

Quantum systems exhibit non-classical correlations that go beyond the capabilities of classical physics, making these correlations a central focus of research in quantum information science. This thesis addresses a seemingly simple yet profound question: *what can we infer about the underlying physics when we observe non-classical correlations?* Specifically, how can we characterize non-classical correlations and certify the underlying quantum systems? Accurate characterization and certification of quantum systems are of fundamental and practical significance for advancing quantum information theory. In this thesis, we develop novel theoretical models for the characterization of non-classical correlations and the certification of underlying quantum systems. Despite the precision of the theoretical models, their implementation in experimental setups often requires consideration of additional factors. Experimentalists must contend with noise and imperfect devices, which can obscure the certification of the underlying quantum systems. Consequently, this thesis also addresses an experimentally significant question: *how can we effectively certify underlying quantum systems in experimental settings despite the presence of imperfections and noise?*

The first two articles derive novel *robust analytical* self-testing statements, which form the most accurate certification of quantum systems underlying the maximum violation of Bell inequalities. The first article deals with the self-testing of Bell inequalities in the sparsely explored multipartite Bell scenarios. We present a novel self-testing technique, which is very simple yet effective in that it can be applied to a substantially large class of multipartite Bell inequalities. The second article addresses the practical challenge of finding the optimal strategies that yield the maximum violation of Bell inequalities in the presence of imperfect devices. We show that the optimal strategies maximally violate a tilted version of the Bell inequality. We derive self-testing statements for the tilted versions of the Clauser-Horne-Shimony-Holt (CHSH) inequality, demonstrating that the optimal strategies are unique. Beyond providing analytical and robust self-testing statements, the articles uncover several pivotal features of quantum correlations in Bell scenarios. In particular, the results in both articles highlight the impracticality of the traditional methods, such as the sum-of-squares (SOS) decomposition method and the Navascués–Pironio–Acín (NPA) hierarchy of semi-definite programming relaxations, for obtaining the self-testing statements. Both articles leverage Jordan’s lemma as a crucial component of the self-testing technique.

The third article investigates the relationship between non-classical correlations and mediated dynamics (dynamics generated by a mediator that couples non-interacting systems). We concentrate on the non-classical characteristics of the interactions involved. We derive conditions that solely use correlations between the coupled systems, excluding the need to measure the mediator, to certify the non-commutativity and non-decomposability of mediated interactions. We also discuss the implications of this formalism, including constraints on possible theories of gravity within a Hilbert space framework and within the theory of quantum simulators.