Precision predictions for scalar leptoquark pair-production at hadron colliders

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We revisit scalar leptoquark pair-production at hadron colliders and significantly improve the level of precision of the cross section calculations. Apart from QCD contributions, we include lepton t-channel exchange diagrams that turn out to be relevant in the light of the recent B-anomalies. We evaluate all contributions at next-to-leading-order accuracy in QCD and resum, in the threshold regime, soft-gluon radiation at next-to-next-to-leading logarithmic accuracy. Our predictions consist hence in the most precise leptoquark cross section calculations available to date, and are necessary for the best exploitation of leptoquark searches at the LHC.

Introduction – Many extensions of the Standard Model (SM) predict the existence of scalar leptoquarks [1–8], i.e. scalar bosons coupling to a quark and a lepton. Evidence for their existence is consequently vastly searched for at the LHC. However, none of the recent ATLAS [9, 10] and CMS [11–15] analyses have managed to find any hint for these leptoquarks, so that their mass is now constrained to be larger than 1–1.5 TeV. Recently, scalar leptoquarks have gained a significant interest as they may provide an explanation [16–20] for the B-meson anomalies [21–28] and address [29] the discrepancy between theoretical predictions [30] and experimental measurements [31] of the anomalous magnetic moment of the muon \((g-2)\mu\). In this context, favored scenarios generally feature large lepton-quark-leptoquark Yukawa couplings \(y\).

The most stringent bounds originating from LHC direct searches for leptoquark pair-production and decay are extracted by assuming that leptoquarks are solely produced via strong interactions. In other words, non-QCD diagrams involving lepton t-channel exchanges of \(\mathcal{O}(y^2)\) are neglected. In the associated limit setting procedure, signal cross sections are evaluated at next-to-leading-order (NLO) accuracy in the strong coupling \(\alpha_s\), sometimes also supplemented by logarithmic threshold corrections. Thus the predictions include contributions at \(\mathcal{O}(\alpha_s^2)\) and \(\mathcal{O}(\alpha_s^3)\), or possibly of higher order in \(\alpha_s\), but are independent of \(y\) [32, 33]. Bearing in mind the B-anomalies and \((g-2)\mu\) motivation, the limits may thus be incorrectly estimated.

In this letter, we perform for the first time a full NLO-QCD cross section calculation for scalar leptoquark pair-production at hadron colliders, in which we include both the QCD and t-channel contributions. Hadronic production of heavy systems, which is the case considered here, inevitably probes partonic center-of-mass energies close to the production threshold given by twice the leptoquark mass \(m_{LQ}\). In this limit, radiative corrections are dominated by soft-gluon emissions, manifesting themselves as large logarithmic terms that must be consistently resummed to all orders [34–37]. We report here on threshold-resummed results at next-to-next-to-leading-logarithmic (NNLL) accuracy and showcase predictions obtained by matching them to our new NLO LHC results. In the following, we first present the considered theoretical framework and provide brief technical computational details. We then show an illustrative selection of results, additional predictions and the computer codes used in this work being available upon request.

Theoretical framework and technicalities – We focus on a simplified model in which the SM is supplemented by several species of scalar leptoquarks \(S_1, \tilde{S}_1, R_2, \tilde{R}_2\) and \(S_3\). Inspired by standard naming conventions [38, 39], these leptoquarks lie in the \((3, 1)_{-1/3}, (3, 1)_{-1}, (3, 2)_{1/6}, (3, 2)_{1/3}\) and \((3, 3)_{-1/3}\) representation of the SM gauge group respectively, and we target their Yukawa interactions involving exactly one lepton and quark. The latter are collected in the Lagrangian

\[
\mathcal{L}_{\text{int.}} = \text{y}_1^{RR} \bar{q}_R \gamma^\mu L_R \sigma_1^{\mu} \ell_L + \text{y}_1^{LL} (\bar{Q}_L \cdot L_L) \sigma_1^{\mu} \ell_L^\dagger + \frac{3}{1} \text{y}_{1/2}^{RR} \bar{q}_R \gamma^\mu L_R \sigma_1^{\mu} \ell_L^\dagger \\
+ \text{y}_2^{LR} \bar{q}_L \gamma^\mu Q_L R_R^\dagger + \text{y}_2^{RL} \bar{u}_R (L_L^\dagger R_R) + \text{y}_2^{RR} \bar{d}_R (L_L^\dagger R_R^\dagger) \\
+ \text{y}_3^{LL} (\bar{Q}_L^\dagger \cdot \sigma_3 L_L) (S_3^{\mu})^\dagger + \text{h.c.}.
\]

In this expression, all flavor indices are suppressed for clarity, \(\sigma_k\) stands for the Pauli matrices and the dot for the invariant product of two fields lying in the (anti)fundamental representation of SU(2). The \(Q_L\) and \(L_L\) spinors denote the SM weak doublets of left-handed quarks and leptons, and \(u_R, d_R\) and \(\ell_R\) are the corresponding weak singlets. Moreover, the \(y/\tilde{y}\) couplings are \(3 \times 3\) matrices in the flavor space, the first index of any element \(y_{ij} / \tilde{y}_{ij}\) referring to the quark generation and the second one to the lepton generation in the gauge basis.

The calculations reported in this work concern scalar leptoquark pair-production and include fixed-order contributions at leading-order (LO) and NLO in QCD. In contrast with previous work [32, 33, 40, 41], we not only consider the QCD components at \(\mathcal{O}(\alpha_s^2)\) and \(\mathcal{O}(\alpha_s^3)\),
but also include the $t$-channel lepton exchange contributions at $\mathcal{O}(y^4)$ and $\mathcal{O}(y^2 \alpha_s)$ as well as the $\mathcal{O}(y^2 \alpha_s^2)$ interference of the $t$-channel diagrams with the QCD ones. The full NLO-accurate predictions are collectively coined “NLO w/ $t$-channel” in the following, in contrast to the pure QCD ones that we refer to as the “NLO-QCD” predictions. The NLO w/ $t$-channel cross sections are then additively matched with the resummed NNLL soft-gluon contributions, resulting in cross section predictions at NLO w/ $t$-channel+NNLL accuracy. Threshold resummation is performed in Mellin space and involves one-loop matching coefficient [42].

To ensure the correctness of the results, we perform the calculations in two independent ways. We first implement the above model into FeynRules [43], that we jointly use with NLOCT [44] and FeynArts [45] to renormalize the bare Lagrangian of eq. (1) at $\mathcal{O}(\alpha_s)$. We then generate a UFO model file [46] that we use to evaluate fixed-order LO and NLO predictions within the MG5_aMC framework [47]. The latter are cross-validated with results obtained within the Powheg-Box framework [48], in which we input virtual corrections calculated with the FeynArts, FormCalc [49] and Collier [50–53] packages. The NNLL corrections are evaluated with two independent in-house Monte Carlo codes.

**Scalar leptoquark pair-production at the LHC** – We present selected predictions for scalar leptoquark pair-production at the 13 TeV LHC for the three most commonly discussed types of scalar leptoquarks in the context of the flavor anomalies: the $SU(2)_L$ singlet state $S_1$ (denoted by $S_1^{(-1/3)}$ due to its electric charge of $-1/3$), doublet state $R_2$ and the triplet state $S_3$. More specifically, in the last two cases, we consider the pair-production of the $R_2$ mass eigenstate of electric charge of $5/3$ (denoted by $R_2^{(5/3)}$) and the one of the $S_3$ mass eigenstate of electric charge of $-4/3$ (denoted by $S_3^{(-4/3)}$). In all our calculations, we treat the leptoquark mass $m_{LQ}$ as a free parameter and assume the CKM matrix to be diagonal. While the determination of a scenario compatible with flavor constraints and $Z$-pole observables is desirable [54], this goes beyond the scope of this study. Motivated by the analysis of ref. [20], we instead consider $S_1 S_1^\dagger$ production with a minimal flavor ansatz for the leptoquark Yukawa couplings, $(y_{\mu L}^{1L})_{22} = -0.15$ and $(y_{\mu L}^{1L})_{32} = 0$ with all other $y_{\mu L}^{1L}$ elements set to 0. For $R_2 R_2^\dagger$ production, we similarly consider the only non-vanishing coupling $(y_{\mu L}^{1L})_{22} = 1.5$, a value still allowed by direct exclusion bounds [20], while for $S_3 S_3^\dagger$ production, we adopt $(y_{\mu L}^{1L})_{22} = -(y_{\mu L}^{1L})_{32} = 0$, keeping the actual coupling value free and setting all other couplings to 0.

Our results are obtained by convoluting the partonic results with two different sets of parton distribution functions (PDFs), NNPDF3.1 [55] and CT18 [56]. Unless stated otherwise, NLO sets are employed for NLO-QCD and NLO w/ $t$-channel predictions, while NNLO sets are used for NLO+NNLL calculations. We set the renormalization ($\mu_R$) and factorization ($\mu_F$) scales equal to a common value $\mu = \mu_R = \mu_F$. The central scale choice $\mu = \mu_0$ is fixed to $\mu_0 = m_{LQ}$, and scale uncertainties are estimated by varying $\mu$ by a factor of 2 up and down.

In fig. 1, we present cross section predictions for $S_1^{(-1/3)} S_1^{(1/3)}$ (left column) and $R_2^{(5/3)} R_2^{(-5/3)}$ (right column) production, both for the NNPDF3.1 (upper row) and CT18 (lower row) parton densities. We estimate the relative importance of the various corrections studied in this work with respect to NLO-QCD predictions, and assess the size of the theoretical uncertainties. Comparing the four subfigures, we observe that depending on the process, the PDFs, the magnitude of the Yukawa couplings and $m_{LQ}$, the considered corrections can influence the predictions in different, often contrasting, ways.

Although providing a positive correction, the $t$-channel contributions depend very differently on $m_{LQ}$ for the two processes (blue dashed curves). On the contrary, NNLL effects, which we estimate through the ratio of the NLO-QCD+NNLL to the NLO-QCD cross sections both calculated with the same NLO PDF set (turquoise dotted curves), are independent of the process and PDF choice. As expected, this ratio is bigger than 1 and grows with increasing $m_{LQ}$, i.e., approaching the production threshold. However, the interplay of the $t$-channel contributions, PDF effects and soft gluon corrections can lead to a vastly different behavior of the NNLL results matched with NLO w/ $t$-channel (red solid curves). The sole effect of evaluating the NLO w/ $t$-channel cross sections with NNLO PDF sets instead of NLO sets is illustrated by the difference between the corresponding ratios to NLO QCD predictions (blue dashed vs. olive dash-dotted curves). For the NNPDF3.1 PDF set (upper row), this effect diminishes the predictions, offsetting the increase stemming from the NNLL contributions. As a consequence, the NLO w/ $t$-channel+NNLL results deliver a positive correction of about 10–20% with respect to the NLO-QCD predictions for $m_{LQ} \in [1, 2]$ TeV. Similarly to the NLO w/ $t$-channel result, the full NLO w/ $t$-channel+NNLL correction exhibits an opposite behavior with increasing $m_{LQ}$ in the $S_1$ (upper left) and $R_2$ (upper right) cases. When CT18 PDFs are used instead (lower row), the corrections are larger and reach a magnitude of about 20–50%, the impact this time increasing with $m_{LQ}$ for both processes. Furthermore, in the NNPDF3.1 case, various contributions to the total correction are often much bigger than the correction itself. For example, the correction due to including $t$-channel diagrams reaches up to 40% of the NLO-QCD result for the pair production of 2 TeV $R_2$ leptoquarks, whereas the complete NLO w/ $t$-channel+NNLL one is only of about 20%. In contrast, results obtained with CT18 densities exhibit an opposite behavior, the cross sections being typically enhanced when switching from NLO to NNLO PDFs. The $t$-channel and soft-gluon resummation pieces are of comparable size and thus equally contribute to the combined correction. Therefore a precise knowledge of the cross section requires calculating all classes of corrections.

In the middle panels of the four subfigures in fig. 1, we focus on the theoretical uncertainties inherent to
FIG. 1. $S_1^{(-1/3)}S_1^{(1/3)}$ (left) and $R_2^{(5/3)}R_2^{(-5/3)}$ (right) production at the 13 TeV LHC, using the NNPDF3.1 (upper) and CT18 (lower) PDF sets. In each subfigure, we present, in the top panel, cross section predictions at the NLO-QCD (magenta dotted), NLO w/ $t$-channel (blue dashed) and NLO w/ $t$-channel+NNLL (red solid) accuracy. We moreover display the associated scale uncertainties (second panel) and PDF errors (third panel), as well as the ratios of the NLO w/ $t$-channel, NLO w/ $t$-channel+NNLL, NLO w/ $t$-channel calculated using NNLO PDFs (olive dash-dotted) and NLO-QCD+NNLL (turquoise dotted) results to the NLO-QCD cross section (fourth panel).
FIG. 2. NLO w/ $t$-channel+NNLL total cross section for $S_{3}^{(-4/3)}S_{3}^{(4/3)}$ production at the 13 TeV LHC as a function of the $S_{3}$ mass $m_{LQ} = m_{S_{3}}$ and the Yukawa couplings $(y_{LL}^{3})_{22} = (y_{LL}^{3})_{32}$ (all other Yukawa couplings being set to 0). We present predictions obtained with the NNPDF3.1 (left) and CT18 (right) PDF set.

the performed computations. We distinguish the impact of scale variations (second panel) from the one originating from the PDF determination (third panel). Our results show that soft-gluon resummation leads to a significant reduction of the scale uncertainties from around 10% (for the NLO predictions) to about 1–2% for $m_{LQ}$ values ranging up to slightly above the current exclusion limits, though the reduction might be underestimated due to the chosen method for the scale uncertainty evaluation. This calls for more detailed studies. Correspondingly, the total theoretical error for our final NLO w/ $t$-channel+NNLL predictions is dominated by its PDF component. The size of the PDF error is however strongly dependent on the PDF choice. For instance, results derived with NNPDF3.1 exhibit, for $m_{LQ} \sim 1$ TeV, PDF errors smaller or comparable in magnitude to the size of the perturbative corrections, whilst at higher $m_{LQ}$ values, the PDF error becomes significantly bigger. In comparison, PDF errors obtained with the CT18 set are larger for small $m_{LQ}$ values, but do not grow as quickly for higher masses. Still, the PDF errors turn out to be of the same order as the full perturbative corrections for large $m_{LQ}$ values. Those large PDF errors at high masses hence obscure the accuracy of the predictions. However, as more and more LHC data will be analyzed, one can expect a substantial improvement of the PDF knowledge, in particular in the large Bjorken-x regime, so that the PDF errors associated with predictions relevant for high-mass system production will get significantly reduced.

In fig. 2, we calculate the NLO w/ $t$-channel+NNLL total cross section for $S_{3}^{(-4/3)}S_{3}^{(4/3)}$ production, and study its dependence on the leptoquark mass and Yukawa coupling strength. We consider both the NNPDF3.1 (left panel) and CT18 (right panel) PDF sets. At small values of the Yukawa coupling, the dominant production mechanism is QCD driven so that the cross section solely depends on $m_{LQ}$. On the contrary, as the coupling is about 1, the $t$-channel contributions become more relevant so that the total rate is significantly increased. This behavior is mostly independent of the chosen PDF set, with CT18 predictions being slightly less sensitive to the $t$-channel diagrams than NNPDF3.1 ones.

Summary – We have significantly advanced the precision of scalar leptoquark pair-production cross section computations. First, we have included all tree-level diagrams, both the QCD ones and those involving the $t$-channel exchange of a lepton. Second, we have consistently evaluated all contributions and their interference at NLO QCD, and moreover resummed at the NNLL accuracy soft-gluon radiation in the threshold regime.

The $t$-channel contributions, threshold resummation, the adopted parton densities and benchmark scenario (in particular when the leptoquark Yukawa couplings are taken as large as suggested by the recent $B$-anomalies) very importantly affect the total rates, in potentially contrasting ways. This emphasizes the necessity of including all contributions whose calculation has been pioneered in this work. While the perturbative series exhibits smaller scale uncertainties, the precision of the predictions is limited by the poor PDF knowledge in the large Bjorken-x regime relevant for the production of high-mass systems. In the light of our findings, we recommend the usage of NLO w/ $t$-channel+NNLL cross sections, to be taken together with the correspondingly reduced scale uncertainties and PDF errors extracted from the envelope spanned by computations, left for future work, performed with different PDF sets. This follows the strategy outlined in various recommendations for LHC cross sections calculations [57–61].

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