned}\tilde{a}(T) &= ac_S^2 + ds_S^2 + 2\,\mathrm{Re}\; bc_S s_S\,,\\ \tilde{b}(T) &= (a-d)c_S s_S - \mathrm{Re}\; b(c_S^2 - s_S^2) - i\,\mathrm{Im}\; b\,,\\ \tilde{d}(T) &= as_S^2 + dc_S^2 + 2\,\mathrm{Re}\; bc_S s_S\,,\\ \bar{b}(T) &= \rho b\,.\end{aligned} \tag{5.6}$$

with $c_S = \cos\theta_S$, $s_S = \sin\theta_S$.

The non-unitary transformation required for CP violation on the unit circle corresponds to non-zero off-diagonal (i.e. not block diagonal) elements in the (light, heavy) basis, for one or more group generators. In the toy model this will be diagnosed by $(1,2)$ and $(2,1)$ entries for the transformations in the mass basis, or by any change under modular transformation in the linear superposition of the original τ making up the mass eigenstates. The (modular invariant) mass eigenvalues are $m_{1,2}^2 = \frac{1}{2}(a + d \pm \sqrt{(a-d)^2 + 4|b|^2})$.

Without further calculation we can see the effect of imposing a self-duality condition corresponding to the behaviour of quark mass matrices at the point $T = 1$. At $T = 1$ we have $\mathcal{S}(T) = T$, thus $\tilde{\mathbf{M}} = \mathbf{M}$. From this it can be deduced that

$$a - d = 2\,\mathrm{Re}\; b\cot\theta_S\,, \qquad \mathrm{Im}\; b = 0 \tag{5.7}$$

and the mass eigenvalues become $\frac{1}{2}(a + d \pm \sqrt{(a-d)\sec\theta_S})$. Because of the mixing in going from the τ basis to the mass basis the mass spectrum can be nondegenerate, although to achieve the desired hierarchy $m_2 \ll m_1$ fine-tuning seems to be required. If we literally implement the assumption of [1] that the τ_i are mass eigenstates, thus $b = 0$, we find an unacceptable spectrum at $T = 1$: the self-duality relation (5.7) reduces to $a = d$ and the states are degenerate.

This value is anyway uninteresting for CP violation; to model the case of T on the unit circle we need to implement the "CP-self-duality" relation $\mathrm{CP}(T) = T^* = \mathcal{S}(T)$ on the mass matrix entries. We require $\tilde{\mathbf{M}} = \mathbf{M}^*$ [6] which reduces to the single condition

$$a - d = 2\,\mathrm{Re}\; b\cot\theta_S \tag{5.8}$$

with no restriction on $\mathrm{Im}\; b$. Thus the mass eigenvalues in the case where the τ are not mass eigenstates are given by three parameters a, d and $\mathrm{Im}\; b$ and there is more freedom to obtain a large hierarchy. But in the case that τ_i are mass eigenstates (so $b = 0$) the spectrum is still degenerate.

Thus, the possibilities that $\langle T\rangle$ lies inside $\mathcal{F}$ with the τ_i being mass eigenstates, or that $\langle T\rangle$ lies on the unit circle with the mass basis distinct from the τ basis, remain viable, but we cannot live in a world where the τ_i are mass eigenstates and $|T| = 1$ (regardless of the status of CP). Note also that if $b = 0$ holds at one value of T it cannot hold at the dual value $\tilde{T}$ since $\tilde{b} = (a-d)s_S c_S$, so one cannot consistently impose $b = 0$ over all of moduli space unless $\theta_S = \pm\pi$. Unless the light and heavy states are *permuted* with no mixing under $\mathcal{S}$

[6] One may also introduce diagonal matrices of constant phases in the CP transformation of $\mathbf{M}$, corresponding to the τ_i receiving complex phases under CP; this possibility does not affect our conclusions.

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(which is inconsistent with any known behaviour of twisted states), or we happen to live at the rather special point(s) in moduli space where the non-modular-invariant condition $b = 0$ holds, the mass eigenstates (modelling the three light and $N_g - 3$ heavy generations) are unitary mixtures of the twist states.

Then the modular properties of the mass eigenstates have to be computed explicitly. We consider transformation of both the modulus and the τ fields together, since this is the symmetry under which the theory is invariant, thus the properties of the theory written in the mass eigenstate basis will be easy to find. We have

$$\tau^\dagger \mathbf{M} \tau = \phi^\dagger \operatorname{diag}(m_i^2) \phi = \phi^\dagger \mathbf{U}^\dagger \mathbf{M} \mathbf{U} \phi \tag{5.9}$$

where $\mathbf{U}$ is given by

$$\mathbf{U} = e^{i\zeta} \begin{pmatrix} \cos\theta & \sin\theta e^{i\varphi} \\ -\sin\theta e^{i\chi} & \cos\theta e^{i(\varphi+\chi)} \end{pmatrix} \tag{5.10}$$

with parameters

$$\chi = -\arg b \,, \qquad \tan 2\theta = -\frac{2|b|}{a-d} \,. \tag{5.11}$$

The phases $e^{i\zeta}$ and $e^{i\varphi}$ are arbitrary. The transformation of the ϕ under $\mathcal{T}$ is simply

$$\phi_i \longmapsto \bar{\phi} = \rho \phi_i \tag{5.12}$$

since the transformation of b cancels against that of $e^{i\chi}$. This result can be further reduced to $\bar{\phi} = \phi$ by an appropriate choice of ζ. On the other hand the $\mathcal{S}$-transformed eigenstates $\tilde{\phi}$ are more complicated functions of the $\tilde{\tau}$, which themselves are mixed relative to the τ under $\mathcal{S}$:

$$\begin{aligned} \tilde{\phi} = \tilde{\mathbf{U}}^\dagger \tilde{\tau} \,, \qquad \tilde{\chi} &= -\arg \left(\frac{a-d}{2} \sin 2\theta_S - \operatorname{Re}\, b \cos 2\theta_S - i \operatorname{Im}\, b \right) , \\ \tan 2\tilde{\theta} &= -\frac{2|\frac{a-d}{2} \sin 2\theta_S - \operatorname{Re}\, b \cos 2\theta_S - i \operatorname{Im}\, b|}{(a-d) \cos 2\theta_S - 2 \operatorname{Re}\, b \sin 2\theta_S} \,. \end{aligned} \tag{5.13}$$

The simplification of these formulae is scarcely practicable given that one requires $\cos\tilde{\theta}$, $\sin\tilde{\theta}$ to be found explicitly in order to write $\tilde{\phi}$ in terms of τ.

Algebraic difficulties are however easily circumvented by a constant change of basis of the original states. Since any unitary matrix is unitarily similar to a diagonal matrix, one can always find a basis $\varsigma = \mathbf{V}^\dagger \tau$ in which any given modular transformation, for example $\mathcal{S}$, is diagonal. The transformation in the new basis is derived as

$$\mathbf{V}^\dagger \tau \longmapsto \mathbf{V}^\dagger \mathbf{S}^{(\tau)} \tau \tag{5.14}$$

(applying the constant linear combination $\mathbf{V}^\dagger$ to $\tau \mapsto \mathbf{S}^{(\tau)} \tau$)

$$\Longrightarrow \varsigma \longmapsto \mathbf{V}^\dagger \mathbf{S}^{(\tau)} \mathbf{V} \varsigma \equiv \mathbf{S}^{(\varsigma)} \varsigma \tag{5.15}$$

(substituting for τ on the RHS). The condition $\mathbf{S}^{(\varsigma)} = \operatorname{diag}(e^{i\beta_1}, e^{i\beta_2})$ is easily solved by

$$\mathbf{V} = \begin{pmatrix} \cos\theta_V & \sin\theta_V \\ -\sin\theta_V & \cos\theta_V \end{pmatrix} \tag{5.16}$$

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with $\theta_V = -\theta_S/2$ and $\beta_1 = -\pi$, $\beta_2 = \pi$.[7] The mass eigenstates ϕ are written

$$\phi = \mathbf{U}'^{\dagger} \varsigma \,, \tag{5.17}$$

where $\mathbf{U}'$ diagonalises the mass matrix $\mathbf{M}'$ in the ς basis. The parameters of $\mathbf{U}'$, defined analogously to (5.10), can be found in terms of the original mass matrix entries a, b, d; the expressions are similar to those for $\tilde{\chi}$ and $\tilde{\theta}$ in (5.13) and equally unenlightening.[8] But since the ς_i have the simple transformation law $\mathcal{S}\colon \varsigma_1 \mapsto -i\varsigma_1,\ \varsigma_2 \mapsto i\varsigma_2$ it is easy to check that the transformed diagonalisation matrix $\tilde{\mathbf{M}}'$ is the same as $\mathbf{M}'$ up to a change of sign of $e^{i\chi'}$. Then under transformation of $\mathbf{M}'$ and ς together the ϕ_i just get an unobservable common factor $-i$, or with an appropriate choice of ζ' can be made invariant.

This result is to be expected since the $\mathcal{S}$ transformation in the ς basis is exactly analogous to $\mathcal{T}$ acting in the τ basis. It is not difficult to show for a representation of arbitrary dimension that one can always find a basis σ in which any given transformation is a diagonal matrix of phases. Then a modulus-dependent matrix analogous to $\mathbf{U}'$ can always be found such that the mass eigenstates are exactly invariant under transformation of both the modulus and the σ_i (see appendix A). Then if the theory is written in the mass basis, all modulus-dependent coupling constants must also be exactly modular invariant smooth functions. This situation was forecast in [2] as a solution to the problem of non-invariant coupling constants. Applied to the case of $\langle T \rangle$ on the unit circle it means that any apparently CP-violating couplings calculated in the original basis of the theory must be killed by the modulus-dependent transformation to the basis of light and heavy states. The only exceptions are if the original basis happens precisely to be the mass basis, such that no diagonalisation is needed, or if the whole modular group acts either diagonally (i.e. trivially) or by a pure permutation (as in the case of KK/winding modes). We argued that the coincidence of the theory basis with the mass basis is highly unlikely, since such a condition cannot be imposed over any extended region of moduli space; also, no known examples of the modular group action on twisted states are purely diagonal or permutation matrices [9].

6. CP as a gauge symmetry and "CP-odd" quantities

Just as for modular invariance, we expect that no physically measurable quantity should allow us to differentiate between CP-conjugate vacua, since CP is an exact symmetry in the underlying higher-dimensional theory, being embeddable in the gauge group [5, 6]. This sounds odd at first: surely in the CP-conjugate vacuum, the CKM phase would have the opposite sign and the vertex (ρ, η) of the unitarity triangle would live in the lower half of the complex plane — with easily measurable consequences? But recall that the exact CP symmetry involves conjugating both the scalar v.e.v. and the particle excitations. Then, imagining a "CP domain wall", what gives the same physics on the other side of the wall

[7] For a more general form of $\mathbf{S}^{(\tau)}$ complex phases may be needed in $\mathbf{V}$.

[8] They turn out to be the same as in (5.13) except for a sign and the substitution of $2\theta_S$ by θ_S.

from us is a world with matter and antimatter exchanged. Combining CP with $SL(2,\mathbb{Z})$ we obtain a fundamental domain half the size of $\mathcal{F}$, with a unique sign for Im T: the "kink" at the real axis is now at the *edge* of the domain.

The gauge aspect of the symmetry was exploited in [5] where "CP strings" were proposed, in the phase where the scalar v.e.v. still left CP intact (see also [12]). In the broken phase, a traveller could conceivably go round a closed loop in space and pass through exactly one "CP domain wall", since the two vacua are gauge-equivalent and can be identified (the domain wall ending on a string). But the traveller "around the string" would, on returning, appear to be made of antimatter; or, deeming himself still matter, he would measure the opposite sign for CP asymmetries, and think that the scalar v.e.v. had flipped (on passing through the wall). A more sophisticated traveller might even, on recognising his (her?) surroundings again (and deducing that the v.e.v. was the same as at the outset) but getting the "wrong" sign for CP asymmetry experiments on board ship, decide that predictions should now be made with hermitean conjugate fields (henceforth called antifields) replacing fields, thus restoring predictive power to his (her) favourite theory.[9]

In order to predict a CP-violating quantity in such a theory, we need to establish a convention for matter vs. antimatter. Otherwise we face a sign ambiguity, since one cannot *a priori* decide whether the fields or the antifields of the theory are to describe the experimental apparatus. This corresponds to a further $\pm$ sign in front of our modular invariant prescription for J_{CP}, which (temporarily) restores the symmetry between the positive and negative values in figure 1. In the light of the traveller's predicament, it may not be possible to establish a globally consistent convention, but locally in regions with a net density of (say) baryon number, it is unambiguous and historically inevitable to pick the prevailing species as matter.[10]

Little attention has been paid to the possible influence of "CP strings" on baryogenesis, perhaps not surprisingly as they erase the distinction between matter and antimatter in their neighbourhood. The usual assumption, valid if symmetry is broken at a high enough scale, is that all strings and domain walls have "cleared out" of the observable Universe, in which case baryogenesis proceeds uniformly over the observable region. This will in the end definitely establish one sign convention, since the baryon asymmetry provides a good definition of matter. On the other side of a putative CP domain wall, both the baryon asymmetry and the CP-violating v.e.v. would be conjugated, and *experimental results would be the same.*

Since such walls are cosmologically excluded, these speculations would seem to be irrelevant. But the point should be addressed in order to predict CP violation at experiments: the status of matter and antimatter in one's theory cannot be set by *fiat*, but must be deduced from a theory of baryogenesis. Otherwise one does not know (even in the correct theory) whether to calculate J_{CP} from the quark mass matrices or from their hermitean conjugates.

[9] The astute deduction that he (she) was now made of antimatter would no doubt forestall the usual catastrophic end to such journey.

[10] The alternative is to take an established experimental result and compare with the theory to fix the convention, so that only relative signs between different measurements can be predicted.

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7. Conclusions

In this paper we investigated the consequences of an exact discrete non-abelian symmetry acting on moduli and matter fields. We were motivated by the claim that the symmetry could be realised in a way that allowed light and heavy states to be mixed, which can lead to interesting consequences for phenomenology. For example, a non-vanishing CKM phase for $\langle T \rangle$ on the unit circle would be desirable since such values appear to arise naturally from gaugino condensation models of moduli stabilization and result in an exactly vanishing modulus F-term, which might be part of a solution of the supersymmetric CP and flavour problems.

We argued that the light-heavy mixing, which leads to noninvariant results for observable moduli-dependent quantities, was possible in principle, but that invariance must be restored by patching together more than one such function, the choice being made by correctly identifying the light fields and using the symmetries of the theory. The result may be a nondifferentiable function on moduli space.

In the second part of the paper we looked more carefully at what mass matrices could be consistent with the assumption of light-heavy mixing. We found that the *ansatz* of [1], in which the original basis of twisted states is also the mass basis, cannot produce a realistic spectrum at points in moduli space invariant under $T \mapsto 1/T$ or $T \mapsto 1/T^*$. Even at other values of T, this *ansatz* is not preserved under modular transformation, so cannot hold except at isolated points and appears unnatural.

A more general *ansatz* with no vanishing mass matrix elements is consistent with a spectrum of light and heavy states after diagonalisation, but we find that these states are separately modular *invariant*, due to the transformation of the diagonalisation matrix. This simple result is significant since it implies that (measurable combinations of) the coupling constants of the light fields are exactly modular invariant functions.

Lastly, we discussed the implications of taking the exact CP symmetry of the underlying theory seriously, set against results which apparently imply different predictions in CP-conjugate vacua. A result such as [1, figure 2] for a physical measure of CP violation tends to produce the impression that, since the two vacua give opposite signs for CP-violating observables and we can't predict which vacuum we live in, the best we can do is predict the magnitude. But, after we realise that the value of such an observable cannot depend on the choice between (CP and modular) equivalent vacua and arrive at the amended result of figure 1, we find that the sign can be predicted, but only in conjunction with the prediction of a non-zero baryon fraction.[11] Once this is done the conjugate vacua give the same physics, as they should. Unfortunately the Jarlskog invariant is just what cannot tell us anything about baryogenesis, since generating the observed baryon asymmetry requires CP violation in physics beyond the Standard Model [13].

[11] Unfortunately for phenomenologists, it is conceivable that the source of CP violation at baryogenesis is unobservably small at the present epoch, and independent of the source of currently observed effects. In this case, which may be realised in Affleck-Dine-type "spontaneous baryogenesis" models, only relative signs between different experimental results can be predicted.

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A. Derivation of the modular invariance of mass eigenstates

The invariance of the mass eigenstate basis is not manifest for the complete modular group simultaneously, hence we treat each group element Γ, acting as a unitary matrix on properly-normalised matter states, separately. By a constant Γ-dependent change of basis one may always find a basis ν where Γ acts as a diagonal matrix of phases:

$$\Gamma\colon \nu_{(L,R)a} \longmapsto e^{i\xi_{(L,R)a}}\nu_{(L,R)a}\,, \tag{A.1}$$

where for greater generality we allow ν to range over left- and right-handed fermions. Then the mass matrix $\mathbf{M}^{(\nu)}$ in this basis is diagonalised as

$$\bar{\nu}_L \mathbf{M}^{(\nu)} \nu_R = \bar{\psi}_L \,\mathrm{diag}(m_i)\psi_R \tag{A.2}$$

with m_i real, where

$$\nu_{(L,R)} = \mathbf{U}_{(L,R)}\psi_{(L,R)}\,, \qquad \mathbf{U}_L{}^\dagger \mathbf{M}^{(\nu)}\mathbf{U}_R = \mathrm{diag}(m_i)\,, \tag{A.3}$$

where $\mathbf{U}_{(L,R)}$ are modulus-dependent unitary matrices. The mass matrix changes under the modular transformation Γ as

$$M^{(\nu)}_{ab} \longmapsto \tilde{M}^{(\nu)}_{ab} = e^{i(\xi_{La}-\xi_{Rb})}M^{(\nu)}_{ab} \tag{A.4}$$

thus the diagonalisation matrices should transform as

$$U_{Lai} \longmapsto \tilde{U}_{Lai} = e^{i\xi_{La}}U_{Lai}\,, \qquad U_{Rai} \longmapsto \tilde{U}_{Rai} = e^{i\xi_{Ra}}U_{Rai} \tag{A.5}$$

and the transformed mass eigenstates are

$$\tilde{\psi}_{(L,R)i} = \tilde{U}^\dagger_{(L,R)ia} e^{i\xi_{(L,R)a}}\nu_{(L,R)a} = \psi_{(L,R)_i} \tag{A.6}$$

formally demonstrating the invariance. This result is significantly different from the case of spontaneously broken continuous symmetry: in that case one can usually redefine the scalar v.e.v. to obtain a mass matrix diagonal in the symmetry space (e.g. imposing $\langle H\rangle = (0, |v|/\sqrt{2})$ in the Standard Model using SU(2) symmetry) and the mass eigenstates can be thought of as charged under the non-abelian group. When considering string models with heavy matter ($\gg m_t$) one may "block-diagonalise" the quark mass matrix by the procedure outlined above, to separate the three light states from the rest, but keep an off-diagonal light quark mass matrix: then, in principle, the light states (in the weak basis) may mix into each other under modular transformation, but V_{CKM} and J_{CP} are invariant.

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