# Detailed closing report of the NKFIH K-125105 research grant

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The aim of this research project was to make significant contributions to the advancement of particle physics theory and phenomenology in two areas: (i) computing radiative corrections to high energy collision processes with particular emphasis on processes at the LHC and also (ii) search for phenomena that cannot be explained by the standard model but can be observed in collider experiments (beyond the standard model, BSM physics). In particular our main goal in area (i) was to develop the theory of computing QCD cross sections at the next-to-next-to-leading order (NNLO) in perturbation theory and also make predictions for LHC processes at the highest available accuracy at the time of publications. In area (ii) we planned to map out the allowed parameter spaces of viable BSM scenarios of scalar extensions. We published many research papers in both fields, although for various reasons we were not able to follow our original plans. In turn, we discuss our achievements in these two fields.

*Computing QCD cross sections at high precision*

In the field of computing QCD cross sections our main goal was to build on our computational scheme – the CoLoRFulNNLO method developed earlier for lepton collisions – to extend it to processes with hadrons in the initial state. This method is based on the rearrangment of infrared (IR) divergences between various contributions to the full higher order prediction by adding and subtracting *the same approximate cross sections*, such that *this rearrangement renders each contribution separately finite without changing the value of the cross section.* As the IR divergences of QCD matrix elements are universal, in principle the approximate cross sections can be explicitly constructed once and for all in a process- and observable-independent way. A straightforward extension of the CoLoRFulNNLO method to processes with coloured partons in the intial state in a completely general way has so far proved to be too difficult technically to our group – we have managed to define the rearrangement, but was unable to perform the emerging integrals –, hence we decided to change the scope of our research.

On the one hand, we defined and validated all subtraction terms needed to regularize double real and real-virtual emission for hadron collision processes resulting in a colorless final state (W, Z or H boson production), which constitutes a subset of our ultimate goal. We made use of the freedom in the precise definitions of the subtraction terms to reduce the number of different momentum mappings that appear in the approximate cross sections and to implement several cancellations among the various counterterms. We also pursued the integration of the subtraction terms over the momenta of the unresolved radiation. We managed to compute the integrated forms of all single and double unresolved counterterms fully analytically and the integration of the iterated single unresolved subtraction terms is ongoing. Such final states belong only to a subset of the interesting processes, hence the reduction of the momentum mappings may not be applicable in more general cases. Nevertheless our failure to find a completely general method had forced us to try to build expertise on processes with simple kinematics.

On the other hand, we also started to explore another computational scheme where the subtractions are aided with a partition of the phase space such that in each partition only a limited set of kinematic singularities may occur. This *sector aided subtraction* was worked out recently for processes without coloured partons in the initial state and we plan to extend this method to the case of hadron collisions. As there is no explicit application of this approach in the literature, we implemented this method in a computer code to regularize the double real radiation corrections emerging in the final state. The advantage of this regularization of the kinematic singularities over the CoLoRFuLNNLO method is the much simpler paramteric integrals that appear in the analytic integration of the subtractions over the unresolved phase space. Indeed, for the case of colourless initial states, we were able to compute these intagrals much easier (in several months versus about ten years) and found much more compact results than in the case of the CoLoRFuLNNLO framework, which makes us beleive that the generalization to hadron collisions will not lead to integrals of extreme complexity.

While we are certainly behind our schedule as compared to the initial plans, our recent advancments make us optimistic that we shall be able to complete these modified plans. We plan to publish the relevant details of both approaches during 2023.

In addition, we were able to make precise predictions to many processes at various level of accuracy, all being the state-of-the-art at the time of publication in the literature, as well as performed phenomenological studies as detailed in the following.

1. We computed the associated production of a Higgs boson with a vector boson, including the decay of the Higgs boson into b quarks, with both the production and the decay computed at NNLO accuracy [1]. For the first time this computation included the leptonic decay of the vector boson with finite-width effects and spin correlations. We considered typical kinematic cuts applied in the experimental analyses at the Large Hadron Collider (LHC) and we found that the full NNLO QCD corrections significantly decrease the accepted cross section and had a substantial impact on the shape of distributions. We pointed out that these additional effects were essential to obtain precise theoretical predictions to be compared with the LHC data.
2. We performed a determination of the strong coupling using our high precision predictions for the energy-energy correlations of hadrons in electron-positron annihilation. We published a result for the strong coupling extraction from LEP, PEP, PETRA, SLC and TRISTAN data with competitively small uncertainties in agreement with the world average [2].
3. We studied new observables (so-called groomed event shapes) of hadronic final states in electron-positron annihilation with reduced higher order corrections. First we computed the distribution of the *soft drop thrust* at the NNLO accuracy [3].
4. We presented the first extraction of the strong coupling $\alpha_S(M_Z)$ based on N$^3$LO+NNLL accurate theoretical predictions for the two-jet rate in the Durham clustering algorithm at electron-positron colliders, using state-of-the-art Monte Carlo event generators to assess the impact of hadronization [4]. We performed a simultaneous fit of the two- and three-jet rates, taking into account the correlation between these observables. In the analysis, we used a large range of data sets form the LEP and PETRA colliders, with center-of-mass energies

ranging from 35 GeV to 207 GeV. Our best determination reads

$$\alpha_S(M_Z) = 0.11881 \pm 0.00063(exp.) \pm 0.00101(hadr.) \pm 0.00045(ren.) \pm 0.00034(res.),$$

and agrees with the latest world average and has a comparable total uncertainty.

5. We computed the cross section of fully exclusive heavy quark-antiquark pair production from a colourless initial state at NNLO in QCD [5] by generalizing the CoLoRFuLNNLO subtraction method. As an example, we calculated the fully differential decay rate of the standard model Higgs boson to massive b-anti-b quark pair at NNLO accuracy in perturbative QCD. To validate our method, we compared our results for the NNLO correction to the inclusive decay rate to the approximate formula available in the literature based on a series expansion in the ratio of the quark mass to the Higgs boson mass. We presented the leading jet rapidity distribution and the two-jet rate emerging from massive b quarks at NNLO accuracy for the first time.
6. We presented the extraction of the strong coupling $\alpha_S(M_Z)$ based on NNLO accurate theoretical predictions for event shape moments measured in electron-positron annihilation into hadrons [6]. We also performed a simultaneous fit of the $N^3LO$ corrections and the strong coupling, providing the first estimate of the $N^3LO$ corrections to event shapes. We used state-of-the-art Monte Carlo event generators as well as analytic models to assess the impact of hadronization and a large range of data sets form the LEP and PETRA colliders, with centre-of-mass energies ranging from 29 GeV to 207 GeV. Our best determination for the strong coupling based on NNLO predictions amended with analytic hadronization model is in agreement with the world average.
7. We published the first ever computation of the two-loop soft function needed for the computation of groomed event shapes of hadronic final states at the $N^3LL$ accuracy [7]. This allowed to make predictions for such an observable resumming the first four towers of large logarithmic contributions to all orders in perturbation theory, and also the matching of the $N^3LL$ prediction to our prediction in fixed-order perturbation theory at NNLO accuracy [8]. This is the fourth event shape variable for which such high accuracy is available in the literature, and the first one in the groomed class, which is expected to be much less sensitive to low energy non-perturbative effects [9].
8. We published a thorough study of different theoretical predictions for the normalised inverse invariant mass distribution of the $t\bar{t}$ quark pair and the leading extra jet not coming from the t quark decays, but with t quark decays included [10]. We studied the impact on the extraction of the t quark mass and quantified the associated uncertainties. We concluded that with the inclusion of quark decays the invariant mass of the $t\bar{t}$ system shows better sensitivity to the t quark mass extraction and smaller dependence on the off-shell effects and non-resonant contributions of the t quark and the W gauge boson than other observables used in previous studies
9. We computed the NLO QCD corrections to $t\bar{t}\gamma$ hadroproduction and made precise predictions for the $R = t\bar{t}\gamma/t\bar{t}$ cross section ratio at the LHC Run II [11]. Depending on the transverse momentum cut on the hard photon a judicious choice of a dynamical scale allowed us to obtain 1 %–3 % percent precision on $R$. We found theoretical uncertainties in the range of 1 %–6 % for differential cross section ratios. Until our work such high precision predictions have only been reserved for the t quark pair production at NNLO QCD. Thus,

$R$ at NLO in QCD represents a very precise observable to be measured at the LHC for example to study the t quark charge asymmetry or to probe the strength and the structure of the $t\bar{t}\gamma$ vertex. The latter can shed some light on possible new physics that can reveal itself only once sufficiently precise theoretical predictions are available.

10. We computed the NLO QCD corrections to $t\bar{t}$ + missing energy production and investigated its connection with Dark Matter searches at the LHC [12]. Good theoretical control over the standard model background is a fundamental prerequisite for a correct interpretation of possible signals of new physics that may arise in this channel. Our work provides a careful study in the presence of more exclusive cuts which is needed for devising realistic strategies for the detection of new physics signals.
11. We also made precise predictions for the hadroproduction of charged vector boson in association with a c quark at the LHC [13]. This work also includes a general implementation of the Narrow Width Approximation in the HELAC-NLO framework.
12. We studied the effect of off-shell versus on-shell modelling of t quarks for the hadroproduction of t quark pair production in association with vector bosons [14]. We also explored the effect of modelling of the t quark decay in different ways in photon associated production [15]. We were able to confirm that for the integrated cross sections the finite t quark width effects are small and of the order of width over the mass of the t quark. However, we found that such effects are strongly enhanced for more exclusive observables. We also investigated the fractions of events where the photon is radiated either in the production or in the decay stage, and found that a large fraction of isolated photons comes from radiative decays of t quarks. Based on our findings, selection criteria can be developed to reduce such contributions that constitute a background for the measurement of the anomalous couplings in the $t\bar{t}\gamma$ vertex.
13. We revisited the computation of the NLO QCD corrections to $t\bar{t} + W^{\pm}$ boson hadroproduction in Ref. [16]. In the computation we described the off-shell t quarks by Breit-Wigner propagators, and we incorporated the double-, single- as well as non-resonant t quark contributions along with all interference effects consistently at the matrix element level for the first time. We presented results at NLO QCD accuracy in the form of fiducial integrated and differential cross sections for two selected renormalisation and factorisation scale choices and three different PDF sets.
14. In light of recent discrepancies between the modeling of $t\bar{t} + W^{\pm}$ signatures in hadroproduction and measurements reported by the LHC experimental collaborations, we investigated the theoretical uncertainties for multi-lepton signatures in this process [17]. We compared results from the state-of-the-art full off-shell calculation and its Narrow Width Approximation to results obtained from the on-shell calculation, with approximate spin-correlations in t quark and W decays, matched to parton showers. In the former case we took into account the double-, single-, and non-resonant contributions together with interference effects, while the latter two cases were only based on the double resonant t quark contributions. We performed the comparison for the LHC at $\sqrt{s} = 13\,\mathrm{TeV}$ colliding energy for which we investigated separately the multi-lepton signatures as predicted from the dominant NLO contributions at the perturbative orders $\alpha_S^3\alpha^6$ and $\alpha_S\alpha^8$. We combined both contributions and proposed a simple way to approximately incorporate the full off-shell effects in the NLO computation of on-shell $t\bar{t} + W^{\pm}$ hadroproduction matched to parton showers.

15. We extended the computation of the NLO QCD corrections to the hadroproduction of $\mathrm{t\bar{t}} + W^{\pm}$ (see previous point) to the estimates of correlations and asymmetries [18]. Discrepancies between theoretical predictions and measurements in multi-lepton plus b-jets analyses for the $pp \to \mathrm{t\bar{t}} + W^{\pm}$ process indicated need for more accurate theoretical predictions and high precision observables to constrain numerous new physics scenarios. Thus we employed NLO QCD computations, with full off-shell t quark effects included, to provide theoretical predictions for the $R = \frac{\sigma(pp\to \mathrm{t\bar{t}}+W^{+})}{\sigma(pp\to \mathrm{t\bar{t}}+W^{-})}$ cross section ratio at the LHC at $\sqrt{s} = 13\,\mathrm{TeV}$. Depending on the transverse momentum cut on the b-jet we obtained 2 %–3 % theoretical precision on $R$ which will help to shed some light on new physics effects that can reveal themselves only once sufficiently precise standard model theoretical predictions are available. We re-examined the charge asymmetry of the t quark and its decay products in the $pp \to \mathrm{t\bar{t}} + W^{\pm}$ production process we achieved theoretical uncertainties below 15 %.
16. We also reported on the calculation of the NLO QCD corrections to the production of a $\mathrm{t\bar{t}}$ pair in association with two heavy-flavour jets with focus on the di-lepton + $\mathrm{t\bar{t}}$ decay channel at the LHC at collision energy $\sqrt{s} = 13\,\mathrm{TeV}$ [19]. This computation was based on $pp \to e^{+} + \nu_e + \mu^{-} + \bar{\nu}_\mu + \mathrm{b} + \bar{\mathrm{b}} + \mathrm{b} + \bar{\mathrm{b}}$ matrix elements (8 particles in the final state!) and included all resonant and non-resonant diagrams, interferences and off-shell effects of the t quark and the W boson. We studied extensively the dependence of our results upon variation of renormalization and factorization scales and parton distribution functions in the quest for an accurate estimate of the theoretical uncertainties. We also studied the impact of the contributions induced by the b quark parton density. Our predictions are particularly relevant for measurements of $\mathrm{t\bar{t}}H(H \to \mathrm{b\bar{b}})$ final states and consequently, the determination of the Higgs coupling to the t quark. They might also be used for precise measurements of the t quark fiducial cross sections and to investigate t quark decay modelling at the LHC.
17. We performed a detailed comparison and provided benchmark predictions at NNLO accuracy for Drell-Yan lepton pair production computed using four publicly available codes [20]. We pointed out that while there is agreement among the predictions at the NLO accuracy, the predictions at NNLO differ, whose extent depends on the observable. The sizes of the differences in general are at least similar, or larger than the sizes of the NNLO corrections themselves, which is clearly unacceptable if we want to achieve the targeted below 1 % theoretical uncertainty for this fundamental process. We demonstrated that the neglected power corrections by the codes that use global slicing methods for the regularization of double real emissions can be the source of the differences. Our findings ignited significant efforts to improve the precision of the computations.

*BSM phenomenology*

During the course of this project our research in the field of BSM phenomenology has also deviated from the original plans. On the one hand Dr. Robens who was on the project at start and was the key person behind the BSM plans had taken a position abroad, and as a result, our collaboration gradually came to an end. Nevertheless, in the first two years a significant part of the plans has been completed. On the other hand, at the same time the PI started a new project in BSM phenomenology that has resulted in several research papers. Below we list the achievements that were published with the support of this research grant.

1. Studying the singlet scalar extension of the SM, we were invited to the working groups of the High Luminosity LHC, as well as CLIC studies. The complete write-up of these activities appeared with the support of this grant in a summary paper [21].
2. We considered the pair-production of inert scalars as signal processes, followed by decays of the charged and neutral scalars into leptonic final states and missing transverse energy [22]. We focused on signal signatures with two muons or an electron and a muon in the final state. A number of selected benchmark scenarios that cover the range of possible collider signatures of the Inert Doublet Model were considered. For the suppression of standard model background with the same visible signature, we employed multivariate analysis methods. We found that for several benchmark points discovery is already possible at the low-energy stage of CLIC.
3. We defined an extension of the standard model with three right-handed neutrinos, a new complex scalar field and a new U(1) gauge interaction [23]. This *super-weak* extension of the standard model (SWSM) is designed to explain the origin of established observations in particle physics that clearly call for a BSM model, such as (i) neutrino masses and mixing matrix elements, (ii) dark matter, (iii) cosmic inflation, (iv) stabilization of the electroweak vacuum and (v) leptogenesis.
4. We studied the allowed parameter space of the SWSM by requiring that the vacuum remains stable up to the Planck scale, and proposed a new particle physics model of cosmic inflation [24].
5. We computed the one-loop corrections to light neutrino masses in gauged U(1) extensions of the standard model [25]. We considered gauged U(1) extensions of the standard model of particle physics with three right-handed sterile neutrinos and a singlet scalar. An example of such extensions is the SWSM. The neutrinos obtain mass after spontaneous symmetry breaking of the new scalar. We computed the one-loop corrections to the elements of the tree level mass matrix of the light neutrinos. We showed explicitly the cancellation of the gauge dependent terms. We estimated the size of the corrections relative to the tree level mass matrix in the super-weak model and found those well below 1 %.
6. We studied the possibility of a dark matter candidate in the SWSM [26]. We explored the parameter space of the model from the point of view of explaining the observed dark matter energy density in the Universe. We studied both freeze-in and freeze-out mechanisms of dark matter production. In both cases, we found regions in the plane of the super-weak coupling vs. the mass of the new gauge boson that are allowed by current experimental constraints. These regions are distinct and the one for freeze-out will be explored in searches for neutral gauge boson in the near future.
7. We started to explore the experimental constraints on the parameter space of the SWSM by focusing on the neutrino and gauge parameters [27]. We discussed the neutrino sector of this model in detail and studied the allowed parameter space of the neutrino Yukawa matrices and mixing matrix elements. The super-weak model also generates nonstandard neutrino interactions, whose allowed experimental limits were used to constrain the parameter space of the model. We provided benchmark points in the relevant parameter space that fall within the sensitivity region of the SHiP and MATHUSLA experiments.
8. We studied the allowed parameter space of the scalar sector in the SWSM [28]. We defined the allowed region by the conditions of (i) stability of the vacuum and (ii) perturbativity

up to the Planck scale, (iii) the pole mass of the Higgs boson falls into its experimentally measured range. We used renormalization group equations and quantum corrections at two-loop accuracy. We also studied the dependence on the Yukawa couplings of the sterile neutrinos at selected values, and checked the exclusion limit set by the precise measurement of the mass of the W boson.

*Additional achievements*

1. We studied decays of neutrinos with possible violation of Lorentz invariance [29].
2. We edited a special issue of the Symmetry journal on recent developments in computing radiative corrections in QCD [30].
3. We published an introductory textbook on particle physics both in English and in Hungarian [31].
4. We were invited to publish a feature article in Europhysics News on the status of particle physics [32].
5. We gave public lectures, participated in several podcasts and wrote outreach publications in Fizikai Szemle in order to disseminate our research to wider audiences.

The mobility restrictions introduced during the COVID pandemic prevented us from fulfilling our budgetary plans as most of our expenses were planned for collaboration meetings and dissemination on workshops and conferences. We spent the smaller portion of the leftover on purchasing programmable computing elements in order to build energetically more efficient targeted computing devices to meet the increasing computing needs of our project.

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[31] Dezső Horváth, Zoltán Trócsányi: Intorduction to particle physics, Cambridge Scholars Publishing, ISBN-13: 978-1-5275-2808-6, 2019. Horváth Dezső, Trócsányi Zoltán: Bevezetés az elemi részek fizikájába, Typotex Kiadó, 2021.

[32] Zoltán Trócsányi, *Status of Particle Physics*, Europhysics News 51/2 (2020) 23-25.

All original research papers listed here contain the reference to the "National Research, Development and Innovation Fund, Hungary under grant number K 125105" and appeared as Open Access articles. On 30 November 2022, there were 794 citations in total to these publications in the INSPIRE database. Our extractions of the strong coupling are part of the world average in the Particle Data Book.