Defects, modular differential equations, and free field realization of $\mathcal{N}=4$ vertex operator algebras

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For all 4D $\mathcal{N}=4$ Super-Yang-Mills theories with simple gauge groups G, we show that a set of residues of the integrands in the $\mathcal{N}=4$ Schur indices, which are related to Gukov-Witten-type surface defects in the theories, equal the vacuum characters of rank$G$ copies of $bc\beta\gamma$ systems that provide the free field realization of associated $\mathcal{N}=4$ vertex operator algebras in [F. Bonetti, C. Meneghelli, and L. Rastelli, J. High Energy Phys. 05 (2019) 155]. This result predicts that these residues, as module characters, are additional solutions to the flavored modular differential equations satisfied by the original Schur index. The prediction is verified in the $G=SU(2)$ case, where an additional logarithmic solution is constructed.

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I. INTRODUCTION

In [1], any four-dimensional $\mathcal{N}=2$ superconformal theory (4D $\mathcal{N}=2$ superconformal field theory (SCFT)) is shown to contain a 2D vertex-operator algebra (VOA) as a protected subsector. The associated VOA encodes important information of the 4D SCFT, which can be accessed using various tools available for 2D VOAs [2–6]. The correspondence also predicts new classes of VOAs [7–11] and inspires novel realizations [12–15] of some existing VOAs. In particular, a free field realization is proposed in [12] of the associated VOAs of the $\mathcal{N}=4$ Super-Yang-Mills (SYM) with gauge groups G in terms of rank G copies of $bc\beta\gamma$ systems.

Another particularly intriguing entry in the 4D/2D dictionary involves BPS (Bogomol'nyi-Prasad-Sommerfield) surface defects in the 4D SCFTs. It is generally believed that they give rise to (twisted) modules of the associated 2D VOAs [16,17]. Interesting progress has been made to elucidate this relation [16,18–22], where a UV class-$\mathcal{S}$ theory $\mathcal{T}'$ is Higgsed with a position-dependent vacuum expectation value [23] to an IR theory $\mathcal{T}$ coupled to certain surface defect.

One simple class of surface defects attracts relatively less attention in the literature on this particular 4D/2D correspondence, namely, those engineered by a singular BPS background profile of a dynamical gauge field in a 4D $\mathcal{N}=2$ SCFT [24]. In this paper, we consider such defects in 4D $\mathcal{N}=4$ SYM with simple gauge groups G. The Schur indices in the presence of the defects are computed by contour integrals that compute the original Schur indices but with shifted contours [25–28], which are related to the residues of the integrand.

What is surprising is that one set of these residues precisely coincide with the vacuum characters of the rank G copies of $bc\beta\gamma$ systems responsible for the free field realization [12]. This observation, first made in [29], helps identify the corresponding modules of the associated VOAs. We will present a detail analysis of the simplest case with $G=SU(2)$, where we identify the simple modules corresponding to the surface defect. Vanishing one-point function of null vectors of the VOA evaluated on modules sometimes lead to flavored modular differential equations (FMDEs) satisfied by all the module characters. To verify this prediction we check that the Schur indices with/without defect satisfy the FMDEs predicted by the nulls studied in [30], and we further propose an additional logarithmic solution using the module characters.

Computationally, our results highlight the fact that for a Lagrangian theory the simple integrand of the Schur index provides easy access to crucial structural information, including potential free field realizations, module characters, and modularity of the associated VOA.

II. DEFECTS AND FREE FIELD CHARACTERS

Let us consider a 4D $\mathcal{N}=4$ SYM with a simply-connected simple gauge group G with Lie algebra $\mathfrak{g}$. The Schur index is well known, given by

$$\mathcal{I}(a,b) \equiv \frac{(-1)^{|\Delta^+|}}{|W|}\oint\left[\frac{da}{2\pi i a}\right]\frac{\eta(\tau)^{3r}}{\vartheta_4(\mathfrak{b}|\tau)^r}\prod_{\alpha\in\Delta}\frac{\vartheta_1(\alpha(\mathfrak{a})|\tau)}{\vartheta_4(\alpha(\mathfrak{a})+\mathfrak{b}|\tau)}. \tag{1}$$

Here $\mathfrak{b}$ (with $b \equiv e^{2\pi i \mathfrak{b}}$) is the flavor symmetry fugacity, $\mathfrak{a} \in \mathfrak{h}$ (also with $a \equiv e^{2\pi i \mathfrak{a}}$) denotes the Cartan-valued flat connection along the temporal S^1 and $[da/2\pi i a]$ an appropriate measure [31]. Also, r denotes the rank of $\mathfrak{g}$, Δ ($\Delta^\pm$) the set of all roots (positive/negative roots) and $|\Delta|$ the number of roots. As usual $\alpha_{i=1,\ldots,r}$ denotes the simple roots of $\mathfrak{g}$. It will prove convenient later to decompose all positive roots according to their "height" H [if $\alpha = \sum_{i=1}^r m_i \alpha_i$, then $H(\alpha) \equiv \sum_{i=1}^r m_i$], and use Δ_H^+ to collect all positive roots of height H. With such a definition, we can rewrite all products over roots into

$$\prod_{\alpha\in\Delta} f(\alpha) = \prod_{H\geq 1} \prod_{\alpha\in\Delta_H^+} f(\alpha) \prod_{\alpha\in\Delta_H^+} f(-\alpha). \tag{2}$$

We are interested in the theory in the presence of a Gukov-Witten-type surface defect specified by a background gauge field with a profile $A^{\mathrm{bg}} = \mathfrak{a}_\varphi d\varphi$ where $\mathfrak{a}_\varphi \in \mathfrak{h}$, which is singular on the torus $T^2_{\theta=\pi/2}$; other component fields in the vector multiplet are set to zero. This background configuration is BPS with respect to the supercharge used for localization [21,32]. As a result, A^{bg} modifies the final path integral on T^2 that computes the Schur index [33], which now reads,

$$\oint \frac{da}{2\pi i a} \int [DbDc]'[D\beta D\gamma] e^{-S_{bc\beta\gamma}[\mathfrak{a},\mathfrak{a}_\varphi,\mathfrak{b}]}. \tag{3}$$

The torus action here is simply

$$S_{bc\beta\gamma}[\mathfrak{a},\mathfrak{a}_\varphi,\mathfrak{b}] = \int_{T^2} (\beta D_{\bar z}\gamma + b D_{\bar z} c), \tag{4}$$

where $D_{\bar z} = \partial_{\bar z} - iA_{\bar z} - iA_{\bar z}^{\mathrm{bg}} - iA_{\bar z}^{\mathrm{flavor}} = \partial_{\bar z} + i\frac{(\mathfrak{a} - \tau\mathfrak{a}_\varphi + \mathfrak{b})}{\tau - \bar\tau}$. When $\mathfrak{a}_\varphi = 0$, the path integral recovers the original index. For nonzero $\mathfrak{a}_\varphi$ the $bc\beta\gamma$ systems are taken to the twisted sector labeled by $\mathfrak{a}_\varphi$, whose character can be computed [34]. In the end, the index in the presence of the surface defect reads

$$\mathcal{I}^{\mathrm{defect}}(a,b) \equiv \frac{(-1)^{|\Delta^+|}}{|W|} \oint \left[\frac{da}{2\pi i a}\right] \frac{\eta(\tau)^{3r}}{\vartheta_4(\mathfrak{b}|\tau)^r} \times \prod_{\alpha\in\Delta} \frac{\vartheta_1(\alpha(\mathfrak{a} - \tau\mathfrak{a}_\varphi)|\tau)}{\vartheta_4(\alpha(\mathfrak{a} - \tau\mathfrak{a}_\varphi) + \mathfrak{b}|\tau)}. \tag{5}$$

We can absorb the shift by $\mathfrak{a}_\varphi$ into the integration variables which effectively shift their contours from unit circles $|a_i| = 1$ to $|a_i| = |q^{-(\mathfrak{a}_\varphi)_i}|$, where we define $\mathfrak{a}_\varphi = \mathrm{diag}((\mathfrak{a}_\varphi)_{i=1,\ldots,N}) \in \mathfrak{h}$.

We argue that this defect index is related to the residues of the integrand. For simplicity we take $G = SU(3)$ temporarily and give $\mathfrak{b}$ a small positive imaginary part so that $|b| < 1$. Now, imagine we gradually turn on the defect parameter $(\mathfrak{a}_\varphi)_1$ from 0 to $-\frac{1}{2}$, which shrinks the a_1 contour from $|a_1| = 1$ to $|a_1| = |q|^{\frac{1}{2}}$. The integral stays the same initially, but right before reaching the final contour, the pole $a_1 = a_1^* \equiv a_2 b^{-1} q^{\frac{1}{2}}$ from the factor $\vartheta_4(\mathfrak{a}_1 - \mathfrak{a}_2 + \mathfrak{b})^{-1}$ crosses the shrunk a_1 contour. As a_1 contour shrinks, the a_2-pole $a_2^2 = (a_2^*)^2 \equiv a_1^{-1} b^{-1} q^{\frac{1}{2}}$ from the factor $\vartheta_4(\mathfrak{a}_1 - \mathfrak{a}_3 + \mathfrak{b})^{-1}$ actually starts venturing outward from inside the a_2 unit circle. In the end, the pole reaches $|a_2^2| = |b^{-1}|$ which is outside of the a_2-integration contour; the pole a_2^* crosses the a_2 contour precisely when the pole a_1^* crosses the a_1 contour [35]. At the end of the movement, $\alpha_i(\mathfrak{a}_\varphi) = -\frac{1}{2}$ for both $i = 1, 2$, and the defect index equals the original Schur index $\mathcal{I}$ with the residue Res of the simultaneous pole $(\frac{a_1}{a_2} = b^{-1} q^{\frac{1}{2}}, \frac{a_2}{a_3} = b^{-1} q^{\frac{1}{2}})$ discussed above subtracted,

$$\mathcal{I}^{\mathrm{defect}} = \mathcal{I} - \mathrm{Res}. \tag{6}$$

Other poles that one might encounter by different ways of turning on $\mathfrak{a}_\varphi$ actually share the same residue, up to numeric constants and a power of q, as an analytic function of $\mathfrak{b}$ and q [36]. One should carefully collect all the poles that crosses the contour when gradually turning on the defect. In the following discussion for more general simple gauge groups G, we will focus on the simplest set of simultaneous poles, and leave the full discussion on other poles to future study.

Let us now consider the simple algebra $\mathfrak{g}$ of a simple Lie group G, and focus on the set of poles of the integrand given by the equations [19,37]

$$e^{2\pi i \alpha_i(\mathfrak{a})} = b q^{\frac{1}{2}}, \quad i = 1, \ldots, r. \tag{7}$$

These equations imply that $e^{2\pi i \alpha(\mathfrak{a})} = (bq^{\frac{1}{2}})^H$ for $\forall\, \alpha \in \Delta_H^+$.

It is straightforward to compute the residue of the full integrand at the poles [19,37]. We first present the raw result before further massage [we have dropped the overall sign and $1/|W|$ to avoid clutter, and written the theta functions in terms of $(z;q)$], which reads

$$\begin{aligned}\mathrm{Res} = {} & \frac{q^{\frac{|\Delta|+r}{8}}(q;q)^{3r}}{[(q;q)(bq^{\frac{1}{2}};q)(b^{-1}q^{\frac{1}{2}};q)]^r} \frac{1}{(q;q)^r} \\ & \times \prod_{H\geq 1} \frac{[((bq^{\frac{1}{2}})^H q;q)((bq^{\frac{1}{2}})^{-H};q)]^{|\Delta_H^+|}}{[((bq^{\frac{1}{2}})^{H+1};q)((bq^{\frac{1}{2}})^{-H-1}q;q)]^{|\Delta_H^+|}} \\ & \times \prod_{H\geq 1} \frac{[((bq^{\frac{1}{2}})^{-H} q;q)((bq^{\frac{1}{2}})^{H};q)]^{|\Delta_H^+|}}{[((bq^{\frac{1}{2}})^{-H+1};q)'((bq^{\frac{1}{2}})^{H-1}q;q)]^{|\Delta_H^+|}}. \end{aligned} \tag{8}$$

Here the prime in the last line indicates that the corresponding factors with $H = 1$ are dropped; they are accounted for by the $(q;q)^{-r}$ in the first line, where the q-Pochhammer symbol is defined by $(z;q) \equiv \prod_{k=0}(1 - zq^k)$.

It is obvious that there are massive cancellations between the second and the third line. Concretely, almost every factor of $(\#;q)^{\#}$ (say, corresponding to a height H) from the second line will find its opponent (corresponding to $H+1$) in the third line:

(a) If a height H is such that $|\Delta_H^+| = |\Delta_{H+1}^+|$, then the two factors completely annihilate each other. However, if $|\Delta_H^+| > |\Delta_{H+1}^+|$, part of the factor from the second line survives.

(b) Additionally, the factors in the second line with the largest H will find no match and therefore always survive.

(c) The factors in the third line with $H=1$ will cancel against those in the first line. Note that $|\Delta_{H=1}^+| = r$.

Finally, with all these cancellations carried out, we are left with

$$q^{\frac{\dim\mathfrak{g}}{8}} \prod_{\substack{H\geq 1\\ |\Delta_H^+|>|\Delta_{H+1}^+|}} \frac{(b^H q^{\frac{1}{2}+\frac{H+1}{2}};q)(b^{-H}q^{\frac{1}{2}-\frac{H+1}{2}};q)}{(b^{H+1}q^{\frac{H+1}{2}};q)(b^{-(H+1)}q^{1-\frac{H+1}{2}};q)}. \tag{9}$$

Here we have used the fact that for all simple Lie algebras, $0 \leq |\Delta_H^+| - |\Delta_{H+1}^+|$. In fact, when the inequality is a strict inequality, $H+1$ coincides with the degree of an invariant of $\mathfrak{g}$ [38,39], which further agrees with the degree of a fundamental invariant of the associated Weyl group. (See Tables I and II for concrete examples.) Hence, we finally recognize the residue to be

$$q^{\frac{\dim\mathfrak{g}}{8}} \prod_{i=1}^{r} \frac{(b^{d_i-1}q^{\frac{d_i+1}{2}};q)(b^{-d_i+1}q^{\frac{1-d_i}{2}};q)}{(b^{d_i}q^{\frac{d_i}{2}};q)(b^{-d_i}q^{1-\frac{d_i}{2}};q)}, \tag{10}$$

which is precisely the vacuum character of the rank $\mathfrak{g}$ copies of $bc\beta\gamma$ systems appearing in the free field realization of $\mathcal{N}=4$ VOAs [12]; see Table 3.4 therein. Therefore (up to some numerical constants)

$$\mathrm{Res} = \mathrm{ch}(V_{bc\beta\gamma}^G). \tag{11}$$

TABLE I. The number of roots at each H for some simplest simple Lie algebras. In the third column, $n_1^{m_1}, n_2^{m_2}, \ldots$ encodes that at m_i consecutive heights there are n_i roots inside. For example, in the row of $\mathfrak{e}_6$, $6, 5^3, 4, \ldots$ means that there are $6, 5, 5, 5, 4, \ldots$ roots at heights $1, 2, 3, 4, 5, \ldots$. From these data we can read off at which height the number of roots decreases.

$\mathfrak{g}$	H	$\lvert\Delta_H^+\rvert$
$\mathfrak{a}_r$	$1, 2, \ldots, r$	$r, r-1, \ldots, 1$
$\mathfrak{d}_{2n}$	$1, 2, \ldots, 2n-1$	$2n, (2n-1)^2, (2n-2)^2, \ldots, (n+1)^2$
	$2n, \ldots, 4n-3$	$(n-1)^2 \ldots, 1^2$
$\mathfrak{e}_6$	$1, 2, \ldots, 11$	$6, 5^3, 4, 3^2, 2, 1^3$
$\mathfrak{e}_7$	$1, 2, \ldots, 17$	$7, 6^4, 5^2, 4^2, 3^2, 2^2, 1^4$
$\mathfrak{e}_8$	$1, 2, \ldots, 29$	$8, 7^6, 6^4, 5^2, 4^4, 3^2, 2^4, 1^6$

TABLE II. The degrees of invariants of the simple Lie algebras.

$\mathfrak{g}$	$d_1, \ldots, d_r$
$\mathfrak{a}_r$	$1, 2, \ldots, r$
$\mathfrak{b}_r$	$2, 4, \ldots, 2r$
$\mathfrak{d}_n$	$2, 4, \ldots, 2(r-1); r$
$\mathfrak{e}_6$	2, 56, 8, 9, 12
$\mathfrak{e}_7$	2, 6, 8, 10, 12, 14, 18
$\mathfrak{e}_8$	2, 8, 12, 14, 18, 20, 24, 30
F_4	2, 6, 8, 12

In particular, the central charge matches as expected, $c = -3\dim\mathfrak{g} = -3\sum_{i=1}^r c_{bc\beta\gamma}^i$.

As proposed in [12], the $\mathcal{N}=4$ VOA $\mathcal{V}_{\mathcal{N}=4}^G$ is embedded as a subalgebra in the $bc\beta\gamma$ system $\mathcal{V}_{bc\beta\gamma}^G$. Consequently, the vacuum module $V_{bc\beta\gamma}^G$ also furnishes a reducible but indecomposable module of the VOA $\mathcal{V}_{\mathcal{N}=4}^G$, with the vacuum module $V_{\mathcal{N}=4}^G$ of $\mathcal{V}_{\mathcal{N}=4}^G$ a submodule of $V_{bc\beta\gamma}^G$.

If $N \in \mathcal{V}_{\mathcal{N}=4}^G$ is a null vector, then one can insert N into the supertrace over any module M of $\mathcal{V}_{\mathcal{N}=4}^G$ and the result should vanish. As discussed in [30,40–42], for N of a special type, one can derive from the supertrace a (flavored) modular differential equation,

$$0 = \mathrm{str}_M N(z) q^{L_0 - \frac{c_{2d}}{24}} b^f = \mathcal{D}_{q,b}\mathrm{ch}(M), \tag{12}$$

where $\mathcal{D}_{q,b}$ denotes a differential operator with simple modular property. In particular, by choosing $M = V_{bc\beta\gamma}^G$ one concludes that the residue Res must be a solution to all the flavored modular differential equations predicted by the nulls of $\mathcal{V}_{\mathcal{N}=4}^G$. Next we will elaborate on the simplest case with $G = SU(2)$.

III. EXAMPLE: 4D $\mathcal{N}=4$ $SU(2)$-SYM

The associated VOA of the 4d $\mathcal{N}=4$ Super-Yang-Mills with an $SU(2)$ gauge group is the small $\mathcal{N}=4$ superconformal algebra $\mathcal{V}_{\mathcal{N}=4}$ with $c_{2d} = -9$, generated by $J^a, G^{\pm}, \tilde{G}^{\pm}$ [1]. Here $\{J^a\}$ generate an $\hat{\mathfrak{su}}(2)_{k=-\frac{3}{2}}$ affine subalgebra, and at this central charge the Sugawara stress tensor coincides with that of the full VOA $\mathcal{V}_{\mathcal{N}=4}$. The flavored Schur index of the theory, or equivalently, the flavored vacuum character of the VOA can be written as the standard contour integral,

$$\begin{aligned}\mathcal{I} &= -\frac{1}{2}\oint_{|a|=1} \frac{da}{2\pi i a} \vartheta_1(\pm 2\mathfrak{a}) \prod_{n=-1}^{+1} \frac{\eta(\tau)}{\vartheta_4(2n\mathfrak{a})} \\ &\equiv \oint \frac{da}{2\pi i z} Z(a,b;q).\end{aligned} \tag{13}$$

As explained in the previous section, we are interested in the theory with a surface defect engineered by turning on a background gauge field of the form $A^{\mathrm{bg}} = \mathfrak{a}_\varphi \mathrm{diag}(1,-1)d\varphi$. Here, $\mathfrak{a}_\varphi \mathrm{diag}(1,-1) \in \mathfrak{h} \subset \mathfrak{su}(2)$. The defect index is then written as

$$\mathcal{I}^{\mathrm{defect}}(b,q) = \oint_{|a|=|q^{-\mathfrak{a}_\varphi}|} \frac{da}{2\pi i a} Z(a,b;q), \tag{14}$$

where we have absorbed the $\mathfrak{a}_\varphi$ into the integration variable which deforms the contour accordingly. The index equals the original Schur index if $|\mathfrak{a}_\varphi|$ is relatively small since the integrand is meromorphic in a. However, as $\mathfrak{a}_\varphi$ varies from 0 towards larger negative values, say, $\mathfrak{a}_\varphi = -\frac{1}{4}$, the shrunk contour will inevitably hit the poles corresponding to $2\mathfrak{a} + \mathfrak{b} = \frac{\tau}{2}$. Concretely, the poles are given by $a = \pm b^{-\frac{1}{2}} q^{\frac{1}{4}}$, whose total residue will be denoted as $\mathrm{Res}(b,q)$. As a result, the defect index reads

$$\mathcal{I}^{\mathrm{defect}}(b;q) = \mathcal{I}(b,q) - \mathrm{Res}(b,q), \tag{15}$$

where the residue equals to

$$\begin{aligned}\mathrm{Res}(b,q) &\equiv -\frac{1}{2} q^{\frac{3}{8}} \frac{(b^{-1}q^{-\frac{1}{2}};q)(bq^{\frac{3}{2}};q)}{(b^{-2};q)(b^2 q;q)} \\ &= -\frac{1}{2}\frac{1}{1-b^{-2}}(-bq^{\frac{1}{8}} + (1+b^{-2})q^{\frac{3}{8}} \\ &\quad - (b^{+1} + b^{-1} + b^{-3})q^{\frac{7}{8}} + \ldots).\end{aligned} \tag{16}$$

Note that the residue is singular in the $b \to 1$ limit, and hence Res and $\mathcal{I}$ are linear independent.

As observed in the previous section, the above residue, up to the factor $-\frac{1}{2}$, is nothing but the character of the character of the vacuum module $V_{bc\beta\gamma}$ of a $bc\beta\gamma$ system $\mathcal{V}_{bc\beta\gamma}$ studied in [12], which is responsible for the free field realization of the small $\mathcal{N}=4$ superconformal algebra $\mathcal{V}_{\mathcal{N}=4}$,

$$-2\,\mathrm{Res}(b,q) = \mathrm{ch}(V_{bc\beta\gamma}) \equiv \mathrm{str}_{V_{bc\beta\gamma}} q^{L_0 - \frac{c_{2d}}{24}} b^f. \tag{17}$$

Given that $\mathcal{V}_{\mathcal{N}=4}$ is a sub-VOA of the $bc\beta\gamma$ system $\mathcal{V}_{bc\beta\gamma}$, its vacuum module $V_{bc\beta\gamma}$ furnishes a reducible but indecomposable module of the $\mathcal{N}=4$ VOA $\mathcal{V}_{\mathcal{N}=4}$. This fact immediately predicts that the residue Res and therefore the defect index $\mathcal{I}^{\mathrm{defect}}$ must satisfy all the relevant flavor modular differential equations coming from the nulls in the $\mathcal{N}=4$ VOA.

A simplest null worth studying is $\mathcal{N} = T - T_{\mathrm{Sug}} = 0$, since the stress tensor of the $\mathcal{N}=4$ VOA coincides with the Sugawara stress tensor of the $\hat{\mathfrak{su}}(2)_{k=-\frac{3}{2}}$ affine subalgebra. One can directly compute the vacuum expectation value $\langle T - T_{\mathrm{Sug}}\rangle$ via localization [32]. On the one hand, the stress tensor T of the 2D VOA descends from the $SU(2)_{\mathcal{R}}$ current in the original four-dimensional theory, while on the other hand, the Sugawara stress tensor $T_{\mathrm{Sug}} = \frac{1}{2(k+h^\vee)}\sum_{a,b} J^a J^b$ where the currents J^a are gauge-invariant bilinears of $\beta\gamma$, $J^{+,3,-} \sim \mathrm{tr}(\beta\beta), \mathrm{tr}(\beta\gamma)$, and $\mathrm{tr}(\gamma\gamma)$. Using the $\mathfrak{a}_\varphi$-twisted Green's functions (C2), (C1) for the bc and $\beta\gamma$ systems and the Wick theorem, we have

$$\langle T\rangle = \oint_{|a|=|q^{-\mathfrak{a}_\varphi}|} \frac{da}{2\pi i a}\frac{1}{4\pi^2}\left[\frac{\vartheta_1''(2\mathfrak{a})}{\vartheta_1(2\mathfrak{a})} + \frac{\vartheta_1'''(0)}{2\vartheta_1'(0)} + \ldots\right],$$

and

$$\langle T_{\mathrm{Sug}}\rangle = \oint_{|a|=|q^{-\mathfrak{a}_\varphi}|} \frac{da}{2\pi i a}\frac{3}{8\pi^2}\left[\frac{\vartheta_1''(0)^2}{\vartheta_1'(0)^2} + \frac{\vartheta_1'''(0)}{\vartheta_1(0)} + \ldots\right].$$

To avoid clutter we only display the first few terms. These integral at small $|\mathfrak{a}_\varphi|$ can be evaluated by picking up the residue at the origin, while for $\mathfrak{a}_\varphi = -\frac{1}{4}$, the residues at $a = \pm b^{-\frac{1}{2}} q^{\frac{1}{4}}$ need to be subtracted off. In either case, we find $\langle T - T_{\mathrm{Sug}}\rangle = 0$.

The null equation $\langle T - T_{\mathrm{Sug}}\rangle = 0$ for general $\mathfrak{a}_\varphi$ is, in fact, a particular flavored modular differential equation [30,40–43]. Indeed, it is straightforward to show that the integral equation can be massaged into [44]

$$\begin{aligned} q\frac{\partial}{\partial q} I = \frac{1}{2(k+h^\vee)}\Bigg(&\frac{1}{2}D_b^2 + kE_2 \\ &+ 2kE_2\begin{bmatrix}1\\ b^2\end{bmatrix} + 2E_1\begin{bmatrix}1\\ b^2\end{bmatrix}D_b\Bigg) I,\end{aligned} \tag{18}$$

for $I = \mathcal{I}, \mathcal{I}^{\mathrm{defect}}$, and $D_b \equiv b\partial_b$; see the Appendix B for more details. In fact, one can further check that both indices also satisfy the flavored modular differential equations corresponding to the nulls studied in [30]. See also [42] for more on FMDEs and their solutions. For example, the nulls in Eq. (6.19) and Eq. (6.21) in [30] lead to

$$\begin{aligned} 0 = {}& q\frac{\partial}{\partial q}\left(b\frac{\partial}{\partial b}\right)I + E_1\begin{bmatrix}-1\\ b\end{bmatrix} q\frac{\partial}{\partial q} I - 3E_3\begin{bmatrix}-1\\ b\end{bmatrix} I \\ &+ 6E_3\begin{bmatrix}1\\ b^2\end{bmatrix} I + \left(E_2 + E_2\begin{bmatrix}-1\\ b\end{bmatrix} - 2E_2\begin{bmatrix}1\\ b^2\end{bmatrix}\right) b\frac{\partial}{\partial b} I,\end{aligned} \tag{19}$$

and

$$\left(D_q^{(2)} + \frac{c_{2d}}{2}E_4\right)I + \left(-2E_2\begin{bmatrix}-1\\b\end{bmatrix}D_q^{(1)} - 4E_3\begin{bmatrix}-1\\b\end{bmatrix}b\partial_b + 18E_4\begin{bmatrix}-1\\b\end{bmatrix}\right)I + \left(3k_{2d}E_4 + 2E_3\begin{bmatrix}1\\b^2\end{bmatrix}b\partial_b - 9E_4\begin{bmatrix}1\\b^2\end{bmatrix}\right)I = 0. \quad (20)$$

Finally, let us define the quotient module $M \equiv V_{bc\beta\gamma}/V_{\mathcal{N}=4}$. It is shown in [45] that M and the vacuum module $V_{\mathcal{N}=4}$ are the only two irreducible $\mathcal{V}_{\mathcal{N}=4}$ modules from the category $\mathcal{O}$. Note that the space $M(0) \subset M$ of lowest conformal weight (*i.e.*, $-\frac{1}{2}$) is an infinite-dimensional irreducible $\mathfrak{su}(2)$ representation with highest weight $-\omega_1$, and is spanned by $\{\gamma_0^n c_{\frac{1}{2}}\mathbf{1} | n \in \mathbb{N}\}$. The zero mode γ_0 lowers the $U(1)$ charge $2m$ by 2, which explains the factor $(1 - b^{-2})^{-1}$ in front of $\mathrm{Res}(b, q)$. As such, we identify

$$\mathcal{I}^{\text{defect}} = \frac{3}{2}\mathcal{I} + \frac{1}{2}\mathrm{ch}(M), \quad (21)$$

where $\mathrm{ch}(M) = -2\,\mathrm{Res} - \mathcal{I}$ is the quotient character, which by construction is a solution to all the flavored modular differential equations mentioned above. Furthermore, one can check that

$$\log b\,\mathrm{ch}(M) + (\log q + \log b)\mathcal{I} \quad (22)$$

is actually an additional logarithmic solution to all the modular differential equations, which is due to the fact that (22) arises as a modular transformation of the Schur index $\mathcal{I}$ [46].

IV. DISCUSSION

In this paper we start from a Gukov-Witten-type surface defects in 4D $\mathcal{N} = 4$ SYMs with simple gauge groups from their Schur indices, which are determined by the residues of the integrands of the contour integrals that compute the original Schur indices. One set of such residues coincide precisely with the vacuum characters of the $bc\beta\gamma$ systems in a free field realization of the $\mathcal{N} = 4$ VOAs. This observation leads to new and easily accessible solutions to the flavored modular differential equations associated to some nulls in the VOAs.

The original construction of the associated VOA of an $\mathcal{N} = 4$ theory is through a BRST (Becchi-Rouet-Stora-Tyutin) reduction of $\dim G$ copies of $bc\beta\gamma$ systems [1]. The computation in this paper reveals a half-way passage from the $\dim G$ to rank G copies of $bc\beta\gamma$ systems, where the actual $\mathcal{N} = 4$ VOA is obtained by additionally taking the kernel of a screening charge $\mathbf{Q}$ [12,45]. The relation between the two approaches deserves further investigation, where the BRST reduction is split into a two-step process, perhaps by a clever split of the BRST charge [47]. Furthermore, the reducible module $V_{bc\beta\gamma}^G$ can be projected down to the irreducible submodule $V_{\mathcal{N}=4}^G$ by a projection $\mathbf{P}$ which establishes the equality

$$\mathcal{I} = \mathrm{ch}(V_{\mathcal{N}=4}^G) = \mathrm{str}_{V_{bc\beta\gamma}^G}\mathbf{P}q^{L_0 - \frac{c_{2d}}{24}}b^f. \quad (23)$$

It would be interesting to identify $\mathbf{P}$ and clarify its relation with the screening charge $\mathbf{Q}$. We conjecture that $\mathbf{P}$ in (23) can be equivalently replaced by some simple difference (or differential) operator $\mathcal{P}$ acting on the vacuum character $\mathrm{ch}(V_{bc\beta\gamma}^G)$, such that

$$\mathcal{I} = \mathcal{P}\,\mathrm{str}_{V_{bc\beta\gamma}^G}q^{L_0 - \frac{c_{2d}}{24}}b^f. \quad (24)$$

As shown in this paper, the flavored vacuum character on the right coincides with some residues of the integrand of the contour integral that computes $\mathcal{I}$ itself. Therefore, this conjecture predicts that the full integral can be simply extracted from the residues of its integrand. This could be achieved by careful application of the elliptic function theory, and as a byproduct, it provides closed-form expressions for the flavored Schur indices. This subject will be studied in [46].

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APPENDIX A: SPECIAL FUNCTIONS

The standard Eisenstein series are defined for $k \in \mathbb{N}_{\geq 1}$ as a q-series (where $q = e^{2\pi i\tau}$ throughout this paper)

$$E_{2k} = -\frac{B_{2k}}{(2k)!} + \frac{2}{(2k-1)!}\sum_{r\geq 1}\frac{r^{2k-1}q^r}{1-q^r}, \quad (A1)$$

with $E_{\text{odd}} = 0$. They are series of integer powers of q, and therefore can arise in the modular differential equations in $\mathbb{Z}$ or $\frac{1}{2}\mathbb{Z}$-graded VOAs.

The twisted Eisenstein series are defined for $k \in \mathbb{N}_{\geq 1}$,

$$E_k\begin{bmatrix}\phi\\\theta\end{bmatrix} = -\frac{B_k(\lambda)}{k!} + \frac{1}{(k-1)!}\sum_{r\geq 0}{}^{\prime}\frac{(r+\lambda)^{k-1}\theta^{-1}q^{r+\lambda}}{1-\theta^{-1}q^{r+\lambda}} + \frac{(-1)^k}{(k-1)!}\sum_{r\geq 1}\frac{(r-\lambda)^{k-1}\theta q^{r-\lambda}}{1-\theta q^{r-\lambda}}, \quad (A2)$$

where $e^{2\pi i\lambda} = \phi$, the prime in the first sum ignores the $r = 0$ term when $\phi = \theta = 1$. They enjoy the symmetry property

$$E_n \begin{bmatrix} \pm 1 \\ \theta^{-1} \end{bmatrix} = (-1)^n E_n \begin{bmatrix} \pm 1 \\ \theta \end{bmatrix} \Rightarrow E_{\text{odd}} \begin{bmatrix} \pm 1 \\ 1 \end{bmatrix} = 0. \tag{A3}$$

They are needed for modular differential equations in $\mathbb{R}$-graded VOAs. When $\phi = \theta = 1$, the twisted Eisenstein series with $k = 2n$ simply reduce to E_{2n}.

The modular differential operators $D_q^{(k\geq 1)}$ are defined as $\partial_{(2k-2)} \dots \partial_{(2)} \partial_{(0)}$ where $\partial_{(k)} \equiv q\partial_q + kE_2$ are the Serre derivatives that map modular forms to higher weight modular forms.

The Jacobi theta functions are defined, in terms of the q-Pochhammer symbol $(x;q) \equiv \prod_{k=0}^{+\infty}(1 - xq^k)$, by

$$\vartheta_1(z) \equiv -ie^{\pi i z} q^{\frac{1}{8}} (q;q)(e^{2\pi i z}q;q)(e^{-2\pi i z};q) \tag{A4}$$

$$\vartheta_4(z) \equiv (q;q)(e^{2\pi i z}q^{\frac{1}{2}};q)(e^{-2\pi i z}q^{\frac{1}{2}};q). \tag{A5}$$

APPENDIX B: FLAVORED MODULAR DIFFERENTIAL EQUATIONS

A VOA $\mathcal{V}$ is characterized by a space of states V (the vacuum module) and a state-operator correspondence Y that builds a local field $Y(a,z)$ out of any state $a \in V$ [48]. We will simply denote the field as $a(z) = \sum_{n\in\mathbb{Z}-h_a} a_n z^{-n-h_a}$ for a weight-h_a state. We also assume the existence and uniqueness of a vacuum state $\mathbf{1} \in V$, such that $Y(\mathbf{1},z) = \mathrm{id}_V$ and $a(0)\mathbf{1} = a$. For a state a with integer weight h_a, one defines its zero mode $o(a) = a_0$, whereas $o(a) = 0$ for nonintegral h_a.

To compute torus correlation functions, it is a common practice to consider $a[z] \equiv e^{izh_a} Y(a, e^{iz} - 1) = \sum_n a_{[n]} z^{-n-h_a}$ where the "square modes" $a_{[n]}$ are defined. Explicitly,

$$a_{[n]} = \sum_{j\geq n} c(j,n,h_a) a_j, \tag{B1}$$

where the coefficients c are defined by the series expansion

$$(1+z)^{h-1}[\log(1+z)]^n = \sum_{j\geq n} c(j,n,h) z^j. \tag{B2}$$

It is worth noting that $o(a_{[-h_a-n]}) = 0, \ \forall\, n \in \mathbb{N}_{\geq 1}$.

Recursion relations for unflavored torus correlation functions were first studied in [48], and later generalized to $\mathbb{R}$-graded super-VOAs [49] and flavored correlation functions [50]. They are the crucial tools for deriving flavored modular differential equations. Consider a $\frac{1}{2}\mathbb{Z}$-graded super-VOA $\mathbf{V}$ containing a $\hat{\mathfrak{u}}(1)$ current h with zero mode h_0, M a module of $\mathbf{V}$ and $a, b \in \mathbf{V}$ are two states of weights h_a, h_b. If $h_0 a = 0$, then [30,51]

$$\begin{aligned}
&\mathrm{str}_M o(a_{[-h_a]}b) x^{h_0} q^{L_0} \\
&\quad = \mathrm{str}_M o(a_{[-h_a]}\mathbf{1}) o(b) x^{J_0} q^{L_0} \\
&\qquad + \sum_{n=1}^{+\infty} E_{2k} \begin{bmatrix} e^{2\pi i h_a} \\ 1 \end{bmatrix} \mathrm{str}_M o(a_{[-h_a+2k]}b) x^{h_0} q^{L_0}.
\end{aligned} \tag{B3}$$

Recall that when a is a conformal descendant, $o(a_{[-h_a]}) = 0$. The first term plays crucial role when dimensionally reducing torus correlators to topological ones on a circle [52,53].

If a is charged with $h_0 a = Qa$, then [42,49]

$$\begin{aligned}
&\mathrm{str}_M o(a_{[-h_a]}b) x^{h_0} q^{L_0} \\
&\quad = \sum_{n=1}^{+\infty} E_n \begin{bmatrix} e^{2\pi i h_a} \\ x^Q \end{bmatrix} \mathrm{str}_M o(a_{[-h_a+n]}b) x^{h_0} q^{L_0}.
\end{aligned} \tag{B4}$$

Using these recursion relations, it is straightforward to write down the modular differential equations associated to the Sugawara relation [42]. Suppose that $\mathbf{V}$ contains an affine subalgebra $\hat{\mathfrak{g}}_k$ and $x^h \equiv x^{\lambda_I H^I} \equiv \prod_{I=1}^r x_I^{H^I}$. Recalling the standard commutation relations

$$[J^a_{[m]}, J^b_{[n]}] = i f^{ab}{}_c J^c_{[m+n]} + kmK^{ab}\delta_{m+n,0}, \tag{B5}$$

where K denotes the Killing form, we have

$$\begin{aligned}
&\mathrm{str}_M K_{ab} o(J^a_{[-1]} J^b_{[-1]}\mathbf{1}) x^h q^{L_0} \\
&\quad = \frac{r}{K(h,h)} \frac{d^2}{dx^2} \mathrm{str}_M x^h q^{L_0} \\
&\qquad + (\dim \mathfrak{g} - r) \sum_{\alpha>0} E_1 \begin{bmatrix} 1 \\ x^{\alpha(h)} \end{bmatrix} K_{IJ} \alpha^I x_J \frac{\partial}{\partial x_J} \mathrm{str}_M x^h q^{L_0} \\
&\qquad + k(\dim \mathfrak{g} - r) \sum_{\alpha>0} E_1 \begin{bmatrix} 1 \\ x^{\alpha(h)} \end{bmatrix} \mathrm{str}_M x^h q^{L_0} \\
&\qquad + kr\, E_2 \mathrm{str}_M x^h q^{L_0},
\end{aligned} \tag{B6}$$

where $\alpha > 0$ denotes all positive roots of $\mathfrak{g}$. For a VOA with a Sugawara relation, we rescale the above by the standard factor $\frac{1}{2(k+h^\vee)}$ and equate it with the torus one-point function $\langle T \rangle = q\partial_q \mathrm{str}_M x^h q^{L_0}$ of the stress tensor, establishing the flavored differential equation. In particular, when $\mathfrak{g} = \mathfrak{su}(2)$, the above reproduces (18) with the variable substitutions $x \to b$, $\mathrm{str}_M x^h q^{L_0 - \frac{c_{2d}}{24}} \to I$.

APPENDIX C: GREEN'S FUNCTIONS

The action (4) of the torus path integral (3) with nonzero $\mathfrak{a}_\varphi$ leads to twisted Green's function for the bc and $\beta\gamma$ ghosts, given by

$$G_{\beta\gamma}(z)^{\rho\rho'} = \frac{K^{\rho\rho'} e^{i\rho(\mathfrak{a}-\tau\mathfrak{a}_\varphi)\frac{z-\bar{z}}{\tau-\bar{\tau}}}}{\pi} \frac{\vartheta_1'(0|\tau)}{\vartheta_4(\rho(\mathfrak{a}-\tau\mathfrak{a}_\varphi)+\mathfrak{b}|\tau)} \times \frac{\vartheta_4(\frac{z}{2\pi}-\rho(\mathfrak{a}-\tau\mathfrak{a}_\varphi)-\mathfrak{b}|\tau)}{\vartheta_1(\frac{z}{2\pi}|\tau)}, \tag{C1}$$

and

$$G_{bc}(z)^{\rho\rho'} = -K^{\rho\rho'}\eta(\tau)^3 e^{i\rho(\mathfrak{a}-\tau\mathfrak{a}_\varphi)\frac{z-\bar{z}}{\tau-\bar{\tau}}} \times \frac{\vartheta_1(\frac{z}{2\pi}+\rho(\mathfrak{a}-\tau\mathfrak{a}_\varphi)|\tau)}{\vartheta_1(\frac{z}{2\pi}|\tau)\vartheta_1(\rho(\mathfrak{a}-\tau\mathfrak{a}_\varphi|\tau))}, \tag{C2}$$

where $\rho, \rho' = 0, \pm 2$ labels the generators of $\mathfrak{su}(2)$.

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