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Towards a Quantum Information Theory of Hadronization: Dihadron Fragmentation and Neutral Polarization in Heavy Baryons

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We pioneer the application of quantum information theory to experimentally distinguish between classes of hadronization models. We adapt the CHSH inequality to the fragmentation of a single parton to hadron pairs, a violation of which would rule out classical dynamics of hadronization altogether. Furthermore, we apply and extend the theory of quantum contextuality and local quantum systems to the neutral polarization of a single spin-1 hadronic system, namely the light constituents of excited Sigma baryons $\Sigma^*_{c,b}$ formed in the fragmentation of heavy quarks.

I. INTRODUCTION

Every single time that quarks and gluons are produced in particle collisions, they combine back into color-neutral bound states like the proton or the pion, collectively called hadrons. Calculating this nonperturbative, strongly coupled phenomenon called hadronization from first principles using the Lagrangian of Quantum Chromodynamics (QCD) remains an open problem, restricting us to phenomenological models. Perhaps surprisingly, and despite the underlying dynamics of quark and gluons clearly being quantum mechanical (QM) in general, classical stochastic models of hadronization [1–4] as e.g. implemented in multi-purpose Monte-Carlo (MC) generators [5–7] are vastly successful in this regard, notably for open, semi-inclusive hadronization observables. A macroscopic, statistical-mechanics approach especially succeeds in the large-multiplicity environment of heavy-ion collisions [8–11]. In this letter we aim to identify experimental measurement outcomes that indicate a departure from classical expectations and − if observed − can only be described by a full QM treatment of hadronization, see e.g. Refs. [12–15]. This, to the reader, will be a familiar task: Asking whether *local reality itself* is quantum in the form of Bell's inequality [16] lies at the root of today's rich field of quantum information (QI) theory. We will therefore adapt and extend QI concepts to hadronization physics to ask, broadly speaking: *Is hadronization quantum?*

Our proposal is part of a larger fruitful effort to bring QI theory to bear on questions in particle physics [17–44], but distinct in that most of the existing work, if not attempting to *explain* the Standard Model (SM) [45, 46], aims to probe quantum foundations either at the highest energy scales or in exclusive hadronic processes, essentially asserting the quantum nature of the perturbative SM Lagrangian or hadronic form factors, respectively. Hadronization then either serves as an analyzer for the perturbative density matrix [31, 42, 47] or, possibly, as a source of decoherence [48, 49] acting on the entangled state created during the perturbative scattering. By contrast, our proposal directly concerns the nature of hadronization itself, and we appeal to principles of effective field theory and factorization theorems to isolate the nonperturbative behavior under study from the (in our view, most likely quantum, and calculable) perturbative scattering and the self-analyzing hadronic decays. Our work is also distinct from proposals to *simulate* hadronization on quantum circuits [50–55].

II. CLASSICAL HADRONIZATION MODELS AS “HIDDEN” VARIABLES

In the picture we are developing, Bell's “hidden variables” λ take on concrete meaning as a point in the phase space of a stochastic hadronization model with an intermediate classical state $p(\lambda)$, i.e., a probability density. Of course, in this case the variables are not really hidden: In an analytic model, one may calculate their statistical distribution; if the model is implicitly defined by a stochastic algorithm, e.g. a Markov process acting on an ensemble of strings or preconfined clusters [3, 4, 56], one can print out and bin the intermediate state to record $p(\lambda)$. Just as in Bell's concise proof [57] of the Clauser-Horne-Shimony-Holt (CHSH) inequality [58], suitable correlation observables $\mathcal{C}$ will have an expectation value $\langle \mathcal{C} \rangle_{p(\lambda)} \leq \mathcal{C}_{\max}$ that is bounded when computed in *any* classical hadronization model, following basic properties of the integral measure in any number of classical phase-space dimensions, while QM expectation values can exceed the bound. Note that $p(\lambda)$ and the conditional measurement probabilities of classical hadronization models must obey the spacetime symmetries of QCD (Lorentz covariance and parity), a constraint that is typically absent in tests of quantum foundations, but which we will make productive use of in this letter.

To fix ideas, consider the fragmentation $i \to h_1 h_2 X$ of an unpolarized parton $i = q, g$ into identified hadrons $h_{1,2}$. If $h_{1,2}$ are spin-1/2 baryons, their most general spin-density matrix compatible with the symmetries of QCD reads

$$\rho = \frac{\mathbb{1}}{4} + \tilde{D}_{LL}\, \hat{S}_{1,L} \otimes \hat{S}_{2,L} + \tilde{D}_{TT}\, \hat{\mathbf{S}}_{1,T} \otimes \hat{\mathbf{S}}_{2,T}\,, \tag{1}$$

where $\hbar = 1$ and $\hat{S}_{j,L}$ ($\hat{\mathbf{S}}_{j,T}$) is the longitudinal (transverse) component of the spin operator of hadron h_j with respect to the fragmentation axis $\mathbf{z}$ pointing back to the hard collision in the hadron's rest frame. (In the last term, a contraction between vector indices is understood.) Eq. (1) is the polarization state of the system at long distances of order the hadron lifetimes, $t_{\text{decay}} \sim 1/\Gamma_h$, where a QM description of the system is appropriate for the exclusive hadronic decays.[1] By contrast, the nonperturbative hadronization physics are encoded in normalized dihadron fragmentation functions (DiFFs) [59–62] $\tilde{D}_{LL}$ [63] and $\tilde{D}_{TT}$, which are determined from experiments or computed in a model. In the latter case, we interpret the DiFFs as matching coefficients that are fixed by computing spin expectation values $T_{k\ell}/4 \equiv \langle S_{1,k} \otimes S_{2,\ell} \rangle$ in a (potentially classical) hadronization model at the scale $t_{\text{confine}} \sim 1/\Lambda_{\text{QCD}} \ll t_{\text{decay}}$ where the hadrons form and decouple. We also have $t_{\text{confine}} \gg t_{\text{hard}}$, where t_{hard} is the very short time scale of the perturbative hard scattering. This separation of all scales allows us to specifically probe the quantum nature of hadronization and, while abstract, mirrors the workflow of MC generators.

The DiFFs completely characterize the system, see Fig. 1: Positivity requires $\tilde{D}_{LL} \geq -1$ and $\tilde{D}_{LL} + 2|\tilde{D}_{TT}| \leq 1$. By the positive-partial-transpose (PPT) criterion [64], the hadrons are entangled if and only if $|\tilde{D}_{TT}| > (\tilde{D}_{LL} - 1)/2$. Most interestingly, we can evaluate the optimal [65] CHSH inequality [58] for Eq. (1) in terms of the DiFFs,

$$\tilde{D}_{TT}^2 + \max\{\tilde{D}_{LL}^2, \tilde{D}_{TT}^2\} \overset{p(\lambda)}{\leq} 1\,. \tag{2}$$

This is the key result for this example process, illustrating our proposal: If Eq. (2) is found to be violated in data, the observation cannot be explained by any classical hadronization model. The proof exactly follows Ref. [57], with one crucial difference: In our case, the "locality" assumption that measurements on h_1 are independent of the reconstruction of h_2 is guaranteed by color confinement, rather than by hypothesizing, like Bell, a local hidden-variable theory (LHVT) of Nature. The CHSH test we propose here therefore does not test quantum nonlocality in the usual way, but instead *uses the identical mathematics* to test whether the blackbox Hamiltonian of hadronization admits a classical description.[2]

III. QUANTUM CONTEXTUALITY AND LOCAL SPIN-1 SYSTEMS

A fundamental aspect of QM systems is their (statistical) *contextuality* [68], the idea that a measurement's outcome may depend on which other properties are being measured. To adapt the notion of statistical contextuality to classical hadronization models, consider a very simple hadronizing system: the production of excited heavy spin-3/2 baryons Σ_Q^* during the fragmentation $Q \to \Sigma_Q^* X$ of beauty or charm quarks, $Q = b, c$. The light hadron constituents that bind to the static heavy quark carry total angular momentum $j = 1$, forming a qutrit. By parity and rotational invariance about the fragmentation axis $\mathbf{z}$, their quantum polarization state ρ at $t_{\text{decay}} \sim 1/\Gamma_{\Sigma_Q^*} \gg t_{\text{confine}}$ is governed by a single nonperturbative Falk-Peskin parameter w_1 [69],

$$\rho = \frac{w_1}{2}\big(|1_z\rangle\langle 1_z| + |{-1}_z\rangle\langle -1_z|\big) + \big(1 - w_1\big)|0_z\rangle\langle 0_z|\,, \tag{3}$$

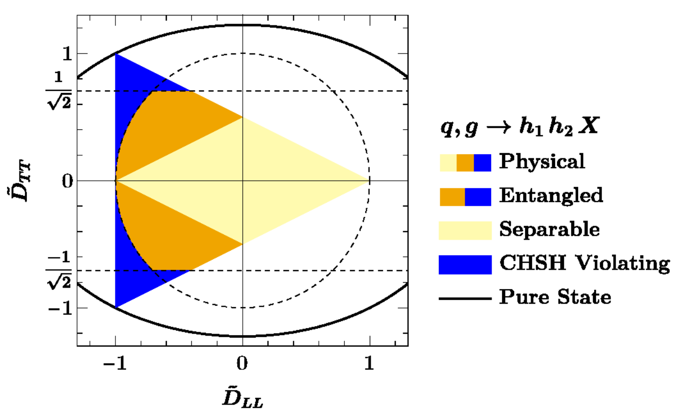

FIG. 1. QI characterization of parton fragmentation to two nearby polarized hadrons. An observation of dihadron fragmentation functions taking values in the blue region is inconsistent with classical models of hadronization. For $\tilde{D}_{LL} = -1$ and $\tilde{D}_{TT} = -1$ (+1), the hadrons are produced in a pure singlet (triplet) Bell state.

[1] Decay matrix elements and differential distributions are collected in the supplemental material.

[2] Another assumption is that Gedanken measurements $\langle (\boldsymbol{e}_\alpha \cdot \boldsymbol{S}_1) \otimes (\boldsymbol{S}_2 \cdot \boldsymbol{e}_\beta) \rangle$ at Bell angles α, β are indeed predicted to evaluate to $\boldsymbol{e}_\alpha \cdot (\mathsf{T}/4) \cdot \boldsymbol{e}_\beta$, where $\mathsf{T} = (T_{k\ell})$. In our case, this property is inherited from the interpolating partonic spin operators defined in the underlying QCD theory. Therefore, the counterexamples of Refs. [66, 67] (*nota bene* constructed to argue against the viability of testing LHVTs *of Nature* at colliders) do not apply.

where the $|m_z\rangle$ are the eigenstates of $\hat{J}_z$. In a classical hadronization model at $t_{\rm confine} \ll t_{\rm decay}$ with intermediate state $p(\lambda)$, the probability of measuring the squared angular momentum $J_e^2 = (\boldsymbol{e}\cdot\boldsymbol{J})^2$ along a unit vector $\boldsymbol{e}$ to be $x \in \{0,1\}$ reads

$$P(x|\boldsymbol{e}) = \int \mathrm{d}\lambda\, p(\lambda)\, P(x|\lambda,\boldsymbol{e})\,, \quad \langle J_e^2\rangle = P(1|\boldsymbol{e}) \qquad (4)$$

and is subject to the constraint $\langle \boldsymbol{J}^2\rangle = 2$ inherited from the interpolating partonic spin operator, i.e., $\langle J_a^2 + J_b^2 + J_c^2\rangle = 2$ for any orthonormal triad $\{\boldsymbol{a},\boldsymbol{b},\boldsymbol{c}\}$. By Gleason's theorem [68, 70], parity, and Lorentz covariance, $P(1|\boldsymbol{e})$ uniquely coincides with the single-parameter form of $\langle J_e^2\rangle$ as computed from Eq. (3) for any $\boldsymbol{e}$. All single-point spin measurements are thus determined by $P(1|\boldsymbol{z}) = \langle J_z^2\rangle = w_1$, which again serves as a matching coefficient connecting the classical (or quantum-mechanical) model at $t_{\rm confine}$ to the quantum state at $t_{\rm decay}$.

In this context, *noncontextuality* of a hadronization model is the statement that in addition to Eq. (4), the model predicts certain joint probabilities

$$P(x_1,\ldots,x_N|\boldsymbol{e}_1,\ldots,\boldsymbol{e}_N) \qquad (5)$$

through a joint conditional measurement probability at given λ. Of particular interest are $\{\boldsymbol{e}_i\}$ arranged in connected Kochen-Specker (KS) graphs [73] where $\boldsymbol{e}_i \perp \boldsymbol{e}_j$ for all edges in the graph. The first nontrivial case of a simple cyclic graph is the Klyachko-Can-Binicioglu-Shumovsky (KCBS) configuration $\bigstar = \{\boldsymbol{e}_i\}$ [74] of $N = 5$ unit vectors $\boldsymbol{e}_i \perp \boldsymbol{e}_{i+1 \bmod 5}$ arranged around a symmetry axis $\boldsymbol{r} = \boldsymbol{z}$, i.e., they form a regular pentagram in the plane of fixed $\boldsymbol{r}\cdot\boldsymbol{e}_i = 1/\sqrt[4]{5}$. Crucially, even though the additional measurements in Eq. (5) are counterfactual in our case, the *existence* of the joint distribution does leave an imprint on experimentally observable distributions. This is the statement of the KCBS inequality [74], which in the general case constrains the sum of two-point correlations. Using $\langle \boldsymbol{J}^2\rangle = 2$, one readily shows (also in the classical case) that Eq. (5) exists for $\bigstar$ if and only if the single-point marginal probabilities satisfy $\sum_{\boldsymbol{e}\in\bigstar} P(1|\boldsymbol{e}) = \sum_{\boldsymbol{e}\in\bigstar}\langle J_e^2\rangle \geq 3$. Importantly, these latter single-point measurements *are* accessible experimentally and determined by w_1. We thus find a KCBS bound for the Falk-Peskin parameter, see Fig. 2,

$$w_1 \geq w_1^\bigstar \equiv \frac{1}{2} - \frac{1}{2\sqrt{5}} \approx 0.276393\,, \qquad (6)$$

which is satisfied if and only if Eq. (5) exists for $\bigstar$. We have verified that the constraint from $\bigstar$ with $N = 5$ is the strongest constraint on w_1 from any simple N-cycle symmetric around $\boldsymbol{z}$. (In practice, we also choose $\boldsymbol{r}$ such that $\sum_{e\in\bigstar}\langle J_e^2\rangle$ is minimized.)

It is important to realize that classical models do not have to be noncontextual, cf. Eq. (7). Instead, the degree of contextuality is a property of the hadronization model that can be assessed by inspecting its dynamics and coupling to the final-state hadron spin. (The intuition of the KCBS-noncontextual limit being "more classical" is valuable nevertheless, cf. the case of a thermal system at high temperatures, where classical and quantum dynamics become indistinguishable and isotropic, $w_1 \to 2/3 > w_1^\bigstar$.) Conversely, the degree to which hadronization models can be coupled to hadron spin in a noncontextual way has fundamental limits. The tightest such constraint for $j = 1$ arises from the Yu-Oh configuration [75], a KS graph with $N = 13$ containing several cycles, whose associated state-independent noncontextuality inequality when combined with $\langle \boldsymbol{J}^2\rangle = 2$ rules out the existence of Eq. (5) for this case altogether.

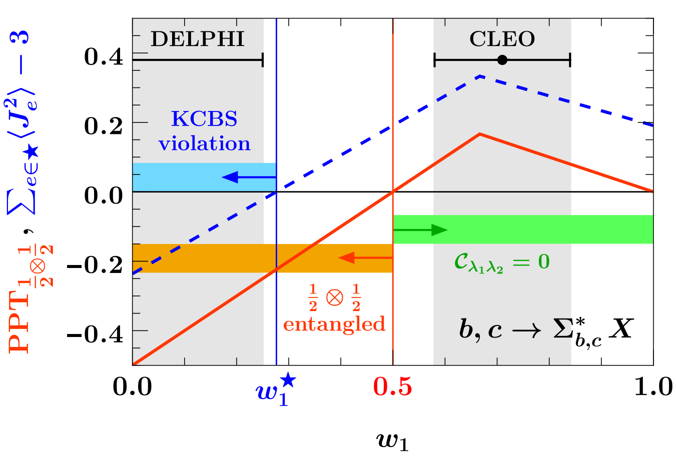

FIG. 2. QI characterization of the Falk-Peskin parameter w_1 for $Q \to \Sigma_Q^* X$ in terms of the KCBS inequality (blue), entanglement in a bipartite QM fragmentation model (orange), and classical correlation strength in a stochastic model (green). Experimental data are from Refs. [71, 72],

IV. CLASSICAL CORRELATION STRENGTH

To explore further interpretations of w_1, consider the "hidden" state of a classical hadronization model that simply consists of a unit vector $\boldsymbol{\lambda}$ in the hadron rest frame. Evaluating $P(1|\boldsymbol{z})$ in this model, we find

$$w_1 = \frac{2}{3} + r\,\Delta_2\,, \quad \Delta_2 \equiv \int \mathrm{d}c_\theta\, p(c_\theta)\left(c_\theta^2 - \frac{1}{3}\right), \qquad (7)$$

where $c_\theta \equiv \boldsymbol{z}\cdot\boldsymbol{\lambda}$ and r is a free parameter governing the strength of the coupling between J_e^2 and $\boldsymbol{\lambda}$ in the Lorentz-invariant conditional measurement probability $P(1|\boldsymbol{\lambda},\boldsymbol{e}) = 2/3 + r[(\boldsymbol{e}\cdot\boldsymbol{\lambda})^2 - 1/3]$. Since $0 \leq P(1|\boldsymbol{\lambda},\boldsymbol{e}) \leq 1$, we have $-1 \leq r \leq \frac{1}{2}$. If $\boldsymbol{\lambda}$ indicates e.g. the average orientation of classical diquark angular momenta near the heavy quark, one physically expects a positive coupling $r > 0$ to the observed angular momentum, in which case $w_1 \geq 1/2$ since $\Delta_2 \geq -1/3$, exhibiting KCBS noncontextuality. However, nothing a priori forbids $r < 0$. Since

$\Delta_2 \leq 2/3$, we can have $w_1 \to 0$ in the extreme limit $r \to -1$ and $p(c_\theta) \to \delta(|c_\theta| - 1)/2$. This is of interest as an example of a classical model that achieves maximal KCBS violation, and thus must be contextual.

Another important insight from this limit is that w_1 measures the degree of *classical* correlation *within* the model. To make this explicit, consider a bipartite classical model consisting of two unit vectors $\{\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2\}$ that couple to the hadron spin through $\boldsymbol{\lambda} = (\boldsymbol{\lambda}_1 + \boldsymbol{\lambda}_2)/|\boldsymbol{\lambda}_1 + \boldsymbol{\lambda}_2|$. In this case we can prove a general bound $w_1 \geq (1 - |\mathcal{C}_{\lambda_1\lambda_2}|)/2$, see Fig. 2, where

$$\mathcal{C}_{\lambda_1\lambda_2} \equiv \left\langle \frac{2\lambda_{1z}\lambda_{2z} - \boldsymbol{\lambda}_1 \cdot \boldsymbol{\lambda}_2 \, (\lambda_{1z}^2 + \lambda_{2z}^2)}{1 - (\boldsymbol{\lambda}_1 \cdot \boldsymbol{\lambda}_2)^2} \right\rangle \leq 1 \,, \tag{8}$$

is a nonlinear correlation coefficient that vanishes e.g. if $\boldsymbol{\lambda}_{1,2}$ are independent, $p(\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2) = p(\boldsymbol{\lambda}_1)\, p(\boldsymbol{\lambda}_2)$. Alternatively, we can bound w_1 for $r < 0$ by linear correlations, leading to

$$w_1 \geq \min\Big\{ \langle \boldsymbol{\lambda}_{1T} \cdot \boldsymbol{\lambda}_{2T} \rangle, \, \frac{2}{3} \Big\} \,, \tag{9}$$

where $\boldsymbol{\lambda}_{iT}$ are the components of $\boldsymbol{\lambda}_i$ transverse to $\boldsymbol{z}$.

V. BIPARTITE QM MODELS AND FACTORIZATION

We conclude our analysis of Eq. (3) by interpreting it in a simple QM model of hadronization where the hadron is formed from the heavy quark and two light spin-1/2 degrees of freedom, which we can e.g. think of as constituent quarks. In this case it is interesting to ask whether the state of the light system is entangled or separable when the hadron is formed. To assess this, we convert Eq. (3) to a two-qubit density matrix (noting that the singlet state, which would correspond to the Λ_Q baryon, is not populated at this binding energy), and again evaluate the PPT criterion [64]. The result for the lowest eigenvalue of the partial transpose is shown in red in Fig. 2: As expected, an overlap of $\mathrm{Tr}[\rho\, |0_z\rangle\langle 0_z|] = 1 - w_1 > 1/2$ with $|0_z\rangle$, which acquires an interpretation as a triplet Bell state in this model, implies entanglement (and eventually leads to KCBS violation [74]).

Importantly, an observation of entanglement at $w_1 < 1/2$ would imply that no factorization can exist (in the technical sense of the word in high-energy physics) in terms of any spin-1/2 degrees of freedom at cross-section level. To see this, compare to the prototypical factorization of the hadronic tensor for the Drell-Yan process at leading-power,

$$W_{\mathrm{DY}}^{\mu\nu} \sim \mathrm{tr}[\gamma^\mu \Phi_q \gamma^\nu \Phi_{\bar{q}}] \,, \tag{10}$$

where $\Phi_{q,\bar{q}}$ are (anti)quark correlation functions of the (possibly polarized) incoming protons, tr denotes a trace over Dirac indices, and μ, ν encode the polarization of the virtual photon. Eq. (10) is manifestly separable with respect to the product $\mathcal{H}_q \otimes \mathcal{H}_{\bar{q}}$ of the (anti)quark Hilbert spaces. Conversely, the neutral polarization state $\frac{1}{\sqrt{2}}\big(|{\uparrow_q\downarrow_{\bar{q}}}\rangle + |{\downarrow_q\uparrow_{\bar{q}}}\rangle\big)$, which is maximally entangled, cannot have large overlap with Eq. (10), and indeed it is well known [76–83] that neutral photon polarization requires an additional spin-1 degree of freedom (and thus subleading-power factorization). The above argument provides a novel perspective on this fact from QI theory.

VI. TMD HEAVY-QUARK FRAGMENTATION

It is experimentally possible [72] that inclusive fragmentation $Q \to \Sigma_Q^* X$ in fact produces an isotropic spin state with $w_1 \approx 2/3$. It is interesting to ask, therefore, whether breaking the azimuthal symmetry by measuring a *transverse* momentum $\boldsymbol{k}_T \perp \boldsymbol{z}$ provides access to richer spin-1 dynamics. Here the transverse momentum-dependent (TMD) observable $\boldsymbol{k}_T \gtrsim \Lambda_{\mathrm{QCD}}$, may e.g. be (a) the recoil of the heavy hadron pair in $e^+e^- \to \Sigma_Q^* H_{\bar{Q}} X$ [84–87], (b) the hadron transverse momentum relative to a jet containing it [87–89], or (c) the transverse momentum of an additional fragmentation pion [87, 90]. In any of these cases, the most general light angular momentum state compatible with the symmetries reads [87]

$$\begin{aligned}\rho = \frac{\mathbb{1}}{3} - \tfrac{1}{2}\hat{J}_y\, w^{(1,1)}(k_T) + \big(\tfrac{3}{2}\hat{J}_z^2 - \mathbb{1}\big)\, w^{(2,0)}(k_T) \\ + \big(\hat{J}_x\hat{J}_z + \hat{J}_z\hat{J}_x\big)\, w^{(2,1)}(k_T) + \big(\hat{J}_x^2 - \hat{J}_y^2\big)\, w^{(2,2)}(k_T) \,,\end{aligned} \tag{11}$$

where $k_T = |\boldsymbol{k}_T|$, $\boldsymbol{x} = \boldsymbol{k}_T/k_T$, $\boldsymbol{y} = \boldsymbol{z} \times \boldsymbol{x}$, and the $w^{(N,n)}$ are the nonperturbative coefficients.

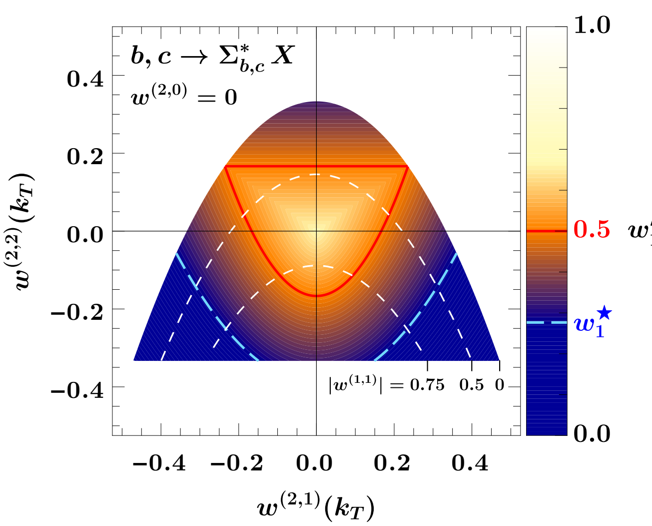

FIG. 3. QI characterization of $Q \to \Sigma_Q^* X$ with a TMD measurement. The heatmap indicates the effective longitudinal polarization w_1'. The bounds at 1/2 and $w_1^\star$ relevant for its QI interpretation are to be compared to Fig. 2.

Our previous discussion elegantly carries over if we define

$$w_1' \equiv \langle J_{z'}^2 \rangle \equiv \min_{\boldsymbol{e}} \langle J_e^2 \rangle = \min_{\boldsymbol{e}} \mathrm{Tr}\big[\rho\, \hat{J}_e^2\big]\,, \tag{12}$$

i.e., by finding the axis $\boldsymbol{z'}$ that maximizes the neutral polarization rate $1 - w_1'$. A rotation from $\boldsymbol{z}$ to $\boldsymbol{z'}$ in fact diagonalizes ρ with eigenvectors $|m_{z'}\rangle$, so we can think of $\boldsymbol{z'}$ as a novel polarization axis that is *spontaneously generated* by the fragmentation dynamics. Here we can make immediate use of $\boldsymbol{z'}$ by repeating our previous QI analysis for w_1', as shown in Fig. 3, where $w^{(2,0)} = 0$ corresponds to $w_1 = 2/3$ after integrating over $\boldsymbol{k}_T$. The value of w_1' is driven by $w^{(2,1)}$ and $w^{(2,2)}$, and even for $w_1 = 2/3$ we find physical regions in their parameter space with nontrivial QI interpretations $w_1' < 1/2$ or $w_1' < w_1^\bigstar$, respectively. (Increasing $w^{(1,1)}$ shrinks the physical region, but leaves w_1' unchanged.) Notably, their scaling for $k_T \gg \Lambda_{\mathrm{QCD}}$ is model-independently predicted to be $w^{(N,n)}(k_T) \sim (\Lambda_{\mathrm{QCD}}/k_T)^n$ [87]. Therefore if heavy-quark fragmentation indeed exhibits “quantum” behavior at $k_T \sim \Lambda_{\mathrm{QCD}}$ as in Fig. 3, there would be the exciting possibility to observe a quantum-to-classical transition as k_T increases.

VII. CONCLUSIONS AND OUTLOOK

In this letter we have initiated the study of applying tools from quantum information (QI) theory to the open problem of hadronization to distinguish between entire classes of classical or quantum-mechanical hadronization models at once. In Eq. (2), we have presented an inequality for light dihadron fragmentation that, if violated in data, would rule out classical hadronization dynamics altogether. We stress that our goal was not to test quantum foundations themselves: Rather, we adapted tools from QI theory to characterize the dynamics of the blackbox Hamiltonian of hadronization, and appealed to effective field theory to separate it from other (very likely quantum) dynamics in the problem. We then adapted the concept of contextuality to the study of hadronization, showcased our ideas using the Falk-Peskin fragmentation parameter w_1 in heavy baryon production, and further interpreted w_1 in terms of classical correlation strength and QM entanglement, with implications for factorizability. Incorporating these insights will impose practical constraints on future hadronization modeling and enable cross-pollination with ongoing QI research.

The experimental status of w_1 is unclear at present, see Fig. 2. Combining $\Sigma_b^{*\pm}$ baryons, DELPHI measured [71]

$$w_1^{\mathrm{DELPHI}} = -0.36 \pm 0.30_{\mathrm{stat}} \pm 0.30_{\mathrm{syst}}\,, \tag{13}$$

which translates to a 95% CL limit of $w_1 \leq 0.25$ after imposing positivity. On the other hand, by combining Σ_c^{*++} and Σ_c^{*0} baryons (that have the identical light valence content and relative rates), CLEO found [72],

$$w_1^{\mathrm{CLEO}} = 0.71 \pm 0.13\,, \tag{14}$$

close to the isotropic limit $w_1 = 2/3$. This disagreement has, to our knowledge, not been resolved [91]. We therefore strongly encourage a new measurement of w_1 using state-of-the-art experimental techniques. We also encourage experimental tests of spin correlations in nearby dihadrons and of the TMD generalizations of w_1 that we introduced, all of which possess deep physical interpretations within the new QI framework of hadronization that we have presented here.

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SUPPLEMENTAL MATERIAL

In this supplemental material we collect explicit expressions for the differential distributions of decay products stemming from the self-analyzing decays of the polarized hadron systems discussed in the main text. These expressions involve the nonperturbative fragmentation coefficients relevant for the analysis in the main text as free parameters, and allow for their experimental determination by fitting them to the observed distributions.

A. Fragmentation to nearby dihadrons

1. Factorization and general structure

Consider the cross section for producing a dihadron pair with general spin $s_{1,2}$ and magnetic quantum numbers $-s_1 \leq m_1, m_1' \leq s_1$ and $-s_2 \leq m_2, m_2' \leq s_2$ with respect to the fragmentation axis $\mathbf{z}$. (In the collinear approximation, the two hadron rest frames only differ by a boost along the $\mathbf{z}$ direction, such that its orientation is common.) We decompose the cross section for an arbitrary spin state in terms of operators $\hat{\mathcal{O}}$ on the product Hilbert space as

$$\frac{\mathrm{d}\sigma_{m_1 m_1', m_2 m_2'}}{\mathrm{d}z_1\, \mathrm{d}z_2\, \mathrm{d}R_T} = \sum_{\mathcal{O}} \frac{\mathrm{d}\sigma_{\mathcal{O}}}{\mathrm{d}z_1\, \mathrm{d}z_2\, \mathrm{d}R_T}\, \mathcal{O}_{m_1 m_1', m_2 m_2'}\,, \tag{S1}$$

where $\mathcal{O}_{m_1 m_1', m_2 m_2'} = \langle m_1 m_2 | \hat{\mathcal{O}} | m_1' m_2' \rangle$ and z_1, z_2 are the longitudinal momentum fractions of hadrons h_1 and h_2, respectively. Here, R_T is the magnitude of the transverse component of the difference of hadron momenta relative to their sum. For pairs of spin-1/2 baryons we have

$$\{\mathcal{O}\} = \left\{ \frac{\mathbb{1}}{4},\, \hat{S}_{1,L} \otimes \hat{S}_{2,L},\, \hat{\mathbf{S}}_{1,T} \otimes \hat{\mathbf{S}}_{2,T} \right\}. \tag{S2}$$

as in Eq. (1), where the coefficients $\mathrm{d}\sigma_{\mathcal{O}}$ are also denoted by $\mathrm{d}\sigma$ (without subscript), $\mathrm{d}\sigma_{LL}$, and $\mathrm{d}\sigma_{TT}$, respectively. They are given in terms of dihadron fragmentation functions $D^{\mathcal{O}}_{i \to h_1 h_2}$ as [59–63]

$$\frac{\mathrm{d}\sigma_{\mathcal{O}}}{\mathrm{d}z_1\, \mathrm{d}z_2\, \mathrm{d}R_T} = \sum_i \int \mathrm{d}y\, C_i(y, \mu)\, D^{\mathcal{O}}_{i \to h_1 h_2}\left(\frac{z_1}{y}, \frac{z_2}{y}, R_T, \mu \right), \tag{S3}$$

where C_i are the usual single-inclusive partonic hard coefficients. (In the case of hadronic collisions, they also contain the parton distribution functions.) Additionally, C_i can include fiducial acceptance cuts on the overall direction of the near-collimated dihadron system; cuts on individual hadron energies or momenta are special cases of the bins we consider below.

We are interested in the yield $N_{\mathcal{O}}$ of dihadron pairs produced in a specific spin state $\mathcal{O}$ and bin of (z_1, z_2), which is proportional to

$$\begin{aligned} \frac{N_{\mathcal{O}}}{\mathcal{L}} = \sigma_{\mathcal{O}} &\equiv \int \mathrm{d}z_1\, \mathrm{d}z_2 \int_0^{R_T^{\mathrm{cut}}} \mathrm{d}R_T\, \frac{\mathrm{d}\sigma_{\mathcal{O}}}{\mathrm{d}z_1\, \mathrm{d}z_2\, \mathrm{d}R_T}\, \Theta(z_1, z_2) \\ &= \sum_i \int \mathrm{d}y\, \mathrm{d}x_1\, \mathrm{d}x_2\, C_i(y, \mu)\, \Theta(y x_1, y x_2) \int_0^{R_T^{\mathrm{cut}}} \mathrm{d}R_T\, D^{\mathcal{O}}_{i \to h_1 h_2}(x_1, x_2, R_T, \mu)\,, \end{aligned} \tag{S4}$$

where $\Theta(z_1, z_2)$ implements the given bin and the normalization factor $\mathcal{L}$ is the total luminosity. By placing an upper cutoff $R_T^{\mathrm{cut}} \sim \Lambda_{\mathrm{QCD}}$ on the relative transverse momentum, we ensure that spin correlations are genuinely sourced by the nonperturbative fragmentation dynamics. The total yield N is given by the $N_{\mathcal{O}}$ with $\mathcal{O} = \mathbb{1}/\operatorname{Tr}[\mathbb{1}]$ the identity on the product Hilbert space. The normalized density matrix of the hadron pair then reads

$$\rho = \frac{1}{N} \sum_{\mathcal{O}} N_{\mathcal{O}}\, \mathcal{O}\,. \tag{S5}$$

For spin-1/2 baryons this results in Eq. (1) if we define the shorthands

$$\tilde{D}_{LL} = \frac{\sigma_{LL}}{\sigma} = \frac{\sum_i \int \mathrm{d}y\, \mathrm{d}x_1\, \mathrm{d}x_2\, C_i(y, \mu)\, \Theta(y x_1, y x_2) \int_0^{R_T^{\mathrm{cut}}} \mathrm{d}R_T\, D^{LL}_{i \to h_1 h_2}(x_1, x_2, R_T, \mu)}{\sum_i \int \mathrm{d}y\, \mathrm{d}x_1\, \mathrm{d}x_2 C_i(y, \mu)\, \Theta(y x_1, y x_2) \int_0^{R_T^{\mathrm{cut}}} \mathrm{d}R_T\, D_{i \to h_1 h_2}(x_1, x_2, R_T, \mu)}\,, \tag{S6}$$

and similarly for $\tilde{D}_{TT}$. We stress that even though the DiFFs enter in a convolution with the perturbative scattering coefficient in this form, the strength of the spin correlation is still uniquely sourced at the low scale, since the DGLAP evolution and the perturbative corrections are all common. In particular, using the leading-order perturbative result for the coefficient $C_i(y,\mu) \propto \delta(1-y) + \mathcal{O}(\alpha_s)$, Eq. (S6) indeed reduces to a ratio of the (binned) DiFFs themselves.

We point out that while the expression for $\tilde{D}_{LL}$ in Eq. (S6) is clearly the most amenable to experimental tests of Eq. (2) in the near future, since it directly relates to the measured cross section at a given collider, we believe it would be valuable in the long run to test Eq. (2) directly at the level of the process and collider-independent ratio

$$\tilde{D}_{LL,i}(x_1,x_2,R_T^{\mathrm{cut}}) \equiv \frac{\int_0^{R_T^{\mathrm{cut}}} \mathrm{d}R_T\, D^{LL}_{i\to h_1h_2}(x_1,x_2,R_T,\mu)}{\int_0^{R_T^{\mathrm{cut}}} \mathrm{d}R_T\, D_{i\to h_1h_2}(x_1,x_2,R_T,\mu)}\,, \tag{S7}$$

with $\tilde{D}_{TT,i}$ again defined in full analogy, where the right-hand side is evaluated at some low input scale $\mu \sim 2\,\mathrm{GeV}$. (In a more sophisticated setup, one may also define $\tilde{D}_{LL}$ and $\tilde{D}_{TT}$ as ratios of Mellin moments of the singlet and gluon or valence DiFFs to form exact renormalization-group invariants.) Eq. (2) equally well applies to $\tilde{D}_{LL,i}$ and $\tilde{D}_{TT,i}$ when defined as in Eq. (S7), where the normalized density matrix is now directly computed in terms of the renormalized fragmentation correlator for given hadron-hadron spin state at the low scale. Using Eq. (S7) in practice requires one to first determine the underlying DiFFs from a global fit to the available collider data for the yields $N_{\mathcal{O}}$ extracted from decay distributions in many different bins. Nevertheless, we believe this would be worth the effort it entails, since one would gain access to the degree of CHSH violation also as a function of e.g. the parton type.

2. *Decay distribution for nearby hyperon pairs*

Differential distributions for the decay products of the hadrons are obtained by tracing Eq. (1) against the (conjugate) decay matrix elements for given hadron helicities $m_{1,2}$ ($m'_{1,2}$), which are specific to each hadron and decay. Here we consider the parity-violating weak decay of hyperons, a standard example of a self-analyzing decay commonly used for reconstructing (transverse) hadron polarization, see e.g. Refs. [18, 34, 48, 96–99].

To fix conventions we begin with the decay of a single, individually polarized (anti)hyperon

$$h_1 = \Lambda \to p\,\pi^-\,, \qquad h_2 = \bar{\Lambda} \to \bar{p}\,\pi^+\,. \tag{S8}$$

The associated decay distributions are standard [100] and read

$$\frac{1}{N}\frac{\mathrm{d}N}{\mathrm{d}\cos\theta_p\,\mathrm{d}\varphi_p} = \frac{1}{4\pi}\big[1 + \alpha_-\,\boldsymbol{P}\cdot\boldsymbol{n}_p\big]\,, \qquad \frac{1}{N}\frac{\mathrm{d}N}{\mathrm{d}\cos\theta_{\bar{p}}\,\mathrm{d}\varphi_{\bar{p}}} = \frac{1}{4\pi}\big[1 + \alpha_+\,\boldsymbol{P}\cdot\boldsymbol{n}_{\bar{p}}\big]\,, \tag{S9}$$

where $\boldsymbol{P} = 2\langle\hat{\boldsymbol{S}}\rangle$ with $|\boldsymbol{P}| \le 1$ is the Bloch vector of the (anti)hyperon, $\boldsymbol{n_p}$ ($\boldsymbol{n_{\bar{p}}}$) is a unit vector pointing in the direction of the (anti)proton in the rest frame of the parent particle, θ_p and φ_p ($\theta_{\bar{p}}$ and $\varphi_{\bar{p}}$) are the polar coordinates of $\boldsymbol{n_p}$ ($\boldsymbol{n_{\bar{p}}}$) in the respective rest frame, and $\alpha_\mp$ are the hyperon decay parameters. With the above common sign for $\alpha_\pm$ for hyperon and antihyperon, one has opposite signs for $\alpha_- = 0.732 \pm 0.014$ and $\alpha_+ = -0.758 \pm 0.012$ [100] (and thus $\alpha_-\alpha_+ < 0$), as required by the approximate CP symmetry.

For the system in Eq. (1), each individual hyperon is indeed unpolarized on average, $\boldsymbol{P} = 0$, such that the distributions $\mathrm{d}N/(\mathrm{d}\cos\theta_p\,\mathrm{d}\varphi_p)$ and $\mathrm{d}N/(\mathrm{d}\cos\theta_{\bar{p}}\,\mathrm{d}\varphi_{\bar{p}})$ are flat. Nevertheless, the spin correlations encoded in Eq. (1) can be readily observed from the joint distribution of their decay products,

$$\begin{aligned}\frac{1}{N}\frac{\mathrm{d}N}{\mathrm{d}\cos\theta_p\,\mathrm{d}\varphi_p\,\mathrm{d}\cos\theta_{\bar{p}}\,\mathrm{d}\varphi_{\bar{p}}} &= \frac{1}{(4\pi)^2}\big[1 + \alpha_-\alpha_+\,\boldsymbol{n}_p\cdot\mathsf{T}\cdot\boldsymbol{n}_{\bar{p}}\big] \\ &= \frac{1}{(4\pi)^2}\big[1 + \alpha_-\alpha_+\,\tilde{D}_{LL}\,\cos\theta_p\,\cos\theta_{\bar{p}} + \alpha_-\alpha_+\,\tilde{D}_{TT}\,\sin\theta_p\,\sin\theta_{\bar{p}}\cos(\varphi_p-\varphi_{\bar{p}})\big]\,,\end{aligned} \tag{S10}$$

where the rank-two tensor $\mathsf{T} = (T_{jk})$ has components $T_{jk}/4 = \langle S_{1,j}\otimes S_{2,k}\rangle$.

B. Inclusive fragmentation to excited heavy baryons

The factorization theorem for the production of a boosted polarized heavy hadron H containing a heavy quark of mass m_Q at strict leading power in $\Lambda_{\rm QCD}/m_Q$ is simply a product [69, 101, 102]

$$\frac{\mathrm{d}\sigma_{HX}^{\mathcal{O}_\ell}}{\mathrm{d}^3\boldsymbol{P}_H} = \frac{\mathrm{d}\sigma_{QX}}{\mathrm{d}^3\boldsymbol{P}_Q}\,\chi_{H,\mathcal{O}_\ell}\Big[1+\mathcal{O}\Big(\frac{\Lambda_{\rm QCD}}{m_Q}\Big)+\mathcal{O}\Big(\frac{m_Q}{|\boldsymbol{P}_H|}\Big)\Big]\,. \tag{S11}$$

The matching coefficient $\mathrm{d}\sigma_{QX}$ is the differential cross section for producing a free unpolarized heavy quark at the same three-momentum in the center-of-mass frame of the collision, $\boldsymbol{P}_Q = \boldsymbol{P}_H$. The nonperturbative dynamics are contained in the fragmentation coefficient $\chi_{H,\mathcal{O}_\ell}$. Note that for hadron colliders, the second set of power corrections in Eq. (S11) scales as $m_Q/|\boldsymbol{P}_T|$ instead, where $\boldsymbol{P}_T$ is the transverse momentum relative to the beam axis. As before, $\mathcal{O}_\ell$ labels a spin operator encoding a generic spin state, in this case for the total angular momentum of the light constituents ℓ of H. The total probability χ_H for Q to fragment into H, which is the coefficient $\chi_{H,\mathcal{O}}$ of $\mathcal{O} = \mathbb{1}_\ell/\operatorname{Tr}[\mathbb{1}_\ell]$, satisfies $\sum_H \chi_H = 1$. Given the multiplicative form of Eq. (S11), cuts acting on the heavy hadron kinematics simply act on the heavy-quark production cross section. Thus, unlike the light dihadron case, no convolution is required to compute the total yields for each spin state. Instead, we have

$$\rho = \frac{1}{N}\sum_{\mathcal{O}_\ell} N_{\mathcal{O}_\ell}\,\mathcal{O}_\ell = \frac{1}{\chi_H}\sum_{\mathcal{O}_\ell}\chi_{H,\mathcal{O}_\ell}\,\mathcal{O}_\ell\,, \tag{S12}$$

i.e., the normalized spin density matrix of the light constituents in any given bin of the heavy-hadron kinematics is directly given by ratios of the nonperturbative coefficients. The normalized coefficients $\chi_{H,\mathcal{O}_\ell}/\chi_H$ for a light state with angular momentum $j = 1$ or $j = 3/2$ are in direct correspondence to the usual Falk-Peskin parameters w_j. Specifically, for the set of operators $\{\mathcal{O}_\ell\} = \{\frac{\mathbb{1}}{4},\, \hat{J}_z^2\}$ allowed by the symmetries in the case $j = 1$, one readily converts the coefficients to the form involving w_1 in Eq. (3) using $\hat{J}_z^2 = \mathbb{1} - |0_z\rangle\langle 0_z|$.

Experimentally, the Falk-Peskin parameter w_1 can be measured from the pion distribution in the dominant decay $\Sigma_Q^* \to \Lambda_Q\pi$. Consistently working to the leading-order in the heavy-quark expansion, the decay amplitude is given by the Isgur-Wise transition matrix element [103], which is proportional to

$$Y_{1m}(\theta,\varphi)\big\langle 1m\,\tfrac{1}{2}k\big|s\,h\big\rangle\,. \tag{S13}$$

Here Y_{jm} is a spherical harmonic, θ (φ) is the pion polar (azimuthal) angle relative to the fragmentation axis in the candidate $\Sigma_Q^{(*)} \to \Lambda_Q\pi$ rest frame, $s = 1/2$ (3/2) and h are the total spin and spin along the $\boldsymbol{z}$ axis of the Σ_Q (Σ_Q^*) baryon, k is the spin of the final-state Λ_Q along the $\boldsymbol{z}$ axis, and $m = h - k$. We now dress Eqs. (3) and (S13) with the appropriate Clebsch-Gordan coefficients, average over the helicities of the unpolarized initial-state heavy-quark, and sum over the helicities of the final-state Λ_Q (whose polarization is not reconstructed). This results in the following angular distributions for the decay products [69],

$$\begin{aligned}\frac{1}{N_{\Sigma_Q}}\frac{\mathrm{d}N_{\Sigma_Q}}{\mathrm{d}\cos\theta} = \frac{1}{2}\,,\qquad \frac{1}{N_{\Sigma_Q^*}}\frac{\mathrm{d}N_{\Sigma_Q^*}}{\mathrm{d}\cos\theta} &= \frac{1}{4}\Big[1+3\cos^2\theta - \frac{9}{2}\omega_1\Big(\cos^2\theta-\frac{1}{3}\Big)\Big] \\ &= \frac{1}{2}\Big\{1-\frac{3}{8}\big[1+3\cos(2\theta)\big]\Big(w_1-\frac{2}{3}\Big)\Big\}\,.\end{aligned} \tag{S14}$$

Here we have performed the integral over the φ dependence, which as expected is flat since no azimuthal direction is preferred. Here we assumed that the Σ_Q and Σ_Q^* form well-separated resonances $\Gamma_{\Sigma_Q}, \Gamma_{\Sigma_Q^*} \ll m_{\Sigma_Q^*} - m_{\Sigma_Q}$ relative to the mass splitting in the heavy-quark spin symmetry doublet, which is reasonably well satisfied [104, 105]. If needed, the decay distributions can readily be generalized to account for their interference [69], and still can be expressed purely in terms of w_1 in that case. We note that the continuum $Q \to \Lambda_Q\pi$ background to Eq. (S14) is in fact described by a heavy-light DiFF that is of interest of its own, with the pion polar angle tracking its residual momentum fraction z_π in this case. Importantly, however, no feature appears around $m_{\Lambda_Q\pi} \approx m_{\Sigma_Q^*}$ in the double-differential $(z_\pi, m_{\Lambda_Q\pi})$ distribution in the background case. We therefore expect that a standard sideband subtraction will remain viable to remove the background also bin by bin in θ. (Signal-background interference is likewise suppressed by the narrow widths of the resonances.) Finally, we stress that care must be taken to avoid biasing the angular distribution in Eq. (S14) when applying acceptance cuts on the pion transverse momentum with respect to the beam axis, as typically done in spectroscopic analyses [104, 105] to enrich the sample with signal events and suppress the $\Lambda_Q\pi$ continuum background. An attractive way to assess systematic uncertainties from correcting for the acceptance (as well as from subleading $1/m_Q$ corrections on the theory side) is offered by the corresponding angular distribution for Σ_Q baryons, which is flat in $\cos\theta$ for unpolarized collisions at leading order in the heavy-quark expansion.

C. Transverse-momentum dependent fragmentation to excited heavy baryons

The precise relation of the coefficients $w^{(N,n)}$ in Eq. (11) to underlying renormalized nonperturbative matrix elements differs, depending on the case considered: In case (c) given in the main text, corresponding to heavy-light dihadron fragmentation, the factorization takes the same multiplicative form as in Eq. (S11). For cases (a) and (b) the matrix elements enter through convolutions with other TMD matrix elements encoding the contributions of soft dynamics or other collinear sectors, none of which however affect the boosted heavy-hadron spin dynamics or the symmetry analysis leading to Eq. (11). Importantly, the resulting decay pion distribution for unpolarized collisions takes a common general form for any of these cases in terms of the cross section-level spin density in Eq. (11), and evaluates to

$$\begin{aligned}
\frac{1}{\mathrm{d}N_{\Sigma_Q}/\mathrm{d}k_T}\,\frac{\mathrm{d}N_{\Sigma_Q}}{\mathrm{d}k_T\,\mathrm{d}\cos\theta\,\mathrm{d}\varphi} &= \frac{1}{4\pi}\,, \\
\frac{1}{\mathrm{d}N_{\Sigma_Q^*}/\mathrm{d}k_T}\,\frac{\mathrm{d}N_{\Sigma_Q^*}}{\mathrm{d}k_T\,\mathrm{d}\cos\theta\,\mathrm{d}\varphi} &= \frac{1}{4\pi}\Big\{1 - \frac{3}{8}\big[1+3\cos(2\theta)\big]\,w^{(2,0)} - 3\cos\theta\,\sin\theta\,\cos\varphi\,w^{(2,1)} - \frac{3}{2}\sin^2\theta\,\cos(2\varphi)\,w^{(2,2)}\Big\}\,,
\end{aligned} \tag{S15}$$

where k_T is the magnitude of the transverse momentum $\boldsymbol{k}_T \perp \boldsymbol{z}$, reconstructed according to the respective experimental scenario. Importantly, φ in this case is the azimuthal angle of the pion *relative* to the azimuth of $\boldsymbol{k}_T$, which provides an azimuthal reference direction $\boldsymbol{x} = \boldsymbol{k}_T/k_T$ in this case, as discussed in the main text.