# Research Statement: An Applied Representation Theorist in a Quantum World

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My work falls into two general veins of research, both of which can be broadly thought of as "applied Lie representation theory in quantum contexts". My dissertation work under advisor Bruno Nachtergaele focuses on ground state phase problems for quantum spin systems with Lie group symmetry. In a different set of projects, first at Los Alamos National Laboratory under Marco Cerezo and Patrick Coles and then at Pacific Northwest National Laboratory and North Carolina State University under Carlos Ortiz Marrero and Bojko Bakalov, we explore and rigorously describe the performance of variational quantum algorithms (VQAs) using tools from Lie representation theory. In a postdoctoral position, I wish to continue this applied representation theory program and attack a variety of problems at the intersection of quantum many-body systems, quantum computation, and quantum information.

## 1 LANL and PNNL: Representation Theory for VQAs

I began working on VQAs at Los Alamos National Laboratory (LANL) with a team spearheaded by Marco Cerezo and Patrick Coles. VQAs broadly refer to a class of variational hybrid quantum-classical algorithms which begin with a given quantum architecture whose unitaries are described by trainable classical parameters (think gates $U(\theta)$ where the angle $\theta \in \mathbb{R}$ controls $U(\theta) = e^{i\theta H}$). Given the dramatic success of classical machine learning, it seems a natural extension worthy of study, especially for learning and predicting the structure of quantum data from e.g. quantum chemistry or condensed matter. Moreover, since VQAs generally require shorter circuit depths and fewer qubits, there is good reason to hope for them to come to practical fruition sooner than their fault-tolerant cousins, like Shor's algorithm or the HHL algorithm.

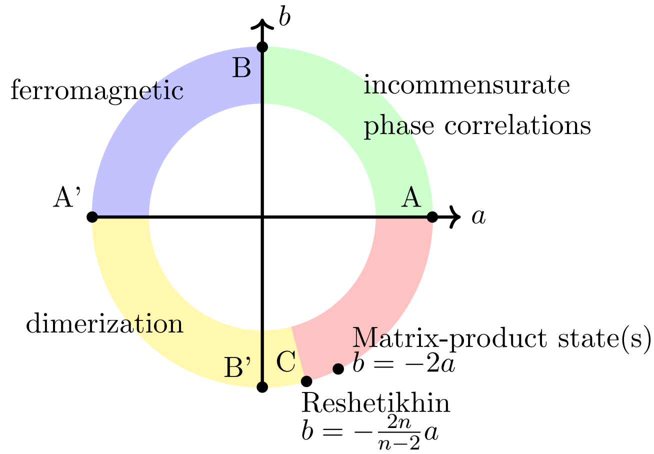
However, over the past five years, it has become clear that generic VQA frameworks typically suffer from severe trainability and performance problems, like barren plateaus and poor generalization. Barren plateaus are particularly worrisome: they describe a situation where the loss function of a VQA model has an exceptionally flat landscape, whose lack of derivative information results in trainability problems. It has become clear that structure and constraints are key to vanquishing these problems, and a rich source of these have been studied for years in the form of symmetry. In physics and mathematics, this is commonly formalized in the language of Lie representation theory: this mathematical formalism captures both discrete and continuous symmetries, like permutation symmetry or unitary rotational symmetry, and it has been intimately tied to quantum theory since its inception. To find examples of VQAs with symmetry, we turn our attention to variational quantum eigensolvers (VQEs), a wide class of algorithms whose cost functions are determined by a given Hamiltonian. When these Hamiltonians come from condensed matter or chemistry, they are often rife with symmetry: translation invariance, spin-rotation symmetry, parity symmetry...the list is enormous, and each is essentially characterized by Lie group representations. But despite the efficacy of symmetry in various domains of quantum science and mathematics, symmetry *was not* *being leveraged for VQAs in any systematic way* until the work of Meyer et.al. [Mey+23] and our work at LANL [Rag+22; Ngu+22]. Again, without problem-specific structural assumptions, we have good reason to believe that VQAs will suffer devastating trainability problems which get worse as quantum computers grow.

The work of our team at LANL is summarized in two papers. Our first paper [Rag+22] contextualizes well-known representation theory results in the language of VQAs. Our second paper [Ngu+22] concretely demonstrates how to use representation theory to construct VQA frameworks which respect the symmetries of a given dataset. Shortly after the conclusion of my summer in LANL, the team successfully exploited symmetry for provable improvements to permutation-symmetric VQA architectures: namely, lack of barren plateaus, rapid solution convergence, and superior generalization features [Sch+22].

I am now working as a graduate student researcher at PNNL under scientist Carlos Ortiz Marrero alongside Lie theorist Bojko Bakalov and condensed matter theorist Lex Kemper at North Carolina State University to pursue the program put forth by the LANL team. Our work rigorously formulates and proves a variety of folklore conjectures for symmetric VQA architectures. The key technical tool is the dynamical Lie algebra $\mathfrak{g}$ of a variational circuit, which grants us precise control over the circuit's expressibility, i.e. the space of unitaries reachable by tuning the circuit's parameters. To find the $\mathfrak{g}$ associated to a parameterized quantum circuit, one lists the Hermitian generators $\{H_1, \ldots, H_k\}$ which generate a pool of unitary gates $U_j(\theta) = e^{i\theta_j H_j}$, and then defines $\mathfrak{g} = \langle iH_1, \ldots, iH_k\} \rangle_{Lie}$, the Lie algebra generated by this set. In the seminal paper [Lar+22], the LANL team posed a conjecture for deep paramaterized quantum circuits, predicting that the presence of a barren plateau is controlled by the dynamical Lie algebra. We proved two results in [Rag+23] which essentially confirm this conjecture. The first result assures us that when the parameters $\theta_j \in [0, 2\pi]$ are equipped with the uniform distribution, a sufficiently deep parameterized quantum circuit forms an $\epsilon$-approximate $G$ $t$-design, where $G = e^{\mathfrak{g}}$. In other words, by wiggling the parameters $\theta$ of a deep circuit $U_\theta$, we approximate moments of the Haar measure on the dynamical Lie group $G$. The second result, which starts by assuming that the circuit forms a $G$ 2-design, *exactly* computes the variance and expectation of a linear loss function $\ell_\theta(\rho) = \mathrm{Tr} U_\theta \rho U_\theta^* O$ for these circuits for any dynamical Lie algebra $\mathfrak{g}$, under the assumption that either the input state $\rho \in i\mathfrak{g}$ or the measurement observable $O \in i\mathfrak{g}$. A wide class of VQAs–including variational quantum eigensolvers, QAOA, and variational compilation algorithms–indeed satisfy this assumption. This serves to unify the zoo of all known sources of barren plateaus in a single mathematical framework [Cer+21], and has spawned a variety of interesting questions which our team continues to study.

## 2 Dissertation work: Symmetric gapped ground states and topological indices

My dissertation work tackles ground state phases of quantum spin systems, a framework which studies models with local degrees of freedom at each site in a lattice, like $\mathbb{Z}$. We focus on a conjectured phase diagram for a class of nearest-neighbor Hamiltonians with a local orthogonal group symmetry (figure from [Bjö+21]):




The yellow "dimerized" phase and the red "Haldane" phase are quite interesting. At the point B', it has been rigorously shown that these models exhibit dimerization, a type of spontaneous symmetry breaking wherein a translation-invariant Hamiltonian has two 2-periodic ground states $\omega_\pm$ which look like translates of each other.[Bjö+21] The matrix product state (MPS) point in the red region contains as a special case the famed AKLT chain, an exactly solvable model which would later serve as a prototypical matrix product state and the premier example of a state in a symmetry protected topological (SPT) phase. [Aff+88] SPT phases are of great interest in condensed matter: they are in some sense the most "tractable" examples of topological materials, and are some for which very concrete data can be extracted.

In our work, we affirmatively prove that the yellow and red phases are indeed distinct phases by constructing a topological invariant which distinguishes them–a group cohomology $H^2(SO(n), U(1))$ invariant, to be precise. While the classification of 1D SPT phases for Hamiltonians with unique gapped ground states is at this point well understood at a high level [Oga20; Che+13], there are many open questions regarding the SPT nature of known models and phase diagrams.

While proving the conjecture was the ultimate goal of the project, it turns out the innocuous MPS point is full of strange and wonderfully unexpected properties when the local dimension $n$ of each on-site Hilbert space is even. Firstly, these states are dimerized, but they have identical entanglement structure and are completely indistinguishable by entanglement measurements. This is in stark contrast to essentially all other examples of dimerization, wherein one typically expects ground states to exhibit alternating "weak-strong" entanglement structures as in the prototypical Majumdar-Ghosh model. Secondly, these states exhibit a "local indistinguishability" feature: given on-site Hilbert dimension $n$, no $k$-local operator with $k < n/2$ can distinguish the two states. This is exceptionally unexpected given 2-periodicity, as it means that when e.g. $n = 6$, no 2-local operator can distinguish these states. Thirdly, these states form an interesting counterexample to a natural conjecture: one might expect that we would need the support of the "smallest" parent Hamiltonian interaction to depend on the correlation length of its ground states. But these MPSs form a class of ground states with a nearest-neighbor parent Hamiltonian whose correlation lengths can be made arbitrarily large by varying $n$.

The project makes heavy use of several mathematical toolboxes. To work on finite chain matrix product ground states in the red region, we used a great deal of Lie representation theory, as well as tools from tensor networks and quantum information theory. Indeed, it was this project that first inspired my fascination with symmetry. The finite chain ground states in the yellow region require methods from probability theory, as they admit a stochastic-geometric description to compute correlations.[Bjö+21] In both cases, extending these insights to the thermodynamic limit and saying something about topological invariants demanded powerful methods from functional analysis and spin systems, like Lieb-Robinson bounds, quasi-adiabatic continuation, and the GNS construction.

## 3 Research Focus 1: Lie Representation Theory in Quantum Computation

The work at LANL and PNNL sparked a promising research program: I want to continue using tools from Lie representation theory to expand our understanding of quantum computation. Firstly, I intend to continue my ongoing work on symmetric VQAs. As I described earlier, without imposing structure on input states, architecture, or measurements, VQAs are doomed to be plagued by insurmountable trainability problems like barren plateaus. Somewhat ironically, the source of these problems seems to be the source of hope for quantum advantage: Hilbert spaces grow exponentially, and so we expect generic VQAs to suffer from trainability problems. But as physicists and chemists have known for many years, a large swath of interesting problems come naturally equipped with structure in the form of symmetries via Lie group representations. Representation theory is a deep and ever-developing field which has enjoyed a variety of successes in closely related disciplines, like condensed matter and quantum information, but we have only just started using it to constrain the behavior of VQAs.

Let us give a more concrete instance of this program. The results of our recent paper [Rag+23] are leading us to more carefully study dynamical Lie algebras. This is one of the first results mathematically describing the vague idea of "expressibility" of a quantum circuit in terms of a concrete algebraic structure. But the consequences of this correspondence for VQAs, as well as Hamiltonian simulation and state preparation, are currently mysterious. For instance, in our calculation of the variance in terms of a measurement operator $O$ and initial state $\rho$, a quantity called the $\mathfrak{g}$-purity appears rather organically. It generalizes the usual purity, which is a crucial measure of mixedness in quantum information theory. $\mathfrak{g}$-purity was initially defined in the thesis [Som05] roughly 20 years ago and has been largely uninvestigated, but it is now clearly an important algebraic quantity to study, as it controls the trainability of a VQA. Thanks to its close connections to the thoroughly studied purity and Killing form of the dynamical Lie algebra, there are no shortage of initial directions to study this quantity, but the full story (and its implications for VQA loss landscapes) is entirely open.

The techniques are hardly restricted to VQAs. Even a cursory look at existing quantum algorithm primitives like the quantum Fourier transform and Haar twirling suggests that lessons from Lie theory can serve as a rich source of useful ideas. Indeed, dynamical Lie algebras themselves originate from quantum control theory, and have close ties to Hamiltonian simulation and ground state preparation. My hope is to amplify the community's existing approaches to such problems by taking into account the symmetry $G$ of a Hamiltonian or quantum circuit at hand and leveraging this geometric data to design better algorithms.

## 4 Research Focus 2: Ground State Phases of Symmetric Hamiltonians

The phase diagram for $SO(n)$-invariant nearest-neighbor Hamiltonians we presented earlier has served as a rich vein of mathematical research for several decades, providing interesting conjectures to prove and revealing previously unheard of physical phenomena. Notably, this study in the $SO(3)$ case lead to the discovery of SPT phases, a rich set of integrable systems at gapless points, and the development of matrix product states. We are seeing signs that the $SO(n)$ case has its own set of interesting behavior even for the case of $SO(4)$, as evidenced by the peculiar properties of the exactly solvable models we stumbled upon. I wish to continue studying models in the $SO(n)$ phase diagram, and begin exploring other analogous (and poorly studied) phase diagrams for Hamiltonians with on-site compact Lie group $G$ symmetries, especially symplectic and special unitary symmetries. In a different direction, the world of 2D $G$-symmetric translation-invariant Hamiltonians beyond $SU(2)$ invariant models is even less explored and will likely provide a wealth of fascinting phenomena and mathematics for years to come.

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