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 noninvariant. We show that physical invariance may arise by patching smooth functions that are separately noninvariant. CP violation for $\langle \mathcal{T} \rangle$ on the unit circle, which requires light and heavy states to mix under transformation, is allowed in principle, although the Jarlskog parameter $J_{CP}(T)$ 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.

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 $T \mapsto T^*$.\textsuperscript{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, SL(2, Z) modular symmetry) \cite{7} to all orders, generated by

$$
T: T \mapsto T + i, \quad S: T \mapsto 1/T,
$$

(1)

where the second generator $S$, which exchanges large and small radii, is loosely referred to as $T$-duality. The action of the symmetry on orbifold twisted sectors \cite{8, 9} 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 $T: T \mapsto T + i$ is diagonalised.

Then we showed in \cite{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 $Z_6$ orbifold model \cite{1} that the Jarlskog parameter $J_{CP}(T)$ does not vanish on the unit circle, and explicit numerical results were presented. Here, the result for $J_{CP}(T)$ changes sign on taking $T \mapsto T^*$, as naively 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 SL(2, 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 \cite{4, 5}, 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.

\textsuperscript{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 \cite{3, 4, 5, 6}. 

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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, noninvariant 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 nonzero, the rotation to the mass eigenstate basis and the non-Abelian 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 original basis are “killed” by the \( \text{modulus-dependent} \) 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.

2 Non-unitary quark transformations

The technical point in [1] that allowed the Jarlskog parameter \( J_{CP}(T) \) as usually defined (as a function of quark mass matrices) to be noninvariant under \( T \mapsto 1/T \), is the transformation of the three generations of light quark
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. [10]). 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 be nonunitary 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,

$$S: q_A \mapsto \tilde{q}_A \equiv S_{AB} q_B, \ A, B = 1, \ldots, N_g$$ (2)

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 $S$, but to simplify the discussion (and also since transformations of the right-handed quarks cancel in the expression for $J_{CP}$) we consider a single matrix. Then for the light quarks $q_i$

$$q_i \mapsto S_{ij} q_j + S_{ia} q_a, \ i = 1, 2, 3, \ a = 1, \ldots, N_g - 3$$ (3)

and $S_{ij}$ will in general be nonunitary (given that some $S_{ia}$ are nonvanishing). Since the mass terms are invariant we have

$$S: M^{u,d}_{AB}(T) \mapsto \tilde{M}^{u,d}_{AB}(T) \equiv M^{u,d}_{AB}(\tilde{T}) = (S M^{u,d}(T) S^\dagger)_{AB}$$ (4)

and for the entries with the light state $q_i$ labels

$$M^{u,d}_{ij} \mapsto \tilde{M}^{u,d}_{ij} = S_{iA} M^{u,d}_{AB}(T) S^\dagger_{Bi} = S_{ik} M^{u,d}_{km}(T) S^\dagger_{mj}$$

+ (terms proportional to $M^{u,d}_{ab}(T)$) (5)

which again is generically a nonunitary transformation and involves the mass matrix of the heavy states $q_a$.

Now the $J_{CP}$ parameter defined by

$$\det[M^{u}_{ij} M^{u\dagger}_{jk}, M^{d}_{mn}, M^{d\dagger}_{np}] = J_{CP}(m_t^2 - m_c^2)(m_c^2 - m_u^2)(m_t^2 - m_u^2)$$

$$(m_b^2 - m_s^2)(m_s^2 - m_d^2)(m_b^2 - m_d^2)$$ (6)

Light meaning compared to the GUT or Planck scales.
or by

\[ J_{CP} = \text{Im} \, V_{11} V_{12}^* V_{22} V_{21}^* \]  

(7)

is invariant precisely under unitary changes of basis for the three quark generations, which appear in the expression (6) as unitary transformations of the quark mass matrices. Thus with a nonunitary modular transformation of quarks \( J_{CP}(T) \), as defined on the mass matrix of the original states \( M_{ij}^{u,d} \), may change in value. The corollary of this is that this value \( J_{CP}(\tilde{T}) \) 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 \( J_{CP} \) 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 \( J'_{CP}(T) \); nevertheless, \( J'_{CP}(\tilde{T}) \) must have the same numerical value as \( J_{CP}(T) \), 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 to be at all meaningful.\(^3\)

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 \( M_{AB}^{u,d}(T_0) \) 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

\[ \bar{q}_A M_{AB}^{u,d}(\tilde{T}_0) q_B = \bar{q}_A (S M_{AB}^{u,d}(T_0) S^\dagger)_{AB} q_B \]  

(8)

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

\[ J'_{CP}(\tilde{T}) = J_{CP}(T). \]

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

\[ J_{CP}(\tilde{T}_0) \propto \det[\bar{M}_{ij} M_{jk}^{u^\dagger}, \bar{M}_{mn} M_{np}^{d^\dagger}] \]  

(9)

\(^3\)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. Thus the symmetry is restored, in this sense.
and the off-diagonal (light-heavy) transformations $S_{iA}$ of (5) do not cancel in the determinant. If one were to use the old function $J_{CP}$ 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 $q_i = S_i A \psi_A$, where the $\psi_A$ are both light and heavy fields, so the calculation is not physically meaningful.

Let us apply this to the model in which $J_{CP}(T)$ is claimed to be noninvariant under the duality $T \mapsto 1/T$. On the unit circle the duality becomes $T \mapsto T^*$ and the noninvariance allows a nonzero value of $J_{CP}$ (see Fig. 2 of [1]). 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 $J_{CP}(T)$ over the complex $T$ plane. Then the result may be correct over some of the unit circle (say, the part with $\text{Im} \, T > 0$) 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 $J_{CP}(T)$ 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 $J_{CP}(T)$ to be nonzero on the unit circle, so the derived function $J_{CP}(T)$ does not remain physical after modular transformation.

Instead we need a new function $J'_{CP}(T)$ valid over the rest of the domain as described above. Since the duality is $Z_2$, we need $J'_{CP}(T) \equiv J_{CP}(\tilde{T})$ as well as $J'_{CP}(\tilde{T}) \equiv J_{CP}(T)$, and realising that the original function $J_{CP}(T)$ is odd under complex conjugation we find that $J'_{CP}(T) = -J_{CP}(T)$ must hold on the unit circle. Thus the physical Jarlskog parameter is given by $J_{CP}(T)$ or $-J_{CP}(T)$, with the sign depending in which domain we find ourselves. In particular, there will be a “join” along which the two prescriptions collide, and the physical result will in general not 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 $Z_6$ orbifold model, one should find the explicit mechanism that makes the heavy fields decouple: the expectation is, contrary to the unstated assumption of [1], 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 $J_{CP}^{(phys)} = \pm |J_{CP}(T)|$, the overall sign depending on which way the prescription turns out (see Fig. 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 by a diagonal matrix of phases, thus the argument of [2] applies to this symmetry and CP symmetry is unbroken at $\text{Im} T = \pm 1/2$.

We briefly return to the result of [2] and ask, what went wrong with the reasoning for the $T \mapsto 1/T$ transformation? Unitary quark transformations were not strictly necessary for the result to hold, but what was needed was the condition 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 we see in the laboratory. Light particles have to remain light under CP.\(^4\) But if and when we can perform experiments with the heavy twisted states and their antiparticles, an unbroken CP symmetry may reappear for $\langle T \rangle$ lying on the unit circle.

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 gedankenexperiment. 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

\(^4\) Within the latitude implied by the CKM mixing, which allows us to mix bottom with down, indeed requires it for CP to be violated.
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

$$m_{\text{detected}} = \min(R, 1/R)$$

(10)

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 nondifferentiable at $R = 1$, just as the prescription for $J_{\text{CP}}^{(\text{phys})}(T)$ is at the real axis. Conversely, extending the smooth function $J_{\text{CP}}(T)$ calculated in [1] over a region containing both $T_0$ and $\tilde{T}_0$ would correspond to choosing either $m = R$ or $m = 1/R$, without the minimum prescription.

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 result 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 $-1/2 < \text{Im} T \leq 1/2$, $|T| \geq 1$. The procedure is analogous to gauge-fixing. Any value in the half-plane $\text{Re} T > 0$ 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 $\text{Im} T \geq 0$. Then if we want to find the value of $J_{\text{CP}}$ 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 Fig. 2 of [1], 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 $\phi = 0$ (Fig. 1). But this replacement creates trouble for the rest of $\mathcal{F}$ away from $|T| = 1$: since the original, non-invariant function $J_{\text{CP}}(T)$ 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
Figure 1: Amended version of Fig. 2 of [1]: the physical $J_{CP}$ 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.

the replacement along $P$ is not enough, since a discontinuity is definitely unphysical.

Thus the calculated smooth function $J_{CP}(T)$ must be amended over a whole region of $F$. 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 SL(2,$\mathbb{Z}$) needs replacement, and our previous answer $J_{CP}^{(phys)} = \pm|J_{CP}(T)|$ is meaningfully extended to the whole of $F$. Given that CP is also an exact symmetry acting on $T$, it makes sense to define a fundamental domain $F'$ for the group SL(2,$\mathbb{Z}$) $\otimes$ CP, which can be taken to be the half of $F$ with Im $T \geq 0$, such that any possible value of $T$ is physically equivalent to precisely one point in $F'$. If we only consider $T$ inside $F'$ then there is no need to patch noninvariant functions.
What happens near $T = 1$? If, as needed for non-unitary 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 $T = 1$ anyway. However, a similar argument applies for values of $T$ near the unit circle: the combination of duality 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 mass eigenstates. Thus a degenerate spectrum also occurs on the “CP self-dual” line $|T| = 1$. If, however, the mass matrix is non-diagonal 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 $J_{CP}(T)$ is a unique modular invariant smooth function odd under $T \mapsto T^*$, which must vanish on the boundary of $\mathcal{F}$, and — as far as modular invariance goes — no “prescriptions” are needed. 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. For a nonabelian duality group with two generators, we can formally write a general modular
invariant mass matrix as
\[ M = \begin{pmatrix} a & b \\ b^* & d \end{pmatrix} \] (11)
where \(a, b, d\) are functions of the modulus, with transformations under the duality group to be determined. The representation of \(\text{SL}(2, \mathbb{Z})\) on the twist fields \(\sigma_i, i = 1, 2, 3\) of the two-dimensional orbifold \(\mathbb{C}/\mathbb{Z}_3\) is
\[ S = -i \sqrt{3} \begin{pmatrix} 1 & 1 & 1 \\ 1 & \alpha & \alpha^2 \\ 1 & \alpha^2 & \alpha \end{pmatrix}, \quad T = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \] (12)
where \(\alpha = e^{2\pi i/3}\).5

This representation is reducible into a singlet \(\tau_0 = \sqrt{2}^{-1}(\sigma_2 - \sigma_3)\) and a doublet
\[ \tau_1 \equiv \sigma_1 \quad \tau_2 \equiv \frac{1}{\sqrt{2}}(\sigma_2 + \sigma_3) \] (13)
for which
\[ S^{(\tau)} = -i \sqrt{3} \begin{pmatrix} 1 & \sqrt{2} \\ \sqrt{2} & -1 \end{pmatrix}, \quad T^{(\tau)} = \begin{pmatrix} \alpha & 0 \\ 0 & 1 \end{pmatrix}. \] (14)
We can generalise the representation slightly without complicating the system by taking
\[ S^{(\tau)} = -i \begin{pmatrix} \cos \theta_S & \sin \theta_S \\ \sin \theta_S & -\cos \theta_S \end{pmatrix}, \quad T^{(\tau)} = \begin{pmatrix} \alpha & 0 \\ 0 & 1 \end{pmatrix}. \] (15)
The modular invariance conditions for the mass matrix analogous to (4) are
\[ S: M \mapsto \tilde{M} = \begin{pmatrix} \tilde{a} & \tilde{b} \\ \tilde{b}^* & \tilde{d} \end{pmatrix}, \quad T: M \mapsto \bar{M} = \begin{pmatrix} a & \bar{b} \\ \bar{b}^* & d \end{pmatrix} \]
where
\[ \tilde{a}(T) = ac_S^2 + ds_S^2 + 2\text{Re} bcs_s s_s, \]
\[ \tilde{b}(T) = (a - d)c_s s_s - \text{Re} b(c_S^2 - s_S^2) - i\text{Im} b, \]
\[ \tilde{d}(T) = as_S^2 + dc_S^2 + 2\text{Re} b c_s s_s, \]
\[ \bar{b}(T) = \rho b. \] (16)

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5There is a sign error in the \(S\) generator in the first reference of [9].
and \(c_S = \cos \theta_S, \quad s_S = \sin \theta_S\).

The nonunitary transformation required for CP violation on the unit circle corresponds to the presence of nonzero elements which are off-diagonal (i.e. not block diagonal) in the (light, heavy) basis, for one or more generators. In our case 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 \(\tau\) 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 which models the behaviour of quark mass matrices at the point \(T = 1\). At \(T = 1\) we have \(S(T) = T\), thus \(\tilde{M} = M\). From this it can be deduced that
\[
a - d = 2\text{Re} \, b \cot \theta_S, \quad \text{Im} \, b = 0 \tag{17}
\]
and the mass eigenvalues become \(\frac{1}{2}(a + d \pm \sqrt{(a - d)^2 + 4|b|^2})\). Because of the mixing in going from the \(\tau\) 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 \(\tau_i\) are mass eigenstates, thus \(b = 0\), we find an unacceptable spectrum at \(T = 1\): the self-duality relation (17) reduces to \(a = d\) and all states are equally massive.

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 \(CP(T) = T^* = S(T)\) on the mass matrix entries. We require \(\tilde{M} = M^*\) which reduces to the single condition
\[
a - d = 2\text{Re} \, b \cot \theta_S \tag{18}
\]
with no restriction on \(\text{Im} \, b\). Thus the mass eigenvalues in the case where the \(\tau\) are not mass eigenstates are given by three parameters \(a, d\) and \(\text{Im} \, b\) and there is more freedom to obtain a large hierarchy. But in the case that \(\tau_i\) are mass eigenstates (so \(b = 0\)) the spectrum is still degenerate.

Thus, the possibilities that \(\langle T \rangle\) lies inside \(\mathcal{F}\) with the \(\tau_i\) being mass eigenstates, or that \(\langle T \rangle\) lies on the unit circle with the mass basis distinct from

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6One may also introduce diagonal matrices of constant phases in the CP transformation of \(M\), corresponding to the \(\tau_i\) receiving complex phases under CP; this possibility does not affect our conclusions.
the \( \tau \) basis, remain viable, but we cannot live in a world where the \( \tau_i \) 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 \( \bar{T} \) since \( \bar{b} = (a - d)s_{SCS} \), 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 \( S \) (which is inconsistent with any known behaviour of twisted matter), or we happen to live at the very 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 \( \tau \) 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

\[
\tau^\dagger M \tau = \phi^\dagger \text{diag}(m_i^2) \phi = \phi^\dagger U^\dagger M U \phi \quad (19)
\]

where \( U \) is given by

\[
U = e^{i\zeta} \begin{pmatrix}
\cos \theta & \sin \theta e^{i\phi} \\
-\sin \theta e^{i\chi} & \cos \theta e^{i(\phi + \chi)}
\end{pmatrix} \quad (20)
\]

with parameters

\[
\chi = -\arg b, \quad \tan 2\theta = -\frac{2|b|}{a - d}. \quad (21)
\]

The phases \( e^{i\zeta} \) and \( e^{i\phi} \) are arbitrary. The transformation of the \( \phi \) under \( T \) is simply

\[
\phi_i \mapsto \bar{\phi} = \rho \phi_i \quad (22)
\]

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 \( \zeta \). On the other hand the \( S \)-transformed eigenstates \( \bar{\phi} \) are more complicated functions of the \( \bar{\tau} \), which themselves are mixed under \( S \) relative to \( \tau \):

\[
\bar{\phi} = \bar{U}^\dagger \bar{\tau}, \quad \bar{\chi} = -\arg\left(\frac{a - d}{2} \sin 2\theta_S - \Re b \cos 2\theta_S - i \Im b\right),
\]

\[
\tan 2\bar{\theta} = -\frac{2|\frac{a - d}{2} \sin 2\theta_S - \Re b \cos 2\theta_S - i \Im b|}{(a - d) \cos 2\theta_S - 2 \Re b \sin 2\theta_S} \quad (23)
\]
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 \( \tau \).

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 of phases, one can always find a basis \( \varsigma = V^\dagger \tau \) in which any given modular transformation, for example \( S \), is diagonal. The transformation in the new basis is derived as

\[
V^\dagger \tau \mapsto V^\dagger S^{(\tau)} \tau
\]

(24)

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

\[
\Rightarrow \varsigma \mapsto V^\dagger S^{(\tau)} V\varsigma \equiv S^{(\varsigma)} \varsigma
\]

(25)

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

\[
V = \begin{pmatrix}
\cos \theta_V & \sin \theta_V \\
-\sin \theta_V & \cos \theta_V
\end{pmatrix}
\]

(26)

with \( \theta_V = -\theta_S/2 \) and \( \beta_1 = -\pi, \beta_2 = \pi \). The mass eigenstates \( \phi \) are written

\[
\phi = U'^\dagger \varsigma
\]

(27)

where \( U' \) diagonalises the mass matrix \( M' \) in the \( \varsigma \) basis. The parameters of \( U' \), defined analogously to (20), 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 (23) and equally unenlightening.\(^8\) But since the \( \varsigma_i \) have the simple transformation law \( S: \varsigma_1 \mapsto -i\varsigma_1, \varsigma_2 \mapsto i\varsigma_2 \) it is easy to check that the transformed diagonalisation matrix \( M' \) is the same as \( M' \) up to a change of sign of \( e^{i\chi'} \). Then under transformation of \( M' \) and \( \varsigma \) together the \( \phi_i \) just get an unobservable common factor \( -i \), or with an appropriate choice of \( \varsigma' \) can be made invariant.

This result is to be expected since the \( S \) transformation in the \( \varsigma \) basis is exactly analogous to \( T \) acting in the \( \tau \) basis. It is not difficult to show for a representation of arbitrary dimension that one can always find

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

\(^8\)They turn out to be the same as in (23) except for a sign and the substitution of \( 2\theta_S \) by \( \theta_S \).
a basis $\sigma$ in which any given transformation is a diagonal matrix of phases. Then a modulus-dependent matrix analogous to $U'$ can always be found such that the mass eigenstates are exactly invariant under transformation of both the modulus and the $\sigma_i$. Then if the theory is written in the mass basis, all modulus-dependent coupling constants must also be exactly modular invariant, and there is no need to patch noninvariant functions to restore invariance. 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 exception is if the original basis happens precisely to be the mass basis, such that no diagonalisation is needed. But we argued that this would be a coincidence, since such a condition cannot be imposed over any extended region of moduli space.

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 [4, 5]. This sounds odd at first: surely in the CP-conjugate vacuum, the CKM phase would have the opposite sign and the vertex $(\rho, \eta)$ 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 from us is a world with matter and antimatter exchanged. Combining CP with SL$(2, Z)$ we obtain a fundamental domain half the size of $F$, 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 [4] where “CP strings” were proposed, in the phase where the scalar v.e.v. still left CP intact (see also [11]). 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 Hermitian conjugate fields (henceforth called antifields) replacing fields, thus restoring predictive power to his (her) favourite theory.\footnote{The astute deduction that he (she) was now made of antimatter would no doubt forestall the usual catastrophic end to such journey.}

In order to predict a CP-violating quantity in such a theory, we need to establish a convention for matter \textit{vs.} antimatter. Otherwise we face a sign ambiguity, since we cannot \textit{a priori} decide whether the fields or the antifields of the theory are to describe our 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 Fig. 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.\footnote{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.}

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 a unique convention, since a symmetry-breaking vacuum will develop a baryon asymmetry, providing 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 \textit{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 Hermitian conjugates. With a baryogenesis mechanism, the absolute sign of CP asymmetries can in principle be predicted, even in a theory of spontaneous CP violation.

7 Conclusions

In this paper we investigated the consequences of an exact discrete non-Abelian symmetry acting on moduli fields and matter. 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 nonvanishing 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 may 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 choosing among 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 non-differentiable 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 $T \mapsto 1/T^*$. This ansatz is not preserved under modular transformation, so cannot hold except at isolated values of $T$ 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 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 Fig. 2 of [1] 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 prediction Fig. 1, we find that the sign can be predicted, but only in conjunction with the prediction of a nonzero baryon fraction.\footnote{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 the 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.} 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 [12].

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