Hidden Topological Angles in Path Integrals

Alireza Behtash, Tin Sulejmanpasic, Thomas Schäfer, and Mithat Ünsal

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Hidden topological angles and Lefschetz thimbles

Alireza Behtash,* Tin Sulejmanpasic,† Thomas Schäfer,‡ and Mithat Ünsal§
Department of Physics, North Carolina State University, Raleigh, NC 27695, USA

We demonstrate the existence of hidden topological angles (HTAs) in a large class of quantum field theories and quantum mechanical systems. HTAs are distinct from theta-parameters in the lagrangian. They arise as *invariant angle* associated with saddle points of the complexified path integral and their descent manifolds (Lefschetz thimbles). Physical effects of HTAs become most transparent upon analytic continuation in n_f to non-integer number of flavors, reducing in the integer n_f limit to a $\mathbb{Z}_2$ valued phase difference between dominant saddles. In $\mathcal{N}=1$ super Yang-Mills theory we demonstrate the microscopic mechanism for the vanishing of the gluon condensate. The same effect leads to an anomalously small condensate in a QCD-like $SU(N)$ gauge theory with fermions in the two-index representation. The basic phenomenon is that, contrary to folklore, the gluon condensate can receive both positive and *negative* contributions in a semi-classical expansion. In quantum mechanics, a HTA leads to a difference in semi-classical expansion of integer and half-integer spin particles.

Introduction. Providing a non-perturbative continuum definition of the path integral in quantum field theory is a challenging but important problem [1]. There is growing evidence that, if an ordinary integral or a path integral admits a Lefschetz-thimble decomposition [2, 3] or resurgent transseries expansion [4–12] then either of these methods gives this long-sought non-perturbative definition. If this is indeed the case, then we expect that these new methods will provide new and deep insight into quantum field theory and quantum mechanics formulated in terms of path integrals. In this article we introduce a new phenomenon of this kind, the appearance of hidden topological angles (HTAs).

The main prescription associated with the Lefschetz-thimble decomposition or the resurgent expansion is the following: Even if an ordinary integral or a path integral is formulated over real fields, the natural space that the critical points (saddles) ρ_σ live in is the complexification of the original space of fields. However, the dimension of the critical point cycles $\mathcal{J}_\sigma$ is that of the original space, or half that of the complexified field space. For example, for an ordinary integral over N-dimensional real space, this procedure is $\mathbb{R}^N \longrightarrow \mathbb{C}^N \longrightarrow \Sigma^N$, where $\Sigma^N = \sum_\sigma n_\sigma \mathcal{J}_\sigma$ and $\dim_{\mathbb{R}}(\mathcal{J}_\sigma) = N$. For $N=1$, this is the well-known steepest descent (stationary phase) approximation.

To each critical point ρ_σ of the complexified action one attributes an action, with real and imaginary parts, and with "weight" e^{-S_σ}. The imaginary part of the action, $\mathrm{Im}S_\sigma$ is an *invariant angle* associated with the critical point ρ_σ and its descent manifold $\mathcal{J}_\sigma$. If there are critical points with the identical real part of the action $\mathrm{Re}S_\sigma$, but different imaginary parts $\mathrm{Im}S_\sigma$, then there may be subtle effects. Indeed, Witten recently studied in [3] the analytic continuation of Chern-Simons theory to non-integer values of the coupling k, finding subtle cancellations among dominant saddle field configurations in the integer k limit, so that the *sub-dominant* saddle gives the main physical contribution. In this work, we show that the effect observed by Witten is not an exotic phenomenon, but that it is possibly quite ubiquitous, and that it is responsible for a variety of interesting physical effects in quantum field theories and quantum mechanics, in which the analytic continuation is now to non-integer "coupling" n_f, which is the number of fermionic flavors for integer values. We also show that the effect is more non-trivial than a simple cancellation between dominant saddles. Indeed, the effect depends on the observable, and the dominant saddles may cancels in certain observables, but contribute to others.

In a field theory with a topological Θ-angle in the Lagrangian, subtle effects may arise at certain values of the Θ-angle [13–16]. For example, at $\Theta=\pi$ in $SU(2)$ gauge theory there is a cancellation of leading order saddle contribution to the mass gap [14]. In this work we study a more exotic phenomenon, which is due to a hidden topological angle not explicitly present in the lagrangian. We define a HTA as the phase associated with a saddle point in the complexified field space. HTA may depend on the number of fermionic flavors n_f or spin of a particle S, and may be interpreted as topology of a saddle in the complexified field space. Below, we will provide examples of this phenomenon in $\mathcal{N}=1$ super Yang-Mills theory (SYM), certain QCD-like theories, and the quantum mechanics of a particle with spin. We also note that a HTA is different from the discrete theta angles discussed recently [17], which comes about as one changes the global gauge group. In contrast, HTAs are present for any gauge group. In the examples discussed below we find that for integer values of the number of fermions n_f there is a $\mathbb{Z}_2$ hidden topological structure.

A prototype in ordinary integration. An elementary example that provides some intuition for field theory is the following. Consider the analytic continuation of the Bessel function to non-integer order, and describe the contour that appears in the integral representation in terms of Lefschetz thimbles. In one complex dimension the Lefschetz thimble is defined as a stationary phase manifold: $\mathrm{Im}[S(w)-S(w_n)]=0$ where w_n is a critical point on the contour. The integral is $I(k,\lambda)=\int_{C_w} dw e^{2\lambda\sinh(w)+kw}$ for complex k, λ. In a certain regime of the analytic continuation, discussed in [3], the integral can be expressed in terms of three cycles, $\mathcal{J}_i, i=1,2,3$ associated with saddles ρ_i, so that $C_w=\mathcal{J}_1+\mathcal{J}_2+\mathcal{J}_3$, see Fig. 1. The sum of the three thimble contribution gives

$$(1+e^{2\pi i(k+\frac{1}{2})})e^{-S_1}+e^{-S_2} \quad (1)$$

where $|e^{-S_1}| = |e^{-S_3}| \gg e^{-S_2}$, i.e, ρ_1 and ρ_3 are dominant over ρ_2. However, they have a relative phase, and the contribution of these two dominant saddles cancel each other exactly for integer k. The mechanism described above is an intuitive example of a mechanism operative in Chern-Simons theory by using analytic continuation, providing confidence for the utility of the idea of analytic continuation of path integrals. Other examples are discussed in [18–20]. We will perform a similar analytic continuation in n_f, the number of fermion flavors in the theory.

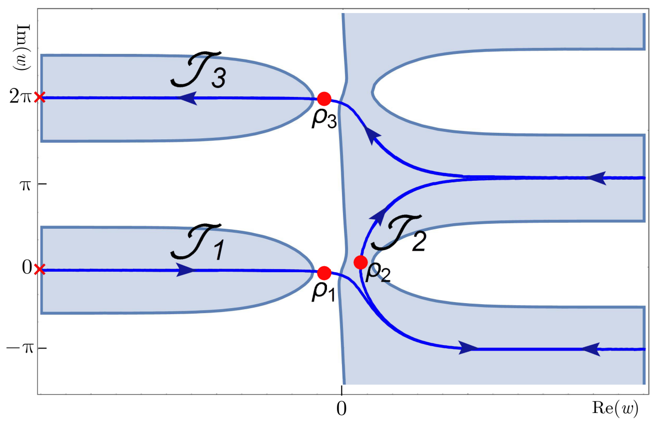

FIG. 1: The blue areas show "good regions" in which the integrand falls sufficiently rapidly at infinity to guarantee convergence. The red dots give the locations of the saddle points, and the blue contours are the Lefschetz thimbles. If the boundary of integration is $(-\infty, -\infty + 2\pi i)$, then the Lefschetz decomposition is $\mathcal{J}_1 + \mathcal{J}_2 + \mathcal{J}_3$. Here, ρ_1 and ρ_3 are equally dominant saddles over ρ_2, but there is an over-all phase difference between the dominant saddles leading to a subtle cancellation for integer k.

Picard-Lefschetz equation and invariant angles. The definition of the Lefschetz thimble based on stationary phase, $\text{Im}[S(w) - S(w_n)] = 0$, is only satisfactory for a one-dimensional integral (it provides one real condition on a one-complex dimensional space). In n complex dimensions, where $n = \infty$ corresponds to field theory or quantum mechanics, this condition defines a co-dimension one (real dimension $2n-1$ space), which is not the desired n real dimensional space. Instead, one needs n real conditions to define the thimble. Guided by these observations, Witten used complex gradient flow equations, the Picard-Lefschetz equations, to describe the Lefschetz-thimbles. In a theory with a field φ and action $S(\varphi)$, this amounts to

$$\frac{\partial \varphi}{\partial \tau} = -\frac{\delta \bar{S}}{\delta \bar{\varphi}}, \qquad \frac{\partial \bar{\varphi}}{\partial \tau} = -\frac{\delta S}{\delta \varphi}, \tag{2}$$

where τ is the flow time. Using (2) and the chain rule,

$$\frac{\partial \text{Im}[S]}{\partial \tau} = \frac{1}{2i}\left(\frac{\delta S}{\delta \varphi}\frac{\partial \varphi}{\partial \tau} - \frac{\delta \bar{S}}{\delta \bar{\varphi}}\frac{\partial \bar{\varphi}}{\partial \tau}\right) = 0, \tag{3}$$

meaning that $\text{Im}[S(\phi)] = \text{Im}[S(\phi_n)]$ is *invariant* under the flow. In a quantum field theory (QFT), or in quantum mechanics (QM), in which semi-classical saddle proliferates (an example is the instanton gas), $\text{Im}[S(\phi_n)]$ will appear as a genuinely new phase in the effective field theory. This is the HTA phenomenon.

The integration in the complexified field space is infinite dimensional. In the background of non-perturbative saddles, this space usually factorizes into finite dimensional zero and quasi-zero modes directions and infinite dimensional gaussian modes. The HTA can be calculated by an exact integration over the complexified finite dimensional quasi-zero mode directions in the field space, dictated by the finite dimensional version of the Picard-Lefschetz theory.

Hidden topological angle in 4d $\mathcal{N} = 1$ SYM: Consider $\mathcal{N} = 1$ SYM on $\mathbb{R}^3 \times S^1_L$, where S^1_L is a circle with period L. We use supersymmetry preserving boundary conditions and take the small L limit in order to be able to use semi-classical methods. According to the trace anomaly relation the gluon condensate $\langle \frac{1}{N}\text{tr}F^2_{\mu\nu}\rangle$ determines the vacuum energy: $\mathcal{E}_{\text{vac}} = \langle\Omega|T_{00}|\Omega\rangle = \frac{1}{4}\langle\Omega|T_{\mu\mu}|\Omega\rangle = \frac{1}{4}\frac{\beta(g)}{g^3}\langle\text{tr}\,F^2_{\mu\nu}\rangle$. This implies that the gluon condensate can serve as an order parameter for supersymmetry breaking. The vacuum energy density, and hence the condensate, vanishes to all orders in perturbation theory in supersymmetric theories. Since supersymmetry is known to be unbroken, the gluon condensate must be zero non-perturbatively as well. In the semi-classical limit this result appears mysterious, because all contributions appear to be positive. The reason is that in euclidean space the fermion determinant is positive definite, and $\text{tr}F^2_{\mu\nu}$ is also positive definite. This implies that the gluon condensate is the average of a positive observable with respect to a positive measure [21]. Then, how does the vanishing of the $\langle\text{tr}\,F^2_{\mu\nu}\rangle$ take place from a semi-classical point of view?

We address this question in the regime of small, but *finite* radii on $\mathbb{R}^3 \times S^1_L$. To do so, recall the Euclidean realization of the vacuum of the theory on small $\mathbb{R}^3 \times S^1_L$, depicted in Fig. 2 for the center-symmetric point of the Wilson line on the Coulomb branch. The vacuum is, primarily, a dilute gas of semi-classical one- and two-events: monopole-instantons [22–25] and bions [5, 26–28]. These are:

a) monopole-instantons, $\mathcal{M}_i = e^{-S_0}(\alpha_i \cdot \lambda)^2$,

b) magnetic bions, $\mathcal{B}_{ij} = [\mathcal{M}_i \overline{\mathcal{M}}_j] = e^{-2S_0}\ldots$,

c) neutral bions, $\mathcal{B}_{ii} = [\mathcal{M}_i \overline{\mathcal{M}}_i] = e^{-2S_0 + i\pi}\ldots$

where α_i, $i = 1, \ldots, N$ are simple roots complemented with the affine root α_N, and $\mathcal{B}_{ij}$ and $\mathcal{B}_{ii}$ are non-vanishing $\forall \hat{A}_{ij} < 0$, and $\forall \hat{A}_{ii} > 0$ entries of the extended Cartan matrix, respectively. The monopole action is $S_0 = \frac{8\pi^2}{g^2 N}$. For small L the coupling is small, the action is large, and fluctuations are suppressed. The $2N$ fermion zero modes of the 4d instanton are distributed uniformly as $(2, 2, \ldots, 2)$ to monopoles $\mathcal{M}_i$.

At leading order $O(e^{-S_0})$ in the semi-classical limit, each monopole-instanton has two fermion zero modes and there-

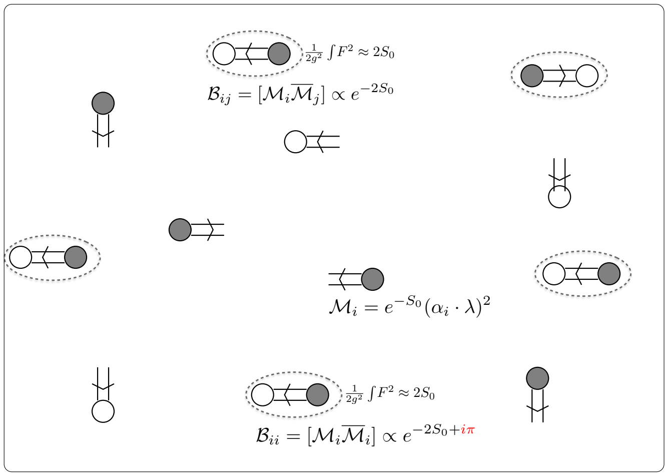

FIG. 2: A snap-shot of the euclidean vacuum of $\mathcal{N}=1$ SYM on small $\mathbb{R}^3\times S^1_L$. Both neutral and magnetic bions carry action $2S_0$, but their contribution to gluon condensate cancels exactly because of the presence of a HTA, a π-phase difference between the two saddles.

fore they do not contribute to the gluon condensate. Two-defects *do contribute* to the gluon condensate. For the sake of making the analogy with the toy example (1) explicit, let us consider analytic continuation away from $n_f = 1$. The density of both types of 2-defects is the same, of order $O(e^{-2S_0})$. However, there is an extra $(4n_f-3)\pi$ phase (invariant angle) associated with the neutral bion saddle/thimble:

$$\mathrm{Arg}(\mathcal{J}_{\mathcal{B}_{ii}}) = \mathrm{Arg}(\mathcal{J}_{\mathcal{B}_{ij}}) + (4n_f-3)\pi\,. \tag{4}$$

Consequently, in contrast to the folklore regarding the positivity of the gluon condensate, the contributions of the two types of 2-defects to the gluon condensate cancel:

$$L^4\langle \tfrac{1}{N}\mathrm{tr}F^2_{\mu\nu}\rangle = 0\times n_{\mathcal{M}_i} + (n_{\mathcal{B}_{ij}} + e^{i(4n_f-3)\pi} n_{\mathcal{B}_{ii}}) = 0\,. \tag{5}$$

at a physical integer value of the parameter, $n_f = 1$, similar to (1). This is the microscopic mechanism for the vanishing of the gluon condensate as well as the vacuum energy in $\mathcal{N}=1$ SYM. The two contributing bion-thimbles are charged oppositely under the $\mathbb{Z}_2^{\mathrm{HTS}}$, and cancel each other out.

The difference with respect to the toy integral and the cancellation in analytically continued Chern-Simons theory is the fact that this cancellation is observable dependent. In fact, the combination of the neutral and magnetic bions, despite giving vanishing contribution to gluon condensate, is responsible for the formation of a mass gap. To see this consider the effective lagrangian for the low energy bosonic modes. As an example, we will use $SU(2)$ gauge theory. Let ϕ denote the fluctuation of the Wilson line around the center symmetric minimum and σ denote the dual photon. The bosonic potential induced by 2-defects is [29]

$$V(\sigma,\phi) = -(\mathcal{B}_{12}+\mathcal{B}_{21}+\mathcal{B}_{11}+\mathcal{B}_{22}) \\ \sim e^{-2S_0}\left(-\cos 2\sigma - e^{i\pi}\cosh 2\phi\right)\,. \tag{6}$$

We observe that the factor $e^{i\pi}$ responsible for the vanishing $\langle \frac{1}{N}\mathrm{tr}F^2_{\mu\nu}\rangle$ is also responsible for the (positive and unsuppressed) mass gap of the ϕ-fluctuations and stabilizes center-symmetry. The HTA explains both the vanishing of the gluon condensate and the non-tachyonic nature of fluctuations of the Polyakov line. It is also not particular to supersymmetric theory, as we discuss next.

QCD(AS/S): In a typical confining asymptotically free $SU(N)$ gauge theory, the "natural" scaling of the (properly normalized) gluon condensate is $O(N^0)$: $\langle \frac{1}{N}\mathrm{tr}F^2_{\mu\nu}\rangle \propto N^0\Lambda^4$. It is natural to expect that the vanishing of the gluon condensate is special to the supersymmetric theory. This is not the case. There exists an *exact* large-N orientifold/orbifold equivalence between $\mathcal{N}=1$ SYM and QCD(AS/S) [30], proven in [31]. Here, AS/S refers to fermions in anti-symmetric/symmetric two-index representations. The large-N equivalence implies that the gluon condensate in QCD(AS/S) is zero at leading order in the $1/N$ expansion, and must scale as [32]:

$$\langle \tfrac{1}{N}\mathrm{tr}\,F^2_{\mu\nu}\rangle^{\mathrm{QCD(AS/S)}} = \tfrac{1}{N}\Lambda^4\,, \tag{7}$$

in sharp contrast with the "natural" value. This result is counter-intuitive, but it is a rigorous consequence of the large N equivalence. However, as in the supersymmetric case, there is no known semi-classical explanation.

Again, we can understand the result based on the presence of HTAs. To achieve this, we use the framework of deformed Yang-Mills theory, and add AS representation fermions (a similar analysis holds for QCD(S)). In QCD(AS), the Atiyah-Singer index theorem implies that the number of fermion zero modes of a 4d instanton is $2N-4$. There are N types of monopole-instantons, with the number of fermion zero modes distributed as $(2,2,\ldots,2,0,0)$ in a center-symmetric background. The difference with respect to $\mathcal{N}=1$ SYM is that 2 out of N monopole-instantons do not possess fermi zero modes. Therefore, at leading order, $O(e^{-S_0})$, in the semi-classical expansion, $N-2$ monopoles do not contribute to the gluon condensate and *only* two do, giving a positive contribution proportional to $1/N$. At second order in the semiclassical expansion, $O(e^{-2S_0})$, there are magnetic and neutral bions that can contribute to gluon condensate. Their contribution cancels at leading order in N, analogous to SYM, leading to (7).

In the older literature on QCD [21, 33, 34], it was assumed that in the semi-classical limit gluon condensate is proportional to the instantons density. This was based on the rationale that a single instanton contributes a finite and positive amount, $\frac{1}{2g^2}\int \mathrm{tr}\,F^2_{\mu\nu} = \frac{8\pi^2}{g^2}$, and that the condensate can be attributed to 4d instantons with a positive weight, $\langle \frac{1}{N}\mathrm{tr}\,F^2_{\mu\nu}\rangle \propto n_I$. In the calculable small S^1_L regime, we see that this is incorrect in at least two ways: *i)* Instantons are sub-leading, i.e.

$O(e^{-N})$, *ii)* The weight of the saddles can be both positive (decreasing energy) and negative (increasing energy). Our work is the first example in which a contribution to condensate has a negative component.

Quantum mechanics: In order to show the generality of hidden topological angles, we also consider the quantum mechanics of a particle with position $x(t)$ and internal spin $(\frac{1}{2})^{n_f}$. The euclidean Lagrangian is that of a bosonic field $x(t)$ coupled to n_f fermionic fields ψ_i:

$$\mathcal{L}_E = \left(\tfrac{1}{2}\dot{x}^2 + \tfrac{1}{2}(W')^2 + (\bar{\psi}_i\dot{\psi}_i + W''\bar{\psi}_i\psi_i)\right) \tag{8}$$

For $n_f = 1$, this theory is supersymmetric [35]. If we choose $W(x)$ to be a periodic function, for example $W(x) = \cos x$, we may identify $x = x + 2\pi$ as the same physical point, corresponding to a particle on a circle, rather than in an infinite lattice. The system contains two types of instantons,

$$I_1 : [0 \to \pi], \qquad I_2 : [0 \to -\pi]\,. \tag{9}$$

Here, I_2 is an instanton (not an anti-instanton), because it satisfies the same BPS equation (or gradient flow equation, if W is viewed as a Morse function) as I_1.

Because of spin, instantons do not contribute to the vacuum energy. A non-vanishing contribution arises from correlated two-events. This parallels the 4d field theory on $\mathbb{R}^3 \times S^1$, and provides a simple system in which the effect of the HTA is not contaminated by first order instanton effects. Following [36, 37], we find that the amplitudes of the two-events are given by $[I_1\bar{I}_1] = [I_2\bar{I}_2] \propto e^{i\pi n_f}e^{-2S_I}$, and $[I_1\bar{I}_2] = [I_2\bar{I}_1] \propto e^{-2S_I}$. Due to the difference in the invariant angles between the two-saddles/thimbles we find

$$\mathrm{Arg}(\mathcal{J}_{[I_1\bar{I}_1]}) = \mathrm{Arg}(\mathcal{J}_{[I_1\bar{I}_2]}) + n_f\pi\,. \tag{10}$$

The non-perturbative contribution to the ground state energy takes the form:

$$\Delta E_0^{\mathrm{np}} = (-2 - 2e^{i\pi n_f})e^{-2S_I} \tag{11}$$

While the $[I_1\bar{I}_2]$ molecule behaves in the expected manner and decreases the ground state energy, the $[I_1\bar{I}_1]$ molecule is sensitive to the HTA governed by the spin and increases the ground state energy for odd n_f (half-integer spin) while decreasing it for even-n_f (integer spin). In the case $n_f = 1$, (10) is the microscopic reason for the non-perturbative vanishing of the ground state energy. We note that this system, despite having Witten index zero [38], $I_W = \mathrm{tr}[(-1)^F] = 0$, has unbroken supersymmetry, and two supersymmetric ground states.

There are two additional interesting features of this system. The first is related to the fact that one can introduce a topological angle into the Lagrangian, $i\frac{\Theta}{2\pi}\int \dot{x}\,d\tau$, and unlike the case of supersymmetric gauge theory, the Θ-angle is physical, and alters the spectrum of the theory. Since $I_W = 0$, the supersymmetry of this system is fragile. The vacuum energy can be written as

$$\Delta E_0^{\mathrm{np}} = (-2\cos\Theta - 2e^{i\pi n_f})e^{-2S_I} \tag{12}$$

which, for the supersymmetric theory ($n_f = 1$), takes the form:

$$\Delta E_0^{\mathrm{np}} = (-2\cos\Theta + 2)e^{-2S_I} = 4\sin^2\tfrac{\Theta}{2}e^{-2S_I} \geq 0 \tag{13}$$

meaning supersymmetry is dynamically broken for $\Theta \neq 0$. Note that the energy remains positive semi-definite, which is a consequence of the supersymmetry of the Hamiltonian. The physical reason for $E > 0$ in the case $\Theta \neq 0$ is that the Θ-angle is equivalent to feeding momentum into the system. Because of supersymmetry, bosonic/fermionic ground state pair is lifted simultaneously by the insertion of momentum, leading to a non-vanishing ground state energy.

The second unusual feature is that the theory has Witten index $I_W = 0$ for any value of Θ, but that the reason for $I_W = 0$ differs in the two cases. For $\Theta = 0$, we get $I_W = 1 - 1 = 0$, where the two contributions arise from the bosonic/fermionic sectors of the Hilbert space, and supersymmetry is unbroken. In the second case, $\Theta \neq 0$, we get $I_W = 0 - 0 = 0$ and supersymmetry is broken.

One may speculate that the invariant angles are related to Berry phases [39], realized in terms of Euclidean saddles, at least in the case of quantum mechanics. Since $(\frac{1}{2})^{n_f} = \bigoplus_S \mathrm{mult}(S)S$, where $\mathrm{mult}(S)$ is the multiplicity, we can rewrite the path integral over the Grassmann variables as spin path integrals [40] $Z = \sum_S \mathrm{mult}(S) Z^{(S)}$ where

$$\begin{aligned} Z^{(S)} &= \int DxD(\cos\theta)D\phi\; e^{-\mathcal{L}_E + i\frac{\Theta}{2\pi}\int \dot{x}\,d\tau} \\ \mathcal{L}_E &= \tfrac{1}{2}(\dot{x}^2 + (W')^2) + SW''\cos\theta + iS(1-\cos\theta)\dot{\phi} \end{aligned} \tag{14}$$

where $(\theta,\phi) \in \mathbf{S}^2$ parameterize the Bloch sphere. There are two spin dependent interactions, a "magnetic field" W''-spin coupling, and the Wess-Zumino term, or Berry phase action. In this language (10) should be replaced by $\mathrm{Arg}(\mathcal{J}_{[I_1\bar{I}_1]}) = \mathrm{Arg}(\mathcal{J}_{[I_1\bar{I}_2]}) + 2S\pi$. This distinguishes half-integer and integer spin particles, similar to anti-ferromagnets in one-spatial dimension [41], leading to qualitative differences.

Conclusion: We have provided several examples of $\mathbb{Z}_2$ hidden topological angles, associated with the saddle point manifolds that appear in the complexified path integral, and have shown that these angles lead to crucial physical effects. We anticipate that HTAs will have crucial impact on the semi-classical analysis of many interesting quantum field theories and quantum mechanical systems. Our examples also show that in an attempt to perform lattice simulations using Lefschetz thimbles, e.g., [42–45], all thimbles whose multipliers are non-zero must be carefully summed over to correctly capture the dynamics of the theory.

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* Electronic address: abehtas@ncsu.edu
† Electronic address: tsulejm@ncsu.edu
‡ Electronic address: tmschaef@ncsu.edu
§ Electronic address: unsal.mithat@gmail.com

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