The quantum monad: towards quantum finite model theory

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This short contribution summarises the article ‘The quantum monad on relational structures’, accepted for MFCS 2017 and available at arXiv:1705.07310 [cs.LO], together with some additional related results. Moreover, we situate this contribution as the starting point of a broader and more ambitious ongoing research programme aiming for a quantum version of finite model theory and descriptive complexity.

Homomorphisms between relational structures play a central role in finite model theory, constraint satisfaction, and database theory. A central theme in quantum computation is to show how quantum resources can be used to gain advantage in information processing tasks. In particular, non-local games have been used to exhibit quantum advantage in boolean constraint satisfaction, and to obtain quantum versions of graph invariants such as the chromatic number. We show how quantum strategies for homomorphism games between relational structures can be viewed as Kleisli morphisms for a quantum monad on the (classical) category of relational structures and homomorphisms. We use these results to exhibit a wide range of examples of contextuality-powered quantum advantage, and to unify several apparently diverse strands of previous work.

Recent work has brought category-theoretic methods into finite model theory. Winning strategies for various kinds of games, such as pebbling or Ehrenfeucht–Fraïssé games, are described as co-Kleisli morphisms for appropriate comonads. This leads to syntax-free characterisations of important logical equivalences between relational structures, as well as coalgebraic characterisations of key combinatorial invariants, including tree-width or tree-depth. By combining this work with our monadic formulation of quantum advantage, we aim to obtain quantum versions of logical equivalences in a syntax-free way. This may pave the way for a ‘quantum finite model theory’ and quantum descriptive complexity. The goal is to study classes of structures arising from these quantum logical equivalences and their correspondence to quantum computational complexity classes, shedding further light into the nature of quantum advantage.

Note: Theorem numbers in this extended abstract refer to the version of our paper at arXiv:1705.07310 [cs.LO]. We direct the reader there for further details and for the proofs of the results.

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1 Summary of paper

Introduction. Finite relational structures and the homomorphisms between them form a mathematical core common to finite model theory [18], constraint satisfaction [9], and relational database theory [17]. Moreover, much of graph theory can be formulated in terms of the existence of graph homomorphisms, as expounded e.g. in the influential text [11]. Thus, implicitly at least, the mathematical setting for all these works is categories of σ-structures and homomorphisms, for relational vocabularies σ.

What could it mean to quantise these structures? More precisely, with the advent of quantum computing, we can now consider the consequences of using quantum resources for carrying out various information-processing tasks. A major theme of current research is to delineate the scope of the *quantum advantage* which can be gained by the use of quantum resources. How can this be related to these fundamental structures?

Our starting point is the notion of *quantum graph homomorphism* introduced in [19] as a generalisation of the notion of quantum chromatic number [5]. Consider the following game, played by Alice and Bob cooperating against a Verifier. Their goal is to establish the existence of a homomorphism $G \to H$ for given graphs G and H. Verifier provides vertices $v_1, v_2 \in V(G)$ to Alice and Bob respectively. They produce outputs $w_1, w_2 \in V(H)$ in response. No communication between Alice and Bob is permitted during the game. They win if the following conditions hold: $v_1 = v_2 \Rightarrow w_1 = w_2$ and $v_1 \sim v_2 \Rightarrow w_1 \sim w_2$, where we write $\sim$ for the adjacency relation.

If only classical resources are permitted, then the existence of a *perfect strategy* for Alice and Bob – one in which they win with probability 1 – is equivalent to the existence of a graph homomorphism between G and H in the standard sense. However, using quantum resources, in the form of an entangled bipartite state where Alice and Bob can each perform measurements on their part, there are perfect strategies in cases where no classical homomorphism exists, thus exhibiting quantum advantage.

Non-local games have also been studied for other tasks, notably for *constraint systems*. Consider the following system of linear equations over $\mathbb{Z}_2$:

$$A \oplus B \oplus C = 0 \qquad D \oplus E \oplus F = 0 \qquad G \oplus H \oplus I = 0$$
$$A \oplus D \oplus G = 0 \qquad B \oplus E \oplus H = 0 \qquad C \oplus F \oplus I = 1$$

Of course, this system is not satisfiable in the standard sense, as we can see by summing over the left- and right-hand sides. Now consider the following game. The Verifier sends Alice an equation, and Bob a variable. Alice returns an assignment to the variables in the equation, and Bob returns an assignment for his variable. They win if Bob's assignment agrees with Alice's, and moreover Alice's assignment satisfies the given equation. Classically, the existence of a perfect strategy is equivalent to the existence of a satisfying assignment for the whole system. Using quantum resources, there is a perfect strategy for the above system, which corresponds to Mermin's "magic square" construction [21]. This can be generalised to a notion of quantum perfect strategies for a broad class of constraint systems [7, 6], which have strong connections both to the study of contextuality in quantum mechanics, and to a number of challenging mathematical questions [27, 25]. Clearly, these games are analogous to those for graph homomorphisms. What is the precise relationship?

In [19], generalising results in [5], the existence of a quantum perfect strategy for the graph homomorphism game from G to H is characterised in terms of the existence of a family $\{E_{vw}\}_{v \in V(G), w \in V(H)}$ of projectors in d-dimensional Hilbert space for some d, subject to certain conditions. Analogous results for constraint systems are proved in [7]. This characterisation eliminates the two-person aspect of the game, and the shared state, leaving a "projector-valued relation" as the witness for existence of a quantum perfect strategy. We call these witnesses *quantum graph homomorphisms*. An important further step is taken in [19]. A construction $H \mapsto \mathsf{M}H$ on graphs is introduced, such that the existence of a quantum graph homomorphism from G to H is equivalent to the existence of a *standard* graph homomorphism $G \to \mathsf{M}H$.

Summary of results. Our contribution begins at this point. We describe a general notion of non-local game for witnessing homomorphisms between structures for any relational signature. We show that the use of quantum resources in these games can be characterised by a notion of *quantum homomorphism*. Moreover, quantum homomorphisms can in turn be characterised as the Kleisli morphisms for a *quantum monad* on the (classical) category of relational structures and homomorphisms. This monad is *graded* [22] by the dimension of the Hilbert space.

Our account refines and generalises the ideas from both [5, 19] and [7]. We characterise quantum solutions for general constraint satisfaction problems, showing as a special case that these subsume the binary constraint systems of [7]. We also show how quantum witnesses for state-independent strong contextuality in the sense of [1] are characterised by quantum homomorphisms. The precise relationship with the quantum graph homomorphisms of [19] turns out to be more subtle. We show that their notion is characterised by a quantum solution in our sense for a related boolean constraint system. Overall, we show that a wide range of notions of quantum advantage is captured in a uniform way by the quantum monad, applied directly to the standard classical structures.

From quantum perfect strategies to quantum homomorphisms. Fix a finite relational vocabulary $\sigma = \{R_1, \ldots, R_p\}$, where R_a has arity k_a, for $a \in \{1, \ldots, p\}$. Consider the following game, played on finite σ-structures $\mathscr{A}$ and $\mathscr{B}$, in which Alice and Bob cooperate to convince a Verifier that there is a homomorphism from $\mathscr{A}$ to $\mathscr{B}$. Verifier sends Alice an index a, and a tuple $\mathbf{x} \in R_a^{\mathscr{A}}$, and Bob an element $x \in A$. Alice returns a tuple $\mathbf{y} \in B^{k_a}$, and Bob returns an element $y \in B$.

Alice and Bob win that play if $\mathbf{y} \in R_a^{\mathscr{B}}$ and $x = \mathbf{x}_i \Rightarrow y = \mathbf{y}_i$ for $i \in \{1, \ldots, k_a\}$. For notational convenience, from now on we focus on the case where the relational signature has a single k-ary relation R.

If only classical resources are allowed, the existence of a perfect strategy is equivalent to the existence of a homomorphism. We now consider the use of (finite-dimensional) quantum resources. There are finite-dimensional Hilbert spaces H and K, belonging to Alice and Bob respectively. The players share a state ρ on $\mathsf{H} \otimes \mathsf{K}$. For each possible input, each player has a POVM on their Hilbert space indexed by the possible outputs. That is, Alice has a POVM $\mathscr{E}_{\mathbf{x}} = \{\mathscr{E}_{\mathbf{x},\mathbf{y}}\}_{\mathbf{y} \in B^k}$ for each $\mathbf{x} \in R^{\mathscr{A}}$; and Bob has a POVM $\mathscr{F}_x = \{\mathscr{F}_{x,y}\}_{y \in B}$ for each $x \in A$. The idea is that each player will perform a measurement depending on their input, using the outcome to determine their output.

We first showed that a quantum perfect strategy can w.l.o.g. be assumed to have a very special form:

Theorem 5. *The existence of a quantum perfect strategy implies the existence of a strategy* $(\psi, \{\mathscr{E}_{\mathbf{x}}\}, \{\mathscr{F}_x\})$ *s.t.:*

- *The state* ψ *is a maximally entangled state* $\psi = 1/\sqrt{d} \sum_{i=1}^{d} e_i \otimes e_i$.
- *The POVMs* $\mathscr{E}_{\mathbf{x}}^i$ *and* $\mathscr{F}_x$ *are projective, where* $\mathscr{E}_{\mathbf{x},y}^i := \sum_{\mathbf{y}_i = y} \mathscr{E}_{\mathbf{x},\mathbf{y}}$.
- *If* $x = \mathbf{x}_i$, *then* $\mathscr{E}_{\mathbf{x},y}^i = \mathscr{F}_{x,y}^T$; *and if* $\mathbf{x} \in R^{\mathscr{A}}$ *and* $\mathbf{y} \notin R^{\mathscr{B}}$, *then* $\mathscr{E}_{\mathbf{x},\mathbf{y}} = \mathbf{0}$.

The proof combines elements from [7] and [19, 5]. It is closest to the argument in [24], but considerably simpler as well as more general. The procedure for obtaining the strategy in special form has three steps: in Step 1, the state and measurements are projected down to the support of the Schmidt decomposition of the state, reducing the Hilbert space dimension, and preserving the probabilities for the strategy exactly; Step 2 is to show that the strategy thus obtained already has strong properties (2nd and 3rd items); Step 3 changes the state to the maximally entangled state, which may change the probabilities for the strategy but preserves possibilities exactly. Note that the dimension is reduced: the process by which we obtain projective measurements is not at all akin to dilation.

The theorem shows that all the information determining the strategy is in Alice's operators. Moreover, these must be chosen non-contextually, so that $\mathscr{E}_{\mathbf{x},y}^i$ is independent of the context $\mathbf{x}$. This leads us to the the notion of *quantum homomorphism* between relational structures $\mathscr{A}$ and $\mathscr{B}$: a family of projectors $\{P_{x,y}\}_{x \in A, y \in B}$ in a d-dimensional Hilbert space satisfying: (1) for all $x \in A$, $\sum_{y \in B} P_{x,y} = I$; (2) for all $x, x' \in A$ adjacent in the Gaifman graph of $\mathscr{A}$ (i.e. belonging to the same tuple in $R^{\mathscr{A}}$) and $y, y' \in B$, $[P_{\mathbf{x}_i,y}, P_{\mathbf{x}_j,y'}] = \mathbf{0}$; and (3) if $\mathbf{x} \in R^{\mathscr{A}}$ and $\mathbf{y} \notin R^{\mathscr{B}}$, then $P_{\mathbf{x},\mathbf{y}} = \mathbf{0}$, where $P_{\mathbf{x},\mathbf{y}} := P_{\mathbf{x}_1,\mathbf{y}_1} \cdots P_{\mathbf{x}_k,\mathbf{y}_k}$ (this is well-defined due to (2)).

Theorem 7. *Let* $\mathscr{A}$ *and* $\mathscr{B}$ *be finite* σ*-structures. Then there is a quantum perfect strategy for the homomorphism game from* $\mathscr{A}$ *to* $\mathscr{B}$ *iff there is a quantum homomorphism from* $\mathscr{A}$ *to* $\mathscr{B}$.

Quantum homomorphisms as Kleisli maps. Quantum homomorphisms can be characterised as the Kleisli morphisms of a monad $\mathscr{Q}_d$ on the category of $\mathscr{R}(\sigma)$ of σ-structures. The monad is *graded* [22] by the dimension of the Hilbert space used as the quantum resource. For the underlying universes of the structures, the construction can be seen as a quantum variant of the discrete distribution monad [14], widely used in coalgebra and semantics. It is well known that this can be defined over any commutative semiring, with $\mathbb{R}_0^+$ being used for the standard case of probabilities [14, 1]. Here we use the projectors $\mathsf{Proj}(d)$ with $d \in \mathbb{N}^+$. For each d, $\mathsf{Proj}(d)$ is a partial commutative semiring, since we can only add projectors if they are orthogonal and multiply them if they commute. Besides, we have a graded multiplication given by the tensor product: if $P \in \mathsf{Proj}(d)$ and $Q \in \mathsf{Proj}(d')$, then $P \otimes Q \in \mathsf{Proj}(dd')$.

For each positive integer d and σ-structure $\mathscr{A}$, we define a σ-structure $\mathscr{Q}_d\mathscr{A}$, whose universe $\mathscr{Q}_dA$ is the set of projector-valued distributions on A in dimension d, i.e. functions $p : A \to \mathsf{Proj}(d)$ satisfying $\sum_{x \in A} p(x) = I$. For each relation R of arity k in σ, we take $R^{\mathscr{Q}_d\mathscr{A}}$ to be the set of tuples $(p_1, \ldots, p_k)$ such that: (1) for all $x, x' \in A$, $[p_i(x), p_j(x')] = \mathbf{0}$ and (2) for all $\mathbf{x} \in A^k \setminus R^{\mathscr{A}}$, $p_1(x_1) \cdots p_k(x_k) = \mathbf{0}$. Note that (1) implies that the product of projectors in (2) is a well-defined projector.

$\mathscr{Q}_d$ extends to an endofunctor on $\mathscr{R}(\sigma)$, and moreover to a $\mathbb{N}^+$-graded monad, in a way analogous to the usual distribution monad over a semiring (generalised to the case with partial addition and graded multiplication). For homomorphisms $h : \mathscr{A} \to \mathscr{B}$, it acts as push-forward: $\mathscr{Q}_d h : \mathscr{Q}_d\mathscr{A} \to \mathscr{Q}_d\mathscr{B}$ given by $\mathscr{Q}_d h(p)(y) := \sum_{h(x)=y} p(x)$. The (graded) unit $\eta_{\mathscr{A}} : \mathscr{A} \to \mathscr{Q}_1\mathscr{A}$ sends $x \in A$ to the "delta distribution": $\eta_{\mathscr{A}}(x)(x') = \delta_{x,x'} I_1$. We also have a graded monad multiplication $\mu_{\mathscr{A}}^{d,d'} : \mathscr{Q}_d\mathscr{Q}_{d'}\mathscr{A} \to \mathscr{Q}_{dd'}\mathscr{A}$ given as $\mu_{\mathscr{A}}^{d,d'}(P)(x) := \sum_{p \in \mathscr{Q}_{d'}\mathscr{A}} P(p) \otimes p(x)$. (See **Theorem 10**.)

We are interested in the Kleisli category for this graded monad. Its objects are the same as those of $\mathscr{R}(\sigma)$. A Kleisli morphism from $\mathscr{A}$ to $\mathscr{B}$ is a standard homomorphism $h : \mathscr{A} \to \mathscr{Q}_d\mathscr{B}$. These correspond bijectively to quantum homomorphisms from $\mathscr{A}$ to $\mathscr{B}$ in dimension d (**Proposition 8**). The graded composition of Kleisli arrows $h : \mathscr{A} \to \mathscr{Q}_d\mathscr{B}$ and $k : \mathscr{B} \to \mathscr{Q}_{d'}\mathscr{C}$ corresponding to quantum homomorphisms $\{P_{x,y}\}_{x \in A, y \in B}$, $\{Q_{y,z}\}_{y \in B, z \in C}$ yields the quantum homomorphism $\{R_{x,z}\}_{x \in A, z \in C}$ given by $R_{x,z} = \sum_{y \in B} P_{x,y} \otimes Q_{y,z}$, recovering the concrete definition given for quantum graph homomorphisms in [19].

Quantum advantage via the quantum monad. The quantum monad provides a unified framework for expressing quantum advantage in a wide range of information processing tasks. We briefly summarise the main results from Section 4 of the paper, where a correspondence is shown between state-independent strong contextuality arguments and quantum advantage in constraint satisfaction, expressed as the existence of a quantum, but not a classical, homomorphism between relational structures.

Classically, solutions to a *constraint satisfaction problem* (CSP) $\mathscr{K}$ correspond to homomorphisms $\mathscr{A}_{\mathscr{K}} \to \mathscr{B}_{\mathscr{K}}$ between a structure $\mathscr{A}_{\mathscr{K}}$ of variables and $\mathscr{B}_{\mathscr{K}}$ of values, where the relations codify the constraints. We now consider how quantum resources enter the picture. Since we have a notion of quantum homomorphism for general relational structures, this provides a ready-made notion of quantum solutions for CSPs, namely a quantum homomorphism $\mathscr{A}_{\mathscr{K}} \xrightarrow{q} \mathscr{B}_{\mathscr{K}}$. In the case of *binary* constraint systems (BCS), our notion of quantum solutions corresponds to the operator solutions considered in [7, 6, 27, 15] (**Proposition 15**).

Empirical models over measurement scenarios were introduced in [1] as a general setting for studying contextuality. Strong contextuality corresponds to the case when no global assignment is consistent with the model, in the sense of yielding *possible* outcomes in all contexts. This form of contextuality is witnessed by the GHZ construction [10, 20], Kochen–Specker paradoxes [16], and post-quantum devices like the PR box [23]. The support of an empirical model e can be described by a CSP $\mathscr{K}_e$, whose solutions are in one-to-one correspondence with consistent global assignments for e. Thus, e is strongly contextual iff $\mathscr{K}_e$ has no (classical) solution (**Proposition 13**). In turn, quantum solutions for this same CSP $\mathscr{K}_e$ are in one-to-one correspondence with state-independent quantum witnesses for e (**Proposition 14**), i.e. choices of quantum measurements with appropriate compatibilities whose outcomes are in the support of e for *any* quantum state. So, if $\mathscr{K}_e$ has a quantum but not a classical solution we have a state-independent quantum realisation of strong contextuality. Examples are the Mermin magic square and pentagram [21] and Kochen–Specker constructions [16, 4]. An interesting point arising from this result, taken together with the description of the homomorphism game, is that state-independent strong contextuality proofs can always be underwritten by non-locality arguments. This is a general form of constructions for turning Kochen–Specker contextuality proofs into Bell non-locality arguments [12]. The role of the entangled state and of Bob in the non-local game provides an operational or physical underpinning for the compatibility or generalised no-signalling assumption that is made for single-site empirical models.

Our notion of quantum homomorphism subsumes a number of existing notions in contextuality and non-local games. However, our definition of quantum graph homomorphism (seeing graphs as special cases of relational structures) differs from that introduced by Mančinska & Roberson (MR) [19], in that the latter does *not* impose the commutativity condition between the PVMs corresponding to adjacent vertices of G. This reflects a difference between the games used to motivate each definition. Clearly, a quantum homomorphism between graphs in the sense of this paper is also an MR quantum graph homomorphism. The converse is not known. However, by adapting a construction by Ji [15], we capture the existence of MR quantum graph homomorphisms in terms of quantum homomorphisms of relational structures, via a BCS (**Theorem 16**). It is worth noting that our approach allows us to avoid ad hoc coding of constraints by polynomials, as in [7, 15]. Instead, we quantise the standard classical notions in a uniform way, using the quantum monad.

Additional results: quantum isomorphisms A notion of quantum graph isomorphism, with an equivalent characterisation via a non-local game, has been studied in [3]. This can be generalised to relational structures. The idea is that each player can be asked a question from either structure, and has to reply in the other. Each player will thus have had an input or output from each structure: $\mathbf{x} \in A^k$ and $\mathbf{y} \in B^k$ for Alice and $x \in A$ and $y \in B$ for Bob. The winning conditions are then $\mathbf{x} \in R^{\mathscr{A}} \Leftrightarrow \mathbf{y} \in R^{\mathscr{B}}$ and $x = \mathbf{x}_i \Leftrightarrow y = \mathbf{y}_i$. Since the Verifier doesn't necessarily send inputs from the same structure to both players, a perfect quantum strategy is more than two quantum homomorphisms, one in each direction. This pair of quantum homomorphisms must be coupled in a certain way. Indeed, adapting the proof of our Theorem 5, we show that there is a quantum perfect strategy for the isomorphism game iff there is a map $A \times B \to \mathrm{Proj}(d)$ such that currying either variable yields a quantum homomorphism.

2 Towards *quantum* finite model theory

We now place the results presented above within a broader research programme, of which it can be seen as a motivation and starting point. The quantum monad provides a uniform way of *quantising* classical notions in the framework of relational structures. We have shown how this captures advantage obtained by the use of quantum resources in certain tasks. We aim to apply this recipe to concepts in finite model theory, which focuses on the study of relational structures with a finite universe from the viewpoint of mathematical logic, with numerous applications to descriptive complexity, database theory, constraint satisfaction, and formal language theory.

The basic idea of model theory is that logics give limited access to the structures they are interpreted over, leading to equivalences coarser than isomorphism. These equivalences are used in finite model theory e.g. to characterise complexity classes. Spoiler–Duplicator games are one of the main tools for characterising these equivalences, and so for proving results in this area. For example, pebble games capture the idea of limited access to a structure through a 'moving window' of size k (the number of pebbles), corresponding to what can be expressed in k-variable logic.

Recent work [2, 26] has brought category-theoretic methods into finite model theory. In [2], a winning strategy for Duplicator in the existential k-pebble game from $\mathscr{A}$ to $\mathscr{B}$ is shown to correspond to a co-Kleisli morphism $\mathbb{T}_k\mathscr{A} \to B$, for a pebbling comonad $\mathbb{T}_k$. In [26], similar comonads were introduced to capture other games, including Ehrenfeucht–Fraïssé (EF) games and (bi)simulation games for the modal fragment. Such comonads capture limitations on how a structure can be accessed, corresponding to limitations on definability imposed by various logics. Thus, they provide syntax-free characterisations of several important logical equivalences. Moreover, key combinatorial parameters such as tree-width or tree-depth can also be described in this formalism. For example, tree-width of a structure $\mathscr{A}$ corresponds to its coalgebra number, the least k such that there is a coalgebra $\mathscr{A} \to \mathbb{T}_k\mathscr{A}$, and tree-depth arises analogously from the EF monad.

As both the quantum monad and these game comonads live in the same setting of $\mathscr{R}(\sigma)$, it is natural to ask whether combining the two can lead to sensible quantum versions of (syntax-free) logical equivalences. The idea is to take one of the comonadic descriptions of logical equivalences in terms of co-Kleisli arrows $\mathbb{T}_k\mathscr{A} \to \mathscr{B}$, and to replace these arrows, which are classical homomorphisms of relational structures, by quantum homomorphisms, i.e. by homomorphisms of the form $\mathbb{T}_k\mathscr{A} \to \mathscr{Q}_d\mathscr{B}$. This would yield a quantum version of the same equivalence and could provide the basis for a 'quantum finite model theory', achieved through a subtle form of quantisation which does not go via a 'quantum logic'. We conclude with some open questions in this direction:

- The first question is whether there is a suitable distributive law between the quantum (graded) monad and the pebble (or other game) comonad, giving a bi-Kleisli category. The obvious candidates don't work. Note that a negative answer could also have significance from the point of view of quantum logic.
- Homomorphisms $\mathbb{T}_k\mathscr{A} \to \mathscr{Q}_d\mathscr{B}$ can be seen either as winning strategies for Duplicator in an asymmetric pebble game played on structures $\mathscr{A}$ and $\mathscr{Q}_d\mathscr{B}$, or as quantum perfect strategies for the non-local game where Alice and Bob aim to convince the Verifier there is a homomorphism between $\mathbb{T}_k\mathscr{A}$ and $\mathscr{B}$. It is not clear how to unravel both aspects simultaneously and define a good notion of quantum pebbling game. Presumably, this would be a game where Spoiler acts as Verifier and Duplicator is Alice and Bob.
- Do the characterisations of tree-width and tree-depth admit a similar 'quantisation'?
- Homomorphisms are intimately related to formulae in the existential positive fragment. Can this be extended to provide a notion of quantum satisfiability ($A \models_q \psi$) for first-order formulae on relational structures?
- Descriptive complexity characterises computational complexity classes in terms of the expressive power of logics, yielding descriptions of complexity classes that do not hinge on a model of computation. For example, NP corresponds exactly to the set of properties expressible in existential second-order logic [8], while the circuit complexity class AC^0 is equivalent to $\mathrm{FO}(+,\times)$, first-order logic with addition and multiplication [13]. Do quantised versions of these (and other) logics correspond to well-known quantum computational complexity classes?

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